



Supplement of

**Synthesis of jadarite in the Li_2O – Na_2O – B_2O_3 – SiO_2 – NaCl – H_2O system:
FTIR, Raman, and Li and B *K*-edge XANES characterizations
and theoretical calculations**

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Validation of Li pseudopotentials

Figure S3 compares the calculated LiCl, Li₂CO₃, and Li₂SiO₃ Li K-edge XANES with experiments. Figure S3a compares the calculated Li-edge XANES spectrum of LiCl with its measured spectra reported by Tsuji et al. (2002), using the total electron yield (TEY) method, and O'Shaughnessy et al. (2018), using the TEY and FYL methods. They all show a strong feature at 6 eV (Position a). The calculated spectrum has an extra shoulder at 6.5 eV (Position b), which is not observed in both measured spectra, probably because the intensity is too weak to be observed. The measured spectra have two small bumps at 7.2 eV (Position c) and 8.2 eV (Position d) in the spectrum of Tsuji et al. (2002) and 9 eV in O'Shaughnessy et al. (2018), which occur in the calculated spectrum at similar positions (i.e. 7.2 eV for Position c and 9.5 eV for Position d). At ~13 eV, all three spectra show a small peak or bump labeled as Position e. The calculated result also shows an extra peak (Position f) at 16 eV, which is not observed in both measured spectra.

Figure S3b compares the calculated Li K-edge XAS spectrum of Li₂CO₃ with its measured spectra reported by de Clermont Gallerande et al. (2018) by the low-q XRS technique and O'Shaughnessy et al. (2018) by the TEY and FYL methods. The calculated spectrum is in very good agreement with that measured by the low-q XRS technique. Positions of the peaks a, b, and c are at 4.0, 5.5, and 6.8 eV, respectively. The calculated spectrum has an extra peak at 10.5 eV (Position d), which is not observed in the measured spectra. All three spectra have a strong and broad peak (Position e), except that its positions in the two measured spectra are at 12.0 eV but at 11.5 eV in the calculated spectrum.

Figure S3c compares the calculated and measured Li K-edge XANES spectra of Li₂SiO₃. Both spectra show five characteristic peaks. It is very interesting to observe that the two spectra have very

similar shapes, but the peak positions in the calculated spectrum are severely shifted to lower energy compared with its measured counterparts. The XANES spectra of Li_2SiO_3 are composed of double peaks in the main edge, with a broad and strong band of triplet peaks at the post-edge region. However, when aligning the first peak at 8 eV (Position a). Position b obtained from the experiment is at 9.4 eV, while this position is at 9.1 eV in the calculation. The discrepancies enlarge for the other peaks. Positions c, d, and e of the experimental spectrum are at 14.1, 15.7, and 17.2 eV, while for the calculated spectrum these values are 11.7, 12.6, and 14.7 eV. We suspect that these discrepancies between the calculated and measured Li K-edge XANES spectra of Li_2SiO_3 probably arise from different polymorphs investigated, rather than problems with the Li pseudopotentials used in this study.

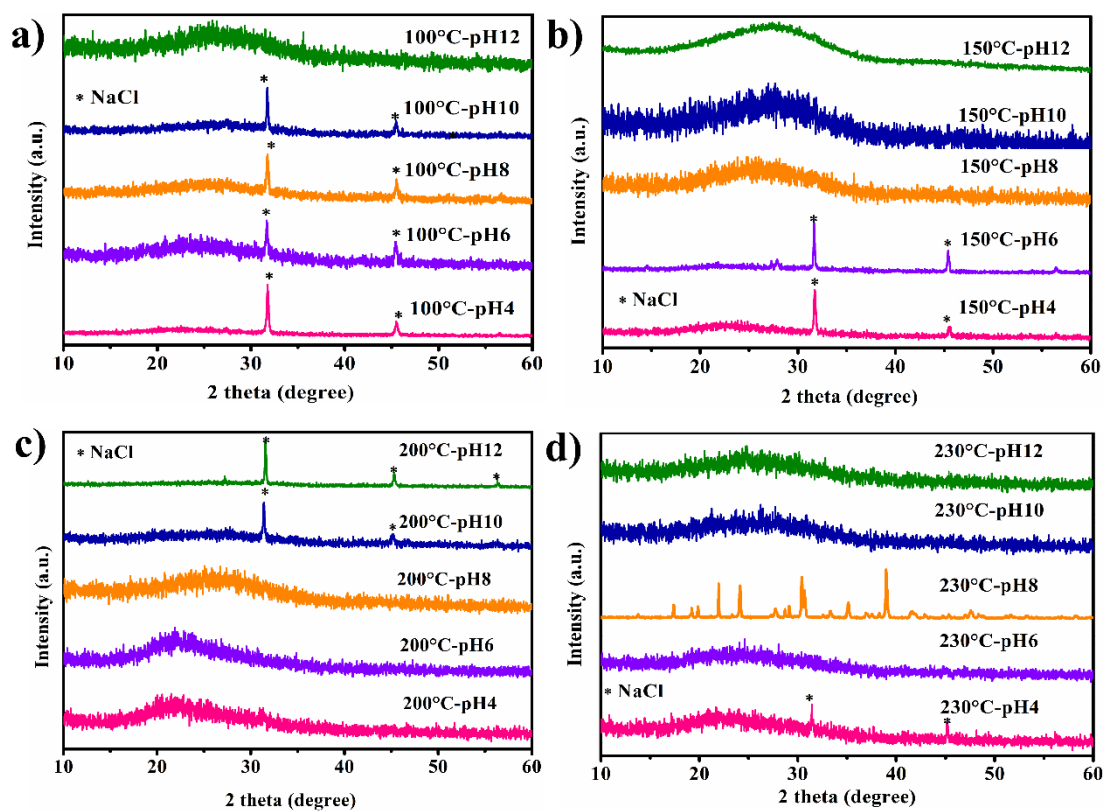


Figure S1. Comparison of the powder X-ray diffraction patterns from different synthetic conditions for the duration of 3 days.

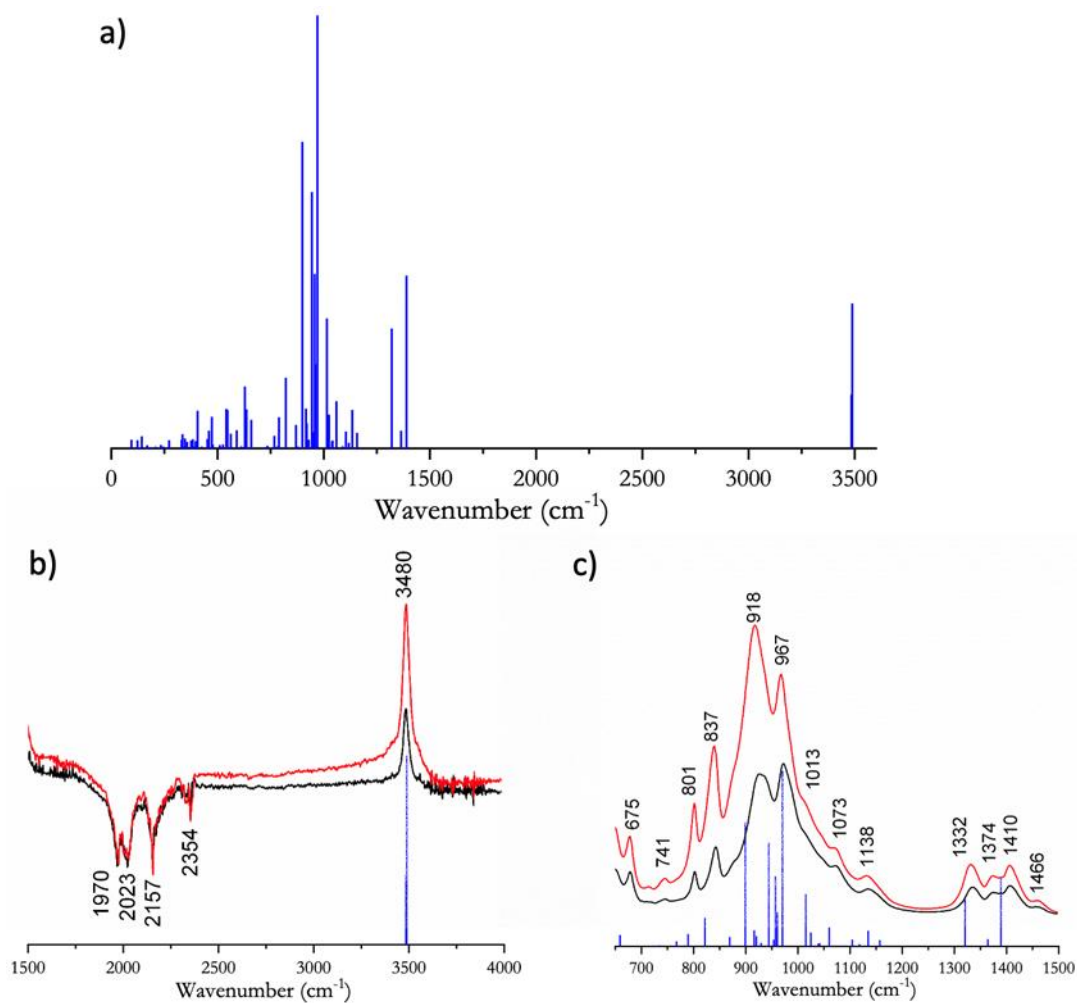


Figure S2. (a) Calculated intensities and wavenumbers of the IR-active vibrational modes of jadarite. (b) Comparison of the FTIR spectra of natural (black) and synthetic (red) in the O-H stretch region. Also included for comparison is the calculation intensities (blue) at the high wavenumber region. (c) Comparison of the measured (red and black) spectra and calculated (blue) FTIR intensities at the low wavenumber region.

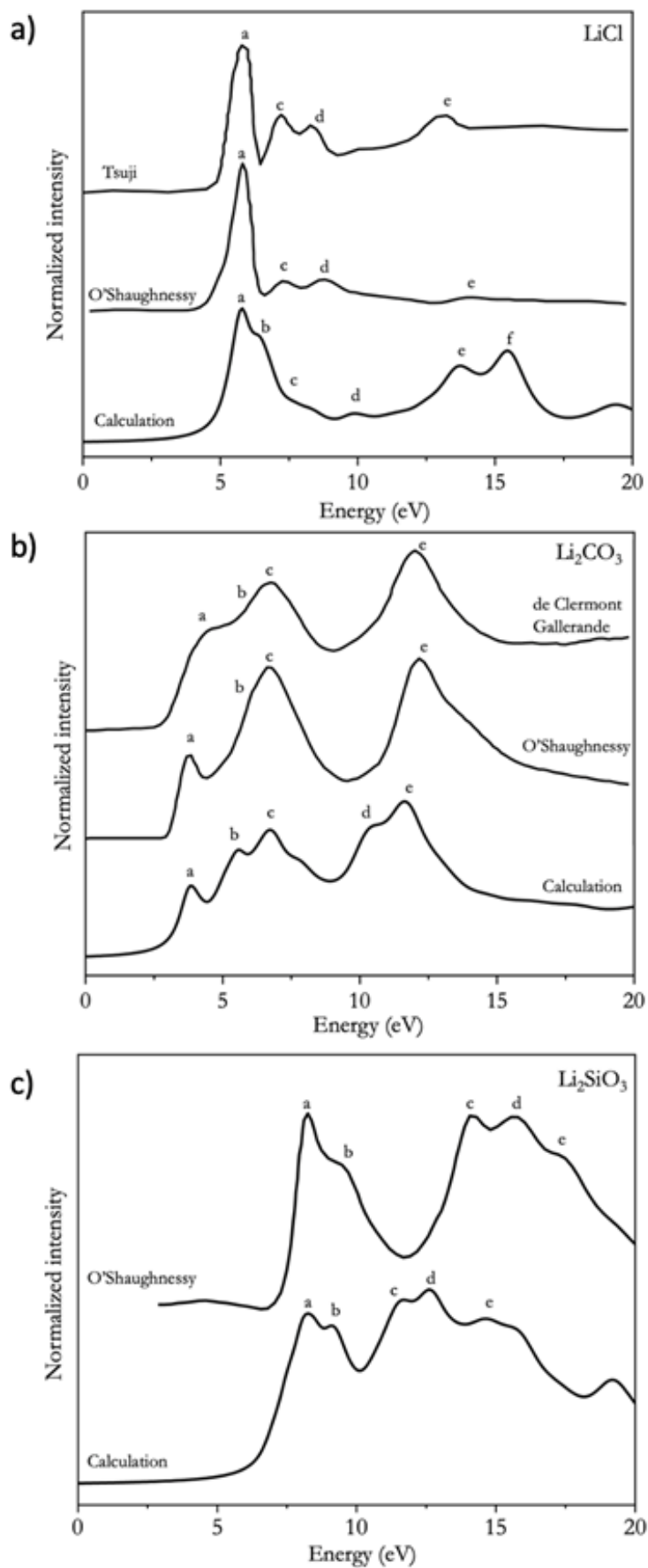


Figure S3. Comparison of calculated Li K-edge XANES spectra of model compounds Li₂CO₃, LiCl, and Li₂SiO₃ from the OCEAN code with measured spectra reported by O'Shaughnessy et al. (2018), de Clermont Gallerande et al. (2018), and Tsuji et al. (2002).

Table S1 Powder X-ray diffraction data of synthetic jadarite

<i>(hkl)</i>	2θ (Cal.)	2θ (Obs.)	Delta (2θ)	d (Obs.)	Intensity (%)
(020)	12.805	12.804	0.001	6.9081	60
(011)	15.386	15.369	0.017	5.7606	8
(-101)	15.760	15.761	-0.002	5.6180	30
(-111)	17.022	17.018	0.004	5.2059	9
(120)	18.924	18.929	-0.005	4.6843	90
(-121)	20.358	20.349	0.008	4.3605	42
(101)	23.076	23.059	0.017	3.8539	8
(130)	23.814	23.843	-0.030	3.7288	43
(-131)	24.980	24.873	0.108	3.5768	4
(040)	25.773	25.754	0.020	3.4564	24
(121)	26.477	26.471	0.006	3.3643	24
(-112)	27.310	27.257	0.054	3.2691	4
(200)	27.959	27.958	0.001	3.1886	100
(002)	28.175	28.154	0.021	3.1669	78
(012)	28.921	28.905	0.015	3.0863	23
(140)	29.385	29.396	-0.011	3.0359	52
(131)	30.228	30.213	0.015	2.9556	85
(022)	31.059	31.060	-0.001	2.8769	9
(-202)	31.827	31.813	0.014	2.8105	11
(-231)	32.846	32.874	-0.027	2.7223	3
(032)	34.356	34.374	-0.018	2.6068	3
(141)	34.865	34.964	-0.099	2.5641	3
(150)	35.375	35.356	0.019	2.5366	3
(211)	36.388	36.347	0.041	2.4697	3
(-142)	37.319	37.383	-0.064	2.4036	4
(240)	38.390	38.361	0.028	2.3445	12
(-301)	39.520	39.519	0.001	2.2784	36
(-311)	40.077	40.091	-0.015	2.2472	56
(160)	41.670	41.691	-0.021	2.1646	14
(-251)	42.213	42.213	0.000	2.1391	7
(250)	43.294	43.259	0.035	2.0897	6
(-223)	44.021	43.995	0.027	2.0565	11
(-133)	44.611	44.613	-0.002	2.0294	8
(161)	45.881	45.826	0.054	1.9784	5
(-233)	46.529	46.522	0.006	1.9505	8
(-261)	47.759	47.766	-0.007	1.9025	8
(062)	48.877	49.072	-0.195	1.8549	11
(-342)	49.708	49.708	-0.001	1.8326	8
(123)	51.997	52.028	-0.031	1.7563	4
(-402)	54.244	54.233	0.011	1.6899	7
(-421)	55.703	55.719	-0.016	1.6483	7

In the FTIR and Raman spectral calculations, the dielectric tensor is given as

$$\epsilon = \begin{pmatrix} 3.748031 & -0.000043 & -0.338468 \\ -0.000043 & 2.395049 & 0.000023 \\ -0.338468 & 0.000023 & 3.068217 \end{pmatrix},$$

and the Born effective charge tensors are listed in Table S2, the optimized structure in Table S3, and the eigenvectors of the dynamical matrix of jadarite in Table S3.

Table S2 Born effective charge tensors (e) in the jadarite structure

Ion	Z_{xx}	Z_{xy}	Z_{xz}	Z_{yx}	Z_{yy}	Z_{yz}	Z_{zx}	Z_{xy}	Z_{zz}
Li1	1.03	-0.08	0.04	-0.05	1.01	-0.03	0.02	0.01	1.08
Li2	1.03	-0.08	0.04	-0.05	1.01	-0.03	0.02	0.01	1.08
Li3	1.03	0.08	0.04	0.05	1.01	0.03	0.02	-0.01	1.08
Li4	1.03	0.08	0.04	0.05	1.01	0.03	0.02	-0.01	1.08
Na1	1.12	-0.01	0.03	-0.03	1.15	-0.03	0.04	-0.08	1.10
Na2	1.12	-0.01	0.03	-0.03	1.15	-0.03	0.04	-0.08	1.10
Na3	1.12	0.01	0.03	0.03	1.15	0.03	0.04	0.08	1.10
Na4	1.12	0.01	0.03	0.03	1.15	0.03	0.04	0.08	1.10
B1	2.55	-0.35	0.28	-0.31	2.34	-0.19	0.02	-0.53	2.37
B2	2.55	-0.35	0.28	-0.31	2.34	-0.19	0.02	-0.53	2.37
B3	2.55	0.35	0.28	0.31	2.34	0.19	0.02	0.53	2.37
B4	2.55	0.35	0.28	0.31	2.34	0.19	0.02	0.53	2.37
B5	2.40	-0.53	-0.10	-0.29	2.34	-0.25	0.25	-0.14	2.45
B6	2.40	-0.53	-0.10	-0.29	2.34	-0.25	0.25	-0.14	2.45
B7	2.40	0.53	-0.10	0.29	2.34	0.25	0.25	0.14	2.45
B8	2.40	0.53	-0.10	0.29	2.34	0.25	0.25	0.14	2.45
B9	1.74	0.13	0.79	0.29	2.52	-0.46	0.72	-0.43	1.44
B10	1.74	0.13	0.79	0.29	2.52	-0.46	0.72	-0.43	1.44
B11	1.74	-0.13	0.79	-0.29	2.52	0.46	0.72	0.43	1.44
B12	1.74	-0.13	0.79	-0.29	2.52	0.46	0.72	0.43	1.44
Si1	3.18	-0.25	-0.08	0.09	2.81	0.20	-0.14	-0.09	3.29
Si2	3.18	-0.25	-0.08	0.09	2.81	0.20	-0.14	-0.09	3.29
Si3	3.18	0.25	-0.08	-0.09	2.81	-0.20	-0.14	0.09	3.29
Si4	3.18	0.25	-0.08	-0.09	2.81	-0.20	-0.14	0.09	3.29
O1	-1.31	0.08	-0.15	0.05	-1.46	-0.70	-0.08	-0.75	-2.28
O2	-1.31	0.08	-0.15	0.05	-1.46	-0.70	-0.08	-0.75	-2.28
O3	-1.31	-0.08	-0.15	-0.05	-1.46	0.70	-0.08	0.75	-2.28
O4	-1.31	-0.08	-0.15	-0.05	-1.46	0.70	-0.08	0.75	-2.28
O5	-2.19	-0.61	0.34	-0.56	-1.47	0.23	0.29	0.30	-1.39
O6	-2.19	-0.61	0.35	-0.56	-1.47	0.23	0.29	0.30	-1.39
O7	-2.19	0.61	0.34	0.56	-1.47	-0.23	0.29	-0.30	-1.39
O8	-2.19	0.61	0.34	0.56	-1.47	-0.23	0.29	-0.30	-1.39
O9	-2.27	0.43	0.13	0.30	-1.50	-0.24	0.18	-0.15	-1.30
O10	-2.27	0.43	0.13	0.30	-1.50	-0.24	0.18	-0.15	-1.30
O11	-2.27	-0.43	0.13	-0.30	-1.50	0.24	0.18	0.15	-1.30
O12	-2.27	-0.43	0.13	-0.30	-1.50	0.24	0.18	0.15	-1.30
O13	-1.13	0.12	-0.10	0.05	-1.49	0.44	-0.18	0.52	-2.30

O14	-1.13	0.12	-0.10	0.05	-1.49	0.44	-0.18	0.52	-2.30
O15	-1.13	-0.12	-0.10	-0.05	-1.49	-0.44	-0.18	-0.52	-2.30
O16	-1.13	-0.12	-0.10	-0.05	-1.49	-0.44	-0.18	-0.52	-2.30
O17	-1.44	-0.56	-0.34	-0.61	-1.92	0.06	-0.32	-0.06	-1.09
O18	-1.44	-0.56	-0.34	-0.61	-1.92	0.06	-0.32	-0.06	-1.09
O19	-1.44	0.56	-0.34	0.61	-1.92	-0.06	-0.32	0.06	-1.09
O20	-1.44	0.56	-0.34	0.61	-1.92	-0.06	-0.32	0.06	-1.09
O21	-1.31	0.23	-0.41	0.11	-1.87	0.55	-0.41	0.45	-1.34
O22	-1.31	0.23	-0.41	0.11	-1.87	0.55	-0.41	0.46	-1.34
O23	-1.31	-0.23	-0.41	-0.11	-1.87	-0.55	-0.41	-0.46	-1.34
O24	-1.31	-0.23	-0.41	-0.11	-1.87	-0.55	-0.41	-0.46	-1.34
O25	-2.02	-0.06	-0.50	-0.05	-1.10	0.12	-0.50	0.06	-1.72
O26	-2.02	-0.06	-0.50	-0.05	-1.10	0.12	-0.50	0.06	-1.72
O27	-2.02	0.06	-0.50	0.05	-1.10	-0.12	-0.50	-0.06	-1.72
O28	-2.02	0.06	-0.50	0.05	-1.10	-0.12	-0.50	-0.06	-1.72
O29	-0.82	0.05	-0.07	-0.01	-1.88	0.29	-0.05	0.26	-0.98
O30	-0.82	0.05	-0.07	-0.01	-1.88	0.29	-0.05	0.26	-0.98
O31	-0.82	-0.05	-0.07	0.01	-1.88	-0.29	-0.05	-0.26	-0.98
O32	-0.82	-0.05	-0.07	0.01	-1.88	-0.29	-0.05	-0.26	-0.98
H1	0.48	-0.12	0.14	-0.18	0.53	-0.22	0.15	-0.15	0.66
H2	0.48	-0.12	0.14	-0.18	0.53	-0.22	0.15	-0.15	0.66
H3	0.48	0.12	0.14	0.18	0.53	0.22	0.15	0.15	0.66
H4	0.48	0.12	0.14	0.18	0.53	0.22	0.15	0.15	0.66

Table S3. Optimized crystal structure of jadarite.

The space group of the optimized jadarite structure is $P2_1/c$. The axial lengths are $a=6.2720$ Å, $b=13.8016$ Å, $c=7.6878$ Å, and $\alpha=\gamma=90^\circ$, $\beta=124.0890^\circ$. The atomic sites are

Li1	0.45798	0.19886	0.12848
Na1	-0.03387	-0.00840	0.75597
B1	0.23143	0.15057	0.68356
B2	0.68011	0.35107	0.41713
B3	0.53748	0.50394	0.78711
Si1	0.04466	0.75263	0.20813
O1	0.81353	0.72265	-0.02222
O2	0.27725	0.78501	0.20978
O3	-0.02544	0.84769	0.29401
O4	0.12540	0.65717	0.35947
O5	0.75340	0.55061	0.88402
O6	0.68129	0.45526	0.35524
O7	0.54853	0.67206	0.61687
O8	0.53471	0.40694	0.83851
H1	0.69386	0.38360	-0.04784

Also attached below is a copy of the CIF file of the optimized crystal structure of hadarite.

CIF file created by FINDSYM, version 7.1.3

data_findsym-output

_audit_creation_method FINDSYM

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_cell_length_b 13.801600000

_cell_length_c 7.687800000

_cell_angle_alpha 90.000000000

_cell_angle_beta 124.088997000

_cell_angle_gamma 90.000000000

_cell_volume 594.1896961515

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_symmetry_Int_Tables_number 14

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2 -x,y+1/2,-z+1/2
3 -x,-y,-z
4 x,-y+1/2,z+1/2

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_symmetry_multiplicity

_atom_site_Wyckoff_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

_atom_site_fract_symmform

Li1	Li	4 e	0.45798	0.19886	0.12848	1.00000	Dx,Dy,Dz
Na1	Na	4 e	-0.03387	-0.00840	0.75597	1.00000	Dx,Dy,Dz
B1	B	4 e	0.23143	0.15057	0.68356	1.00000	Dx,Dy,Dz
B2	B	4 e	0.68011	0.35107	0.41713	1.00000	Dx,Dy,Dz
B3	B	4 e	0.53748	0.50394	0.78711	1.00000	Dx,Dy,Dz
Si1	Si	4 e	0.04466	0.75263	0.20813	1.00000	Dx,Dy,Dz
O1	O	4 e	0.81353	0.72265	-0.02222	1.00000	Dx,Dy,Dz
O2	O	4 e	0.27725	0.78501	0.20978	1.00000	Dx,Dy,Dz
O3	O	4 e	-0.02544	0.84769	0.29401	1.00000	Dx,Dy,Dz
O4	O	4 e	0.12540	0.65717	0.35947	1.00000	Dx,Dy,Dz
O5	O	4 e	0.75340	0.55061	0.88402	1.00000	Dx,Dy,Dz
O6	O	4 e	0.68129	0.45526	0.35524	1.00000	Dx,Dy,Dz
O7	O	4 e	0.54853	0.67206	0.61687	1.00000	Dx,Dy,Dz
O8	O	4 e	0.53471	0.40694	0.83851	1.00000	Dx,Dy,Dz
H1	H	4 e	0.69386	0.38360	-0.04784	1.00000	Dx,Dy,Dz

end of cif

Table S4. Eigenvectors of the dynamic matrix of jadarite.

1 f =	104.566043 THz	657.007825 2PiTHz	3487.947645 cm ⁻¹	432.450548 meV			
	X	Y	Z	dx	dy	dz	
Li	3.769818	9.645336	4.001386	0.000043	-0.000709	0.000767	
Li	-1.316675	4.156264	2.365404	0.000043	-0.000711	0.000768	
Li	-3.471104	2.744536	5.548798	0.000043	0.000707	0.000765	
Li	5.924247	11.057064	0.817991	0.000044	0.000714	0.000772	
Na	2.049025	6.784862	1.629696	-0.000007	-0.000273	0.000017	
Na	0.404117	7.016739	4.737094	-0.000007	-0.000273	0.000018	
Na	2.558546	13.685662	1.553699	-0.000007	0.000272	0.000018	
Na	-0.105403	0.115939	4.813091	-0.000008	0.000274	0.000017	
B	4.155007	8.978944	1.168663	0.001449	-0.000201	-0.000021	
B	-1.701865	4.822656	5.198127	0.001451	-0.000201	-0.000023	
B	0.452564	2.078144	2.014732	0.001443	0.000197	-0.000020	
B	2.000578	11.723457	4.352058	0.001459	0.000205	-0.000024	
B	-2.733891	11.746082	5.839177	-0.000095	0.000403	0.000005	
B	5.187034	2.055518	0.527613	-0.000095	0.000396	0.000004	
B	3.032605	4.845282	3.711007	-0.000095	-0.000400	0.000005	
B	-0.579463	8.956318	2.655782	-0.000095	-0.000399	0.000003	
B	-0.983708	0.054306	1.827988	0.000890	-0.000487	0.000911	
B	3.436850	13.747295	4.538802	0.000886	-0.000474	0.000901	
B	5.591279	6.955106	1.355407	0.000888	0.000480	0.000906	
B	-3.138137	6.846495	5.011383	0.000887	0.000479	0.000905	
Si	0.631772	3.486686	4.508512	-0.000297	0.000544	0.000171	
Si	1.821370	10.314915	1.858278	-0.000296	0.000544	0.000170	
Si	-0.333059	10.387486	5.041673	-0.000299	-0.000546	0.000173	
Si	2.786201	3.414115	1.325117	-0.000295	-0.000542	0.000170	
O	0.061445	3.072947	3.041906	-0.000159	-0.000051	-0.000135	
O	2.391697	10.728653	3.324884	-0.000161	-0.000053	-0.000135	
O	4.546126	9.973747	0.141489	-0.000160	0.000053	-0.000137	
O	-2.092984	3.827853	6.225301	-0.000160	0.000052	-0.000134	
O	2.197450	3.933608	4.519003	0.000286	-0.000068	0.000012	
O	0.255692	9.867992	1.847787	0.000286	-0.000069	0.000014	
O	-1.898737	10.834409	5.031182	0.000287	0.000068	0.000012	
O	4.351879	2.967192	1.335608	0.000285	0.000069	0.000014	

O	-0.212316	4.798696	5.055280	-0.000542	-0.000359	-0.000661
O	2.665458	9.002905	1.311510	-0.000541	-0.000359	-0.000659
O	0.511030	11.699496	4.494905	-0.000545	0.000361	-0.000664
O	1.942113	2.102105	1.871885	-0.000538	0.000357	-0.000657
O	0.525580	2.169271	5.472081	0.000061	-0.000348	0.000013
O	1.927562	11.632329	0.894709	0.000061	-0.000349	0.000014
O	-0.226867	9.070071	4.078104	0.000061	0.000350	0.000014
O	2.680009	4.731529	2.288686	0.000061	0.000348	0.000013
O	0.058846	0.698526	2.444964	0.000038	0.000140	0.000080
O	2.394296	13.103075	3.921826	0.000031	0.000132	0.000079
O	4.548725	7.599326	0.738431	0.000035	-0.000136	0.000080
O	-2.095583	6.202275	5.628359	0.000033	-0.000135	0.000079
O	-2.459230	13.184059	5.445139	-0.000265	0.000185	-0.000335
O	4.912372	0.617542	0.921651	-0.000269	0.000192	-0.000339
O	2.757943	6.283259	4.105046	-0.000266	-0.000188	-0.000336
O	-0.304801	7.518342	2.261744	-0.000268	-0.000188	-0.000338
O	-0.175430	2.374756	0.744070	-0.000330	-0.000051	-0.000244
O	2.628573	11.426844	5.622720	-0.000333	-0.000053	-0.000246
O	4.783002	9.275557	2.439325	-0.000331	0.000051	-0.000245
O	-2.329859	4.526044	3.927465	-0.000332	0.000053	-0.000244
O	-1.223866	12.517207	2.155216	0.017560	-0.011164	0.022441
O	3.677009	1.284394	4.211574	0.017386	-0.011056	0.022221
O	5.831438	5.616407	1.028179	0.017468	0.011108	0.022324
O	-3.378295	8.185194	5.338611	0.017451	0.011096	0.022304
H	-0.637445	12.195109	2.878812	-0.282545	0.170066	-0.358956
H	3.090587	1.606491	3.487978	-0.279741	0.168387	-0.355403
H	5.245016	5.294309	0.304583	-0.281072	-0.169188	-0.357091
H	-2.791874	8.507292	6.062207	-0.280789	-0.169014	-0.356729

2 f = 104.467378 THz 656.387895 2PiTHz 3484.656537 cm-1 432.042503

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000080	-0.000702	0.000831
Li	-1.316675	4.156264	2.365404	-0.000079	0.000666	-0.000758
Li	-3.471104	2.744536	5.548798	0.000080	0.000671	0.000764
Li	5.924247	11.057064	0.817991	-0.000080	-0.000699	-0.000828

Na	2.049025	6.784862	1.629696	-0.000061	-0.000158	0.000005
Na	0.404117	7.016739	4.737094	0.000060	0.000147	-0.000004
Na	2.558546	13.685662	1.553699	-0.000060	0.000149	0.000004
Na	-0.105403	0.115939	4.813091	0.000062	-0.000157	-0.000005
B	4.155007	8.978944	1.168663	0.001785	-0.000731	-0.000510
B	-1.701865	4.822656	5.198127	-0.001667	0.000761	0.000485
B	0.452564	2.078144	2.014732	0.001678	0.000764	-0.000486
B	2.000578	11.723457	4.352058	-0.001779	-0.000731	0.000511
B	-2.733891	11.746082	5.839177	-0.000051	-0.000699	-0.000330
B	5.187034	2.055518	0.527613	0.000041	0.000710	0.000289
B	3.032605	4.845282	3.711007	-0.000042	0.000707	-0.000289
B	-0.579463	8.956318	2.655782	0.000051	-0.000700	0.000331
B	-0.983708	0.054306	1.827988	-0.000453	0.001368	-0.001131
B	3.436850	13.747295	4.538802	0.000394	-0.001280	0.001055
B	5.591279	6.955106	1.355407	-0.000388	-0.001276	-0.001049
B	-3.138137	6.846495	5.011383	0.000457	0.001368	0.001134
Si	0.631772	3.486686	4.508512	0.000347	-0.000360	-0.000374
Si	1.821370	10.314915	1.858278	-0.000372	0.000413	0.000412
Si	-0.333059	10.387486	5.041673	0.000371	0.000411	-0.000412
Si	2.786201	3.414115	1.325117	-0.000349	-0.000363	0.000376
O	0.061445	3.072947	3.041906	-0.000202	0.000058	0.000358
O	2.391697	10.728653	3.324884	0.000216	-0.000092	-0.000406
O	4.546126	9.973747	0.141489	-0.000217	-0.000092	0.000405
O	-2.092984	3.827853	6.225301	0.000201	0.000058	-0.000359
O	2.197450	3.933608	4.519003	-0.000254	-0.000225	0.000180
O	0.255692	9.867992	1.847787	0.000264	0.000220	-0.000192
O	-1.898737	10.834409	5.031182	-0.000263	0.000220	0.000192
O	4.351879	2.967192	1.335608	0.000257	-0.000225	-0.000180
O	-0.212316	4.798696	5.055280	0.000698	0.000239	0.000602
O	2.665458	9.002905	1.311510	-0.000742	-0.000284	-0.000660
O	0.511030	11.699496	4.494905	0.000739	-0.000283	0.000657
O	1.942113	2.102105	1.871885	-0.000702	0.000241	-0.000606
O	0.525580	2.169271	5.472081	-0.000033	-0.000028	-0.000048
O	1.927562	11.632329	0.894709	0.000038	0.000011	0.000064
O	-0.226867	9.070071	4.078104	-0.000037	0.000012	-0.000064
O	2.680009	4.731529	2.288686	0.000034	-0.000026	0.000048

O	0.058846	0.698526	2.444964	-0.000601	-0.000823	0.000020
O	2.394296	13.103075	3.921826	0.000591	0.000789	-0.000028
O	4.548725	7.599326	0.738431	-0.000589	0.000787	0.000029
O	-2.095583	6.202275	5.628359	0.000601	-0.000823	-0.000019
O	-2.459230	13.184059	5.445139	-0.000247	0.000623	-0.000433
O	4.912372	0.617542	0.921651	0.000269	-0.000660	0.000468
O	2.757943	6.283259	4.105046	-0.000271	-0.000659	-0.000470
O	-0.304801	7.518342	2.261744	0.000244	0.000621	0.000430
O	-0.175430	2.374756	0.744070	-0.000337	-0.000229	-0.000159
O	2.628573	11.426844	5.622720	0.000362	0.000229	0.000182
O	4.783002	9.275557	2.439325	-0.000364	0.000228	-0.000183
O	-2.329859	4.526044	3.927465	0.000336	-0.000229	0.000157
O	-1.223866	12.517207	2.155216	-0.018221	0.011183	-0.023066
O	3.677009	1.284394	4.211574	0.016960	-0.010408	0.021460
O	5.831438	5.616407	1.028179	-0.016838	-0.010330	-0.021304
O	-3.378295	8.185194	5.338611	0.018289	0.011228	0.023154
H	-0.637445	12.195109	2.878812	0.291398	-0.174784	0.369933
H	3.090587	1.606491	3.487978	-0.271188	0.162708	-0.344237
H	5.245016	5.294309	0.304583	0.269204	0.161515	0.341716
H	-2.791874	8.507292	6.062207	-0.292510	-0.175457	-0.371350

3 f = 104.459650 THz 656.339336 2PiTHz 3484.398748 cm-1 432.010541 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000001	-0.000380	0.000845
Li	-1.316675	4.156264	2.365404	0.000006	-0.000443	0.000920
Li	-3.471104	2.744536	5.548798	-0.000005	-0.000432	-0.000906
Li	5.924247	11.057064	0.817991	-0.000000	-0.000390	-0.000858
Na	2.049025	6.784862	1.629696	-0.000012	-0.000123	0.000012
Na	0.404117	7.016739	4.737094	-0.000018	-0.000138	0.000013
Na	2.558546	13.685662	1.553699	0.000017	-0.000135	-0.000013
Na	-0.105403	0.115939	4.813091	0.000013	-0.000126	-0.000012
B	4.155007	8.978944	1.168663	0.001344	0.000441	-0.000312
B	-1.701865	4.822656	5.198127	0.001508	0.000368	-0.000354
B	0.452564	2.078144	2.014732	-0.001477	0.000382	0.000350
B	2.000578	11.723457	4.352058	-0.001374	0.000426	0.000316

B	-2.733891	11.746082	5.839177	-0.000114	0.000134	-0.000522
B	5.187034	2.055518	0.527613	-0.000119	0.000091	-0.000548
B	3.032605	4.845282	3.711007	0.000118	0.000079	0.000546
B	-0.579463	8.956318	2.655782	0.000115	0.000145	0.000524
B	-0.983708	0.054306	1.827988	-0.000799	0.001123	-0.000995
B	3.436850	13.747295	4.538802	-0.000823	0.001201	-0.001059
B	5.591279	6.955106	1.355407	0.000831	0.001226	0.001080
B	-3.138137	6.846495	5.011383	0.000791	0.001098	0.000976
Si	0.631772	3.486686	4.508512	-0.000321	0.000675	0.000488
Si	1.821370	10.314915	1.858278	-0.000288	0.000635	0.000453
Si	-0.333059	10.387486	5.041673	0.000293	0.000645	-0.000457
Si	2.786201	3.414115	1.325117	0.000315	0.000665	-0.000484
O	0.061445	3.072947	3.041906	0.000194	-0.000435	-0.000609
O	2.391697	10.728653	3.324884	0.000181	-0.000425	-0.000576
O	4.546126	9.973747	0.141489	-0.000178	-0.000429	0.000580
O	-2.092984	3.827853	6.225301	-0.000197	-0.000431	0.000606
O	2.197450	3.933608	4.519003	0.000124	-0.000053	-0.000158
O	0.255692	9.867992	1.847787	0.000098	-0.000071	-0.000144
O	-1.898737	10.834409	5.031182	-0.000103	-0.000070	0.000144
O	4.351879	2.967192	1.335608	-0.000118	-0.000054	0.000158
O	-0.212316	4.798696	5.055280	-0.000580	-0.000561	-0.000724
O	2.665458	9.002905	1.311510	-0.000513	-0.000534	-0.000662
O	0.511030	11.699496	4.494905	0.000525	-0.000540	0.000674
O	1.942113	2.102105	1.871885	0.000567	-0.000554	0.000711
O	0.525580	2.169271	5.472081	0.000058	-0.000216	0.000216
O	1.927562	11.632329	0.894709	0.000054	-0.000211	0.000211
O	-0.226867	9.070071	4.078104	-0.000055	-0.000217	-0.000212
O	2.680009	4.731529	2.288686	-0.000056	-0.000210	-0.000215
O	0.058846	0.698526	2.444964	-0.000123	-0.000441	-0.000122
O	2.394296	13.103075	3.921826	-0.000158	-0.000489	-0.000120
O	4.548725	7.599326	0.738431	0.000169	-0.000504	0.000120
O	-2.095583	6.202275	5.628359	0.000112	-0.000426	0.000122
O	-2.459230	13.184059	5.445139	0.000312	-0.000506	0.000493
O	4.912372	0.617542	0.921651	0.000297	-0.000469	0.000468
O	2.757943	6.283259	4.105046	-0.000292	-0.000457	-0.000459
O	-0.304801	7.518342	2.261744	-0.000317	-0.000518	-0.000503

O	-0.175430	2.374756	0.744070	0.000343	0.000005	0.000295
O	2.628573	11.426844	5.622720	0.000321	-0.000011	0.000285
O	4.783002	9.275557	2.439325	-0.000316	-0.000013	-0.000282
O	-2.329859	4.526044	3.927465	-0.000350	0.000007	-0.000298
O	-1.223866	12.517207	2.155216	-0.016973	0.010475	-0.021651
O	3.677009	1.284394	4.211574	-0.018005	0.011109	-0.022958
O	5.831438	5.616407	1.028179	0.018344	0.011317	0.023387
O	-3.378295	8.185194	5.338611	0.016655	0.010280	0.021248
H	-0.637445	12.195109	2.878812	0.272554	-0.163007	0.346634
H	3.090587	1.606491	3.487978	0.289073	-0.172924	0.367616
H	5.245016	5.294309	0.304583	-0.294487	-0.176170	-0.374482
H	-2.791874	8.507292	6.062207	-0.267468	-0.159960	-0.340184

4 f = 104.442827 THz 656.233635 2PiTHz 3483.837595 cm-1 431.940967 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000066	-0.000573	0.000705
Li	-1.316675	4.156264	2.365404	-0.000067	0.000568	-0.000692
Li	-3.471104	2.744536	5.548798	-0.000067	-0.000575	-0.000708
Li	5.924247	11.057064	0.817991	0.000066	0.000565	0.000688
Na	2.049025	6.784862	1.629696	-0.000064	-0.000131	0.000000
Na	0.404117	7.016739	4.737094	0.000064	0.000130	-0.000000
Na	2.558546	13.685662	1.553699	0.000064	-0.000132	-0.000001
Na	-0.105403	0.115939	4.813091	-0.000064	0.000129	-0.000000
B	4.155007	8.978944	1.168663	0.001671	-0.000765	-0.000227
B	-1.701865	4.822656	5.198127	-0.001651	0.000774	0.000221
B	0.452564	2.078144	2.014732	-0.001676	-0.000766	0.000226
B	2.000578	11.723457	4.352058	0.001643	0.000772	-0.000220
B	-2.733891	11.746082	5.839177	-0.000089	0.000648	-0.000121
B	5.187034	2.055518	0.527613	0.000088	-0.000648	0.000111
B	3.032605	4.845282	3.711007	0.000090	0.000650	0.000121
B	-0.579463	8.956318	2.655782	-0.000087	-0.000646	-0.000111
B	-0.983708	0.054306	1.827988	0.000409	-0.001311	0.001071
B	3.436850	13.747295	4.538802	-0.000428	0.001335	-0.001095
B	5.591279	6.955106	1.355407	-0.000413	-0.001314	-0.001076
B	-3.138137	6.846495	5.011383	0.000425	0.001334	0.001092

Si	0.631772	3.486686	4.508512	0.000294	-0.000530	-0.000209
Si	1.821370	10.314915	1.858278	-0.000299	0.000540	0.000217
Si	-0.333059	10.387486	5.041673	-0.000293	-0.000528	0.000208
Si	2.786201	3.414115	1.325117	0.000300	0.000542	-0.000218
O	0.061445	3.072947	3.041906	0.000171	0.000181	0.000183
O	2.391697	10.728653	3.324884	-0.000167	-0.000188	-0.000194
O	4.546126	9.973747	0.141489	-0.000170	0.000180	-0.000182
O	-2.092984	3.827853	6.225301	0.000167	-0.000189	0.000194
O	2.197450	3.933608	4.519003	-0.000304	-0.000006	-0.000005
O	0.255692	9.867992	1.847787	0.000305	0.000006	0.000002
O	-1.898737	10.834409	5.031182	0.000302	-0.000007	0.000005
O	4.351879	2.967192	1.335608	-0.000306	0.000005	-0.000002
O	-0.212316	4.798696	5.055280	0.000651	0.000331	0.000657
O	2.665458	9.002905	1.311510	-0.000659	-0.000339	-0.000667
O	0.511030	11.699496	4.494905	-0.000649	0.000329	-0.000653
O	1.942113	2.102105	1.871885	0.000661	-0.000341	0.000669
O	0.525580	2.169271	5.472081	-0.000078	0.000324	-0.000075
O	1.927562	11.632329	0.894709	0.000079	-0.000326	0.000079
O	-0.226867	9.070071	4.078104	0.000078	0.000322	0.000075
O	2.680009	4.731529	2.288686	-0.000079	-0.000328	-0.000079
O	0.058846	0.698526	2.444964	0.000587	0.000809	0.000004
O	2.394296	13.103075	3.921826	-0.000590	-0.000819	-0.000007
O	4.548725	7.599326	0.738431	-0.000588	0.000811	-0.000004
O	-2.095583	6.202275	5.628359	0.000590	-0.000819	0.000007
O	-2.459230	13.184059	5.445139	0.000269	-0.000637	0.000487
O	4.912372	0.617542	0.921651	-0.000262	0.000627	-0.000476
O	2.757943	6.283259	4.105046	-0.000268	-0.000636	-0.000486
O	-0.304801	7.518342	2.261744	0.000264	0.000628	0.000478
O	-0.175430	2.374756	0.744070	0.000324	0.000113	0.000169
O	2.628573	11.426844	5.622720	-0.000316	-0.000112	-0.000162
O	4.783002	9.275557	2.439325	-0.000323	0.000112	-0.000168
O	-2.329859	4.526044	3.927465	0.000319	-0.000113	0.000163
O	-1.223866	12.517207	2.155216	0.017388	-0.010663	0.021997
O	3.677009	1.284394	4.211574	-0.017793	0.010915	-0.022515
O	5.831438	5.616407	1.028179	-0.017480	-0.010722	-0.022116
O	-3.378295	8.185194	5.338611	0.017730	0.010874	0.022433

H	-0.637445	12.195109	2.878812	-0.278032	0.166658	-0.352701
H	3.090587	1.606491	3.487978	0.284539	-0.170559	0.360982
H	5.245016	5.294309	0.304583	0.279518	0.167557	0.354594
H	-2.791874	8.507292	6.062207	-0.283523	-0.169944	-0.359686

5 f = 41.915422 THz 263.362364 2PiTHz 1398.147943 cm-1 173.348314 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.001791	-0.000291	-0.001589
Li	-1.316675	4.156264	2.365404	0.001792	0.000291	0.001590
Li	-3.471104	2.744536	5.548798	0.001787	-0.000293	0.001588
Li	5.924247	11.057064	0.817991	-0.001786	0.000294	-0.001590
Na	2.049025	6.784862	1.629696	0.001237	0.000104	-0.002613
Na	0.404117	7.016739	4.737094	-0.001237	-0.000105	0.002616
Na	2.558546	13.685662	1.553699	-0.001243	0.000105	0.002625
Na	-0.105403	0.115939	4.813091	0.001241	-0.000104	-0.002624
B	4.155007	8.978944	1.168663	-0.000211	-0.015942	-0.011073
B	-1.701865	4.822656	5.198127	0.000206	0.015939	0.011070
B	0.452564	2.078144	2.014732	0.000206	-0.016006	0.011113
B	2.000578	11.723457	4.352058	-0.000208	0.015997	-0.011106
B	-2.733891	11.746082	5.839177	-0.007930	-0.013025	0.002933
B	5.187034	2.055518	0.527613	0.007940	0.013046	-0.002939
B	3.032605	4.845282	3.711007	0.007905	-0.012986	-0.002926
B	-0.579463	8.956318	2.655782	-0.007901	0.012981	0.002924
B	-0.983708	0.054306	1.827988	0.090814	-0.007096	0.079543
B	3.436850	13.747295	4.538802	-0.090717	0.007102	-0.079465
B	5.591279	6.955106	1.355407	-0.090423	-0.007086	-0.079210
B	-3.138137	6.846495	5.011383	0.090437	0.007062	0.079212
Si	0.631772	3.486686	4.508512	-0.004120	0.001295	-0.002776
Si	1.821370	10.314915	1.858278	0.004120	-0.001294	0.002773
Si	-0.333059	10.387486	5.041673	0.004127	0.001298	0.002761
Si	2.786201	3.414115	1.325117	-0.004130	-0.001297	-0.002761
O	0.061445	3.072947	3.041906	0.000488	0.005529	0.003938
O	2.391697	10.728653	3.324884	-0.000487	-0.005525	-0.003934
O	4.546126	9.973747	0.141489	-0.000488	0.005505	-0.003919
O	-2.092984	3.827853	6.225301	0.000490	-0.005504	0.003920

O	2.197450	3.933608	4.519003	0.004218	0.004749	-0.001245
O	0.255692	9.867992	1.847787	-0.004218	-0.004749	0.001244
O	-1.898737	10.834409	5.031182	-0.004225	0.004763	0.001247
O	4.351879	2.967192	1.335608	0.004229	-0.004770	-0.001252
O	-0.212316	4.798696	5.055280	0.006649	-0.005831	-0.002629
O	2.665458	9.002905	1.311510	-0.006649	0.005831	0.002633
O	0.511030	11.699496	4.494905	-0.006672	-0.005852	0.002644
O	1.942113	2.102105	1.871885	0.006678	0.005855	-0.002644
O	0.525580	2.169271	5.472081	0.000510	-0.005020	0.007611
O	1.927562	11.632329	0.894709	-0.000511	0.005015	-0.007602
O	-0.226867	9.070071	4.078104	-0.000512	-0.005001	-0.007579
O	2.680009	4.731529	2.288686	0.000512	0.005001	0.007579
O	0.058846	0.698526	2.444964	-0.028583	-0.012901	-0.019387
O	2.394296	13.103075	3.921826	0.028548	0.012882	0.019363
O	4.548725	7.599326	0.738431	0.028456	-0.012839	0.019303
O	-2.095583	6.202275	5.628359	-0.028464	0.012847	-0.019305
O	-2.459230	13.184059	5.445139	0.027010	-0.014841	0.027308
O	4.912372	0.617542	0.921651	-0.027035	0.014856	-0.027332
O	2.757943	6.283259	4.105046	-0.026922	-0.014791	-0.027216
O	-0.304801	7.518342	2.261744	0.026922	0.014798	0.027220
O	-0.175430	2.374756	0.744070	-0.008035	0.000506	-0.006829
O	2.628573	11.426844	5.622720	0.008022	-0.000510	0.006826
O	4.783002	9.275557	2.439325	0.008003	0.000507	0.006804
O	-2.329859	4.526044	3.927465	-0.008001	-0.000508	-0.006805
O	-1.223866	12.517207	2.155216	-0.010375	-0.004264	-0.009315
O	3.677009	1.284394	4.211574	0.010365	0.004255	0.009309
O	5.831438	5.616407	1.028179	0.010331	-0.004240	0.009279
O	-3.378295	8.185194	5.338611	-0.010332	0.004248	-0.009278
H	-0.637445	12.195109	2.878812	0.060742	0.152588	0.012801
H	3.090587	1.606491	3.487978	-0.060686	-0.152437	-0.012780
H	5.245016	5.294309	0.304583	-0.060480	0.151960	-0.012756
H	-2.791874	8.507292	6.062207	0.060499	-0.151988	0.012755

6 f = 41.899846 THz 263.264500 2PiTHz 1397.628395 cm-1 173.283898
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.001417	0.000611	-0.000249
Li	-1.316675	4.156264	2.365404	0.001417	-0.000610	0.000246
Li	-3.471104	2.744536	5.548798	-0.001424	-0.000610	-0.000251
Li	5.924247	11.057064	0.817991	0.001424	0.000609	0.000255
Na	2.049025	6.784862	1.629696	-0.001285	-0.000077	0.002653
Na	0.404117	7.016739	4.737094	0.001283	0.000078	-0.002657
Na	2.558546	13.685662	1.553699	-0.001277	0.000076	0.002649
Na	-0.105403	0.115939	4.813091	0.001282	-0.000077	-0.002642
B	4.155007	8.978944	1.168663	-0.000520	0.016554	0.010397
B	-1.701865	4.822656	5.198127	0.000526	-0.016535	-0.010383
B	0.452564	2.078144	2.014732	-0.000523	-0.016469	0.010340
B	2.000578	11.723457	4.352058	0.000524	0.016502	-0.010358
B	-2.733891	11.746082	5.839177	-0.008642	-0.014200	0.002995
B	5.187034	2.055518	0.527613	0.008617	0.014156	-0.003002
B	3.032605	4.845282	3.711007	-0.008658	0.014223	0.003011
B	-0.579463	8.956318	2.655782	0.008661	-0.014229	-0.003007
B	-0.983708	0.054306	1.827988	0.090751	-0.006917	0.079354
B	3.436850	13.747295	4.538802	-0.091002	0.006886	-0.079549
B	5.591279	6.955106	1.355407	0.091254	0.006939	0.079784
B	-3.138137	6.846495	5.011383	-0.091166	-0.006916	-0.079704
Si	0.631772	3.486686	4.508512	0.002334	-0.000845	-0.003695
Si	1.821370	10.314915	1.858278	-0.002336	0.000843	0.003707
Si	-0.333059	10.387486	5.041673	0.002322	0.000840	-0.003715
Si	2.786201	3.414115	1.325117	-0.002318	-0.000839	0.003707
O	0.061445	3.072947	3.041906	-0.000297	0.006214	0.004419
O	2.391697	10.728653	3.324884	0.000295	-0.006228	-0.004434
O	4.546126	9.973747	0.141489	-0.000294	-0.006246	0.004446
O	-2.092984	3.827853	6.225301	0.000294	0.006238	-0.004437
O	2.197450	3.933608	4.519003	-0.002438	-0.004690	0.001443
O	0.255692	9.867992	1.847787	0.002444	0.004692	-0.001445
O	-1.898737	10.834409	5.031182	-0.002429	0.004679	0.001443
O	4.351879	2.967192	1.335608	0.002422	-0.004668	-0.001436
O	-0.212316	4.798696	5.055280	-0.006943	0.006109	0.003458
O	2.665458	9.002905	1.311510	0.006951	-0.006113	-0.003466
O	0.511030	11.699496	4.494905	-0.006931	-0.006093	0.003455
O	1.942113	2.102105	1.871885	0.006915	0.006086	-0.003450

O	0.525580	2.169271	5.472081	-0.000442	-0.004504	0.007266
O	1.927562	11.632329	0.894709	0.000440	0.004513	-0.007284
O	-0.226867	9.070071	4.078104	-0.000439	0.004529	0.007305
O	2.680009	4.731529	2.288686	0.000440	-0.004526	-0.007300
O	0.058846	0.698526	2.444964	-0.028597	-0.012987	-0.019273
O	2.394296	13.103075	3.921826	0.028671	0.013031	0.019316
O	4.548725	7.599326	0.738431	-0.028754	0.013061	-0.019375
O	-2.095583	6.202275	5.628359	0.028725	-0.013051	0.019357
O	-2.459230	13.184059	5.445139	0.027196	-0.014630	0.027399
O	4.912372	0.617542	0.921651	-0.027116	0.014604	-0.027326
O	2.757943	6.283259	4.105046	0.027239	0.014662	0.027448
O	-0.304801	7.518342	2.261744	-0.027272	-0.014681	-0.027477
O	-0.175430	2.374756	0.744070	-0.007363	0.000280	-0.006354
O	2.628573	11.426844	5.622720	0.007385	-0.000280	0.006372
O	4.783002	9.275557	2.439325	-0.007410	-0.000284	-0.006393
O	-2.329859	4.526044	3.927465	0.007397	0.000281	0.006383
O	-1.223866	12.517207	2.155216	-0.010385	-0.004006	-0.009184
O	3.677009	1.284394	4.211574	0.010430	0.004049	0.009203
O	5.831438	5.616407	1.028179	-0.010454	0.004045	-0.009233
O	-3.378295	8.185194	5.338611	0.010438	-0.004041	0.009224
H	-0.637445	12.195109	2.878812	0.060793	0.145778	0.009517
H	3.090587	1.606491	3.487978	-0.060938	-0.146207	-0.009585
H	5.245016	5.294309	0.304583	0.061109	-0.146630	0.009612
H	-2.791874	8.507292	6.062207	-0.061069	0.146478	-0.009585

7 f = 41.706288 THz 262.048336 2PiTHz 1391.171978 cm-1 172.483404 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000930	-0.000365	-0.001739
Li	-1.316675	4.156264	2.365404	-0.000934	-0.000362	-0.001740
Li	-3.471104	2.744536	5.548798	0.000934	-0.000363	0.001740
Li	5.924247	11.057064	0.817991	0.000929	-0.000365	0.001739
Na	2.049025	6.784862	1.629696	-0.001944	0.000489	-0.001675
Na	0.404117	7.016739	4.737094	-0.001947	0.000488	-0.001670
Na	2.558546	13.685662	1.553699	0.001948	0.000489	0.001673
Na	-0.105403	0.115939	4.813091	0.001946	0.000488	0.001675

B	4.155007	8.978944	1.168663	-0.000081	0.013315	0.009587
B	-1.701865	4.822656	5.198127	-0.000085	0.013353	0.009609
B	0.452564	2.078144	2.014732	0.000089	0.013357	-0.009609
B	2.000578	11.723457	4.352058	0.000080	0.013334	-0.009599
B	-2.733891	11.746082	5.839177	-0.007601	-0.015462	0.001693
B	5.187034	2.055518	0.527613	-0.007618	-0.015473	0.001700
B	3.032605	4.845282	3.711007	0.007614	-0.015465	-0.001702
B	-0.579463	8.956318	2.655782	0.007592	-0.015439	-0.001689
B	-0.983708	0.054306	1.827988	-0.090544	0.014476	-0.080595
B	3.436850	13.747295	4.538802	-0.090422	0.014473	-0.080490
B	5.591279	6.955106	1.355407	0.090300	0.014457	0.080382
B	-3.138137	6.846495	5.011383	0.090505	0.014484	0.080566
Si	0.631772	3.486686	4.508512	-0.002390	-0.001328	0.004367
Si	1.821370	10.314915	1.858278	-0.002385	-0.001332	0.004363
Si	-0.333059	10.387486	5.041673	0.002389	-0.001330	-0.004360
Si	2.786201	3.414115	1.325117	0.002390	-0.001327	-0.004366
O	0.061445	3.072947	3.041906	0.000077	-0.004621	-0.003504
O	2.391697	10.728653	3.324884	0.000078	-0.004611	-0.003500
O	4.546126	9.973747	0.141489	-0.000079	-0.004606	0.003496
O	-2.092984	3.827853	6.225301	-0.000077	-0.004618	0.003501
O	2.197450	3.933608	4.519003	0.004722	0.005722	-0.002962
O	0.255692	9.867992	1.847787	0.004717	0.005713	-0.002963
O	-1.898737	10.834409	5.031182	-0.004723	0.005721	0.002965
O	4.351879	2.967192	1.335608	-0.004721	0.005724	0.002963
O	-0.212316	4.798696	5.055280	0.005218	-0.002504	-0.001934
O	2.665458	9.002905	1.311510	0.005208	-0.002488	-0.001929
O	0.511030	11.699496	4.494905	-0.005214	-0.002492	0.001931
O	1.942113	2.102105	1.871885	-0.005221	-0.002505	0.001934
O	0.525580	2.169271	5.472081	-0.000222	0.006211	-0.007906
O	1.927562	11.632329	0.894709	-0.000225	0.006205	-0.007898
O	-0.226867	9.070071	4.078104	0.000225	0.006195	0.007888
O	2.680009	4.731529	2.288686	0.000222	0.006210	0.007905
O	0.058846	0.698526	2.444964	0.026564	0.012519	0.018000
O	2.394296	13.103075	3.921826	0.026520	0.012498	0.017968
O	4.548725	7.599326	0.738431	-0.026483	0.012482	-0.017945
O	-2.095583	6.202275	5.628359	-0.026551	0.012508	-0.017993

O	-2.459230	13.184059	5.445139	0.027492	-0.015677	0.027690
O	4.912372	0.617542	0.921651	0.027534	-0.015697	0.027731
O	2.757943	6.283259	4.105046	-0.027522	-0.015694	-0.027720
O	-0.304801	7.518342	2.261744	-0.027457	-0.015657	-0.027654
O	-0.175430	2.374756	0.744070	0.008082	-0.000048	0.006157
O	2.628573	11.426844	5.622720	0.008077	-0.000047	0.006156
O	4.783002	9.275557	2.439325	-0.008067	-0.000047	-0.006148
O	-2.329859	4.526044	3.927465	-0.008079	-0.000048	-0.006156
O	-1.223866	12.517207	2.155216	0.010211	0.001398	0.010470
O	3.677009	1.284394	4.211574	0.010196	0.001390	0.010457
O	5.831438	5.616407	1.028179	-0.010182	0.001385	-0.010444
O	-3.378295	8.185194	5.338611	-0.010206	0.001394	-0.010466
H	-0.637445	12.195109	2.878812	-0.048300	-0.152489	-0.022383
H	3.090587	1.606491	3.487978	-0.048222	-0.152319	-0.022372
H	5.245016	5.294309	0.304583	0.048144	-0.152112	0.022350
H	-2.791874	8.507292	6.062207	0.048289	-0.152438	0.022370

8 f = 41.649065 THz 261.688792 2PiTHz 1389.263219 cm-1 172.246748

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000922	-0.000481	0.000172
Li	-1.316675	4.156264	2.365404	0.000922	-0.000480	0.000173
Li	-3.471104	2.744536	5.548798	0.000922	0.000481	0.000173
Li	5.924247	11.057064	0.817991	0.000923	0.000479	0.000175
Na	2.049025	6.784862	1.629696	-0.001957	0.000068	-0.001656
Na	0.404117	7.016739	4.737094	-0.001956	0.000068	-0.001659
Na	2.558546	13.685662	1.553699	-0.001956	-0.000068	-0.001656
Na	-0.105403	0.115939	4.813091	-0.001954	-0.000068	-0.001656
B	4.155007	8.978944	1.168663	-0.001153	0.012917	0.006864
B	-1.701865	4.822656	5.198127	-0.001156	0.012895	0.006848
B	0.452564	2.078144	2.014732	-0.001157	-0.012894	0.006849
B	2.000578	11.723457	4.352058	-0.001153	-0.012895	0.006846
B	-2.733891	11.746082	5.839177	0.008160	0.018730	-0.001104
B	5.187034	2.055518	0.527613	0.008163	0.018738	-0.001108
B	3.032605	4.845282	3.711007	0.008165	-0.018736	-0.001105
B	-0.579463	8.956318	2.655782	0.008172	-0.018759	-0.001110

B	-0.983708	0.054306	1.827988	0.093036	-0.004240	0.078999
B	3.436850	13.747295	4.538802	0.093011	-0.004240	0.078976
B	5.591279	6.955106	1.355407	0.093164	0.004264	0.079115
B	-3.138137	6.846495	5.011383	0.093039	0.004243	0.079001
Si	0.631772	3.486686	4.508512	-0.002197	0.001755	-0.002133
Si	1.821370	10.314915	1.858278	-0.002202	0.001755	-0.002131
Si	-0.333059	10.387486	5.041673	-0.002197	-0.001759	-0.002138
Si	2.786201	3.414115	1.325117	-0.002198	-0.001753	-0.002134
O	0.061445	3.072947	3.041906	0.000453	0.005012	0.003809
O	2.391697	10.728653	3.324884	0.000452	0.005010	0.003808
O	4.546126	9.973747	0.141489	0.000453	-0.005017	0.003813
O	-2.092984	3.827853	6.225301	0.000452	-0.005014	0.003810
O	2.197450	3.933608	4.519003	0.003244	0.005743	-0.001853
O	0.255692	9.867992	1.847787	0.003250	0.005752	-0.001856
O	-1.898737	10.834409	5.031182	0.003241	-0.005741	-0.001851
O	4.351879	2.967192	1.335608	0.003245	-0.005744	-0.001853
O	-0.212316	4.798696	5.055280	0.005279	-0.002969	-0.001101
O	2.665458	9.002905	1.311510	0.005287	-0.002976	-0.001105
O	0.511030	11.699496	4.494905	0.005279	0.002973	-0.001102
O	1.942113	2.102105	1.871885	0.005278	0.002968	-0.001101
O	0.525580	2.169271	5.472081	0.000507	-0.006499	0.006667
O	1.927562	11.632329	0.894709	0.000509	-0.006495	0.006664
O	-0.226867	9.070071	4.078104	0.000509	0.006509	0.006679
O	2.680009	4.731529	2.288686	0.000507	0.006497	0.006667
O	0.058846	0.698526	2.444964	-0.028534	-0.015246	-0.018455
O	2.394296	13.103075	3.921826	-0.028527	-0.015238	-0.018447
O	4.548725	7.599326	0.738431	-0.028573	0.015262	-0.018479
O	-2.095583	6.202275	5.628359	-0.028534	0.015243	-0.018454
O	-2.459230	13.184059	5.445139	-0.026954	0.013068	-0.026503
O	4.912372	0.617542	0.921651	-0.026959	0.013071	-0.026509
O	2.757943	6.283259	4.105046	-0.026960	-0.013072	-0.026509
O	-0.304801	7.518342	2.261744	-0.027002	-0.013094	-0.026549
O	-0.175430	2.374756	0.744070	-0.007698	-0.000665	-0.005431
O	2.628573	11.426844	5.622720	-0.007692	-0.000663	-0.005432
O	4.783002	9.275557	2.439325	-0.007706	0.000662	-0.005441
O	-2.329859	4.526044	3.927465	-0.007698	0.000664	-0.005433

O	-1.223866	12.517207	2.155216	-0.010772	-0.004659	-0.009631
O	3.677009	1.284394	4.211574	-0.010772	-0.004662	-0.009630
O	5.831438	5.616407	1.028179	-0.010786	0.004661	-0.009647
O	-3.378295	8.185194	5.338611	-0.010775	0.004660	-0.009632
H	-0.637445	12.195109	2.878812	0.050344	0.148282	0.020636
H	3.090587	1.606491	3.487978	0.050335	0.148266	0.020638
H	5.245016	5.294309	0.304583	0.050420	-0.148499	0.020662
H	-2.791874	8.507292	6.062207	0.050343	-0.148315	0.020652

9 f = 40.897808 THz 256.968503 2PiTHz 1364.203975 cm-1 169.139797 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000165	0.000275	-0.001773
Li	-1.316675	4.156264	2.365404	-0.000165	0.000272	-0.001773
Li	-3.471104	2.744536	5.548798	-0.000166	-0.000274	-0.001774
Li	5.924247	11.057064	0.817991	-0.000165	-0.000273	-0.001772
Na	2.049025	6.784862	1.629696	-0.000014	-0.003450	0.000239
Na	0.404117	7.016739	4.737094	-0.000015	-0.003449	0.000239
Na	2.558546	13.685662	1.553699	-0.000015	0.003450	0.000240
Na	-0.105403	0.115939	4.813091	-0.000014	0.003450	0.000238
B	4.155007	8.978944	1.168663	-0.004794	-0.008727	-0.007581
B	-1.701865	4.822656	5.198127	-0.004786	-0.008742	-0.007585
B	0.452564	2.078144	2.014732	-0.004789	0.008733	-0.007585
B	2.000578	11.723457	4.352058	-0.004792	0.008735	-0.007582
B	-2.733891	11.746082	5.839177	0.008611	0.009168	0.004620
B	5.187034	2.055518	0.527613	0.008620	0.009175	0.004621
B	3.032605	4.845282	3.711007	0.008615	-0.009170	0.004619
B	-0.579463	8.956318	2.655782	0.008615	-0.009174	0.004622
B	-0.983708	0.054306	1.827988	0.022914	0.123205	-0.026106
B	3.436850	13.747295	4.538802	0.022908	0.123219	-0.026111
B	5.591279	6.955106	1.355407	0.022924	-0.123192	-0.026089
B	-3.138137	6.846495	5.011383	0.022896	-0.123225	-0.026127
Si	0.631772	3.486686	4.508512	0.000682	0.000207	-0.000815
Si	1.821370	10.314915	1.858278	0.000682	0.000206	-0.000814
Si	-0.333059	10.387486	5.041673	0.000684	-0.000207	-0.000815
Si	2.786201	3.414115	1.325117	0.000680	-0.000207	-0.000814

O	0.061445	3.072947	3.041906	0.000986	0.000456	0.001992
O	2.391697	10.728653	3.324884	0.000983	0.000449	0.001989
O	4.546126	9.973747	0.141489	0.000982	-0.000457	0.001989
O	-2.092984	3.827853	6.225301	0.000988	-0.000447	0.001992
O	2.197450	3.933608	4.519003	-0.001962	0.000512	-0.000583
O	0.255692	9.867992	1.847787	-0.001969	0.000518	-0.000586
O	-1.898737	10.834409	5.031182	-0.001973	-0.000516	-0.000591
O	4.351879	2.967192	1.335608	-0.001958	-0.000514	-0.000577
O	-0.212316	4.798696	5.055280	0.001419	0.000830	-0.000508
O	2.665458	9.002905	1.311510	0.001416	0.000825	-0.000507
O	0.511030	11.699496	4.494905	0.001419	-0.000824	-0.000509
O	1.942113	2.102105	1.871885	0.001415	-0.000830	-0.000506
O	0.525580	2.169271	5.472081	-0.001220	-0.001496	-0.001545
O	1.927562	11.632329	0.894709	-0.001214	-0.001478	-0.001543
O	-0.226867	9.070071	4.078104	-0.001217	0.001486	-0.001541
O	2.680009	4.731529	2.288686	-0.001217	0.001488	-0.001547
O	0.058846	0.698526	2.444964	-0.021737	-0.029573	-0.006460
O	2.394296	13.103075	3.921826	-0.021744	-0.029579	-0.006467
O	4.548725	7.599326	0.738431	-0.021729	0.029574	-0.006456
O	-2.095583	6.202275	5.628359	-0.021751	0.029577	-0.006470
O	-2.459230	13.184059	5.445139	0.009617	-0.024603	0.015899
O	4.912372	0.617542	0.921651	0.009607	-0.024585	0.015896
O	2.757943	6.283259	4.105046	0.009629	0.024598	0.015913
O	-0.304801	7.518342	2.261744	0.009595	0.024589	0.015881
O	-0.175430	2.374756	0.744070	-0.001159	-0.002291	0.001025
O	2.628573	11.426844	5.622720	-0.001146	-0.002288	0.001011
O	4.783002	9.275557	2.439325	-0.001147	0.002285	0.001019
O	-2.329859	4.526044	3.927465	-0.001159	0.002293	0.001018
O	-1.223866	12.517207	2.155216	-0.005366	-0.042034	0.010782
O	3.677009	1.284394	4.211574	-0.005368	-0.042033	0.010784
O	5.831438	5.616407	1.028179	-0.005367	0.042029	0.010778
O	-3.378295	8.185194	5.338611	-0.005364	0.042035	0.010787
H	-0.637445	12.195109	2.878812	0.004398	-0.014391	0.014436
H	3.090587	1.606491	3.487978	0.004382	-0.014411	0.014435
H	5.245016	5.294309	0.304583	0.004402	0.014353	0.014442
H	-2.791874	8.507292	6.062207	0.004363	0.014451	0.014437

10 f = 39.585589 THz 248.723592 2PiTHz 1320.433080 cm-1 163.712896
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.001108	0.007968	-0.000577
Li	-1.316675	4.156264	2.365404	-0.001110	0.007969	-0.000578
Li	-3.471104	2.744536	5.548798	0.001110	0.007967	0.000576
Li	5.924247	11.057064	0.817991	0.001107	0.007970	0.000580
Na	2.049025	6.784862	1.629696	-0.000272	-0.001748	0.000124
Na	0.404117	7.016739	4.737094	-0.000272	-0.001747	0.000127
Na	2.558546	13.685662	1.553699	0.000273	-0.001747	-0.000127
Na	-0.105403	0.115939	4.813091	0.000271	-0.001747	-0.000124
B	4.155007	8.978944	1.168663	-0.005957	0.010418	-0.007339
B	-1.701865	4.822656	5.198127	-0.005958	0.010417	-0.007335
B	0.452564	2.078144	2.014732	0.005964	0.010424	0.007336
B	2.000578	11.723457	4.352058	0.005951	0.010411	0.007337
B	-2.733891	11.746082	5.839177	-0.013049	0.006338	-0.006827
B	5.187034	2.055518	0.527613	-0.013061	0.006341	-0.006834
B	3.032605	4.845282	3.711007	0.013056	0.006336	0.006829
B	-0.579463	8.956318	2.655782	0.013055	0.006343	0.006832
B	-0.983708	0.054306	1.827988	-0.035098	-0.121889	0.017013
B	3.436850	13.747295	4.538802	-0.035040	-0.121783	0.017015
B	5.591279	6.955106	1.355407	0.035059	-0.121847	-0.017027
B	-3.138137	6.846495	5.011383	0.035083	-0.121831	-0.017001
Si	0.631772	3.486686	4.508512	0.000363	0.006314	0.002130
Si	1.821370	10.314915	1.858278	0.000361	0.006312	0.002127
Si	-0.333059	10.387486	5.041673	-0.000362	0.006312	-0.002128
Si	2.786201	3.414115	1.325117	-0.000363	0.006313	-0.002129
O	0.061445	3.072947	3.041906	0.000053	-0.008370	-0.007849
O	2.391697	10.728653	3.324884	0.000057	-0.008368	-0.007842
O	4.546126	9.973747	0.141489	-0.000056	-0.008371	0.007845
O	-2.092984	3.827853	6.225301	-0.000053	-0.008368	0.007847
O	2.197450	3.933608	4.519003	-0.004392	-0.005767	0.001243
O	0.255692	9.867992	1.847787	-0.004395	-0.005770	0.001246
O	-1.898737	10.834409	5.031182	0.004393	-0.005769	-0.001246
O	4.351879	2.967192	1.335608	0.004394	-0.005768	-0.001243

O	-0.212316	4.798696	5.055280	0.005737	-0.006358	-0.002522
O	2.665458	9.002905	1.311510	0.005739	-0.006358	-0.002519
O	0.511030	11.699496	4.494905	-0.005735	-0.006356	0.002519
O	1.942113	2.102105	1.871885	-0.005741	-0.006360	0.002522
O	0.525580	2.169271	5.472081	0.001513	-0.004684	0.005025
O	1.927562	11.632329	0.894709	0.001513	-0.004681	0.005021
O	-0.226867	9.070071	4.078104	-0.001512	-0.004684	-0.005023
O	2.680009	4.731529	2.288686	-0.001513	-0.004681	-0.005023
O	0.058846	0.698526	2.444964	0.025049	0.027319	0.009280
O	2.394296	13.103075	3.921826	0.025013	0.027289	0.009261
O	4.548725	7.599326	0.738431	-0.025024	0.027304	-0.009263
O	-2.095583	6.202275	5.628359	-0.025042	0.027307	-0.009280
O	-2.459230	13.184059	5.445139	-0.005285	0.016555	-0.010271
O	4.912372	0.617542	0.921651	-0.005287	0.016564	-0.010277
O	2.757943	6.283259	4.105046	0.005285	0.016556	0.010271
O	-0.304801	7.518342	2.261744	0.005288	0.016563	0.010277
O	-0.175430	2.374756	0.744070	0.002023	-0.002991	0.001947
O	2.628573	11.426844	5.622720	0.002022	-0.002992	0.001941
O	4.783002	9.275557	2.439325	-0.002022	-0.002995	-0.001946
O	-2.329859	4.526044	3.927465	-0.002023	-0.002987	-0.001943
O	-1.223866	12.517207	2.155216	0.004512	0.039855	-0.012354
O	3.677009	1.284394	4.211574	0.004513	0.039830	-0.012341
O	5.831438	5.616407	1.028179	-0.004515	0.039851	0.012347
O	-3.378295	8.185194	5.338611	-0.004509	0.039836	0.012348
H	-0.637445	12.195109	2.878812	0.007949	0.054675	-0.004293
H	3.090587	1.606491	3.487978	0.007935	0.054616	-0.004282
H	5.245016	5.294309	0.304583	-0.007944	0.054641	0.004290
H	-2.791874	8.507292	6.062207	-0.007949	0.054666	0.004286

11 f = 39.328217 THz 247.106475 2PiTHz 1311.848070 cm-1 162.648490 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002783	0.001029	-0.007081
Li	-1.316675	4.156264	2.365404	-0.002784	-0.001035	0.007081
Li	-3.471104	2.744536	5.548798	0.002784	-0.001034	-0.007083
Li	5.924247	11.057064	0.817991	-0.002783	0.001031	0.007081

Na	2.049025	6.784862	1.629696	0.000849	0.000035	0.000498
Na	0.404117	7.016739	4.737094	-0.000849	-0.000034	-0.000501
Na	2.558546	13.685662	1.553699	0.000850	-0.000034	0.000501
Na	-0.105403	0.115939	4.813091	-0.000849	0.000035	-0.000498
B	4.155007	8.978944	1.168663	0.012843	-0.011692	0.007966
B	-1.701865	4.822656	5.198127	-0.012845	0.011683	-0.007968
B	0.452564	2.078144	2.014732	0.012847	0.011686	0.007967
B	2.000578	11.723457	4.352058	-0.012844	-0.011694	-0.007967
B	-2.733891	11.746082	5.839177	0.012212	-0.008920	0.011141
B	5.187034	2.055518	0.527613	-0.012213	0.008915	-0.011144
B	3.032605	4.845282	3.711007	0.012211	0.008915	0.011141
B	-0.579463	8.956318	2.655782	-0.012212	-0.008917	-0.011142
B	-0.983708	0.054306	1.827988	-0.030243	-0.121228	0.026496
B	3.436850	13.747295	4.538802	0.030247	0.121249	-0.026503
B	5.591279	6.955106	1.355407	-0.030254	0.121255	0.026497
B	-3.138137	6.846495	5.011383	0.030229	-0.121185	-0.026494
Si	0.631772	3.486686	4.508512	0.002724	0.004418	0.001464
Si	1.821370	10.314915	1.858278	-0.002722	-0.004423	-0.001464
Si	-0.333059	10.387486	5.041673	0.002723	-0.004423	0.001465
Si	2.786201	3.414115	1.325117	-0.002723	0.004418	-0.001464
O	0.061445	3.072947	3.041906	-0.001245	-0.006241	-0.008574
O	2.391697	10.728653	3.324884	0.001247	0.006247	0.008575
O	4.546126	9.973747	0.141489	-0.001250	0.006247	-0.008576
O	-2.092984	3.827853	6.225301	0.001242	-0.006240	0.008572
O	2.197450	3.933608	4.519003	-0.007727	-0.004190	0.002030
O	0.255692	9.867992	1.847787	0.007729	0.004191	-0.002030
O	-1.898737	10.834409	5.031182	-0.007727	0.004193	0.002033
O	4.351879	2.967192	1.335608	0.007729	-0.004189	-0.002027
O	-0.212316	4.798696	5.055280	0.007553	-0.004240	0.000106
O	2.665458	9.002905	1.311510	-0.007557	0.004253	-0.000104
O	0.511030	11.699496	4.494905	0.007559	0.004252	0.000104
O	1.942113	2.102105	1.871885	-0.007553	-0.004243	-0.000106
O	0.525580	2.169271	5.472081	0.001114	-0.005213	0.007558
O	1.927562	11.632329	0.894709	-0.001114	0.005206	-0.007557
O	-0.226867	9.070071	4.078104	0.001112	0.005210	0.007554
O	2.680009	4.731529	2.288686	-0.001116	-0.005208	-0.007559

O	0.058846	0.698526	2.444964	0.022705	0.023359	0.007402
O	2.394296	13.103075	3.921826	-0.022702	-0.023366	-0.007397
O	4.548725	7.599326	0.738431	0.022714	-0.023369	0.007409
O	-2.095583	6.202275	5.628359	-0.022688	0.023350	-0.007389
O	-2.459230	13.184059	5.445139	0.007178	-0.016852	0.013742
O	4.912372	0.617542	0.921651	-0.007185	0.016851	-0.013746
O	2.757943	6.283259	4.105046	0.007171	0.016844	0.013735
O	-0.304801	7.518342	2.261744	-0.007191	-0.016853	-0.013748
O	-0.175430	2.374756	0.744070	-0.001159	-0.002427	0.003168
O	2.628573	11.426844	5.622720	0.001158	0.002432	-0.003170
O	4.783002	9.275557	2.439325	-0.001157	0.002429	0.003170
O	-2.329859	4.526044	3.927465	0.001160	-0.002429	-0.003167
O	-1.223866	12.517207	2.155216	0.004690	0.041740	-0.013138
O	3.677009	1.284394	4.211574	-0.004682	-0.041746	0.013142
O	5.831438	5.616407	1.028179	0.004685	-0.041745	-0.013142
O	-3.378295	8.185194	5.338611	-0.004684	0.041727	0.013133
H	-0.637445	12.195109	2.878812	0.007050	0.035003	-0.011828
H	3.090587	1.606491	3.487978	-0.007060	-0.035053	0.011820
H	5.245016	5.294309	0.304583	0.007071	-0.035056	-0.011826
H	-2.791874	8.507292	6.062207	-0.007046	0.035003	0.011820

12 f = 39.143158 THz 245.943716 2PiTHz 1305.675174 cm-1 161.883148 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000870	0.004062	-0.004458
Li	-1.316675	4.156264	2.365404	-0.000870	-0.004059	0.004459
Li	-3.471104	2.744536	5.548798	-0.000869	0.004062	0.004458
Li	5.924247	11.057064	0.817991	0.000870	-0.004058	-0.004457
Na	2.049025	6.784862	1.629696	0.000871	-0.000055	0.000510
Na	0.404117	7.016739	4.737094	-0.000871	0.000054	-0.000512
Na	2.558546	13.685662	1.553699	-0.000871	-0.000055	-0.000512
Na	-0.105403	0.115939	4.813091	0.000871	0.000054	0.000510
B	4.155007	8.978944	1.168663	0.011217	-0.012495	0.004417
B	-1.701865	4.822656	5.198127	-0.011219	0.012503	-0.004414
B	0.452564	2.078144	2.014732	-0.011215	-0.012493	-0.004413
B	2.000578	11.723457	4.352058	0.011217	0.012502	0.004416

B	-2.733891	11.746082	5.839177	-0.010387	0.010755	-0.008863
B	5.187034	2.055518	0.527613	0.010381	-0.010752	0.008858
B	3.032605	4.845282	3.711007	0.010387	0.010757	0.008865
B	-0.579463	8.956318	2.655782	-0.010385	-0.010753	-0.008859
B	-0.983708	0.054306	1.827988	0.031763	0.122411	-0.025590
B	3.436850	13.747295	4.538802	-0.031795	-0.122480	0.025590
B	5.591279	6.955106	1.355407	-0.031775	0.122438	0.025591
B	-3.138137	6.846495	5.011383	0.031794	-0.122488	-0.025595
Si	0.631772	3.486686	4.508512	-0.000497	-0.000203	-0.000542
Si	1.821370	10.314915	1.858278	0.000498	0.000206	0.000544
Si	-0.333059	10.387486	5.041673	0.000498	-0.000203	0.000543
Si	2.786201	3.414115	1.325117	-0.000498	0.000206	-0.000543
O	0.061445	3.072947	3.041906	0.000456	0.005466	0.004792
O	2.391697	10.728653	3.324884	-0.000460	-0.005469	-0.004802
O	4.546126	9.973747	0.141489	-0.000461	0.005467	-0.004800
O	-2.092984	3.827853	6.225301	0.000456	-0.005471	0.004796
O	2.197450	3.933608	4.519003	-0.003490	-0.004320	0.001454
O	0.255692	9.867992	1.847787	0.003490	0.004317	-0.001453
O	-1.898737	10.834409	5.031182	0.003490	-0.004319	-0.001454
O	4.351879	2.967192	1.335608	-0.003487	0.004317	0.001453
O	-0.212316	4.798696	5.055280	0.006777	-0.003373	0.000029
O	2.665458	9.002905	1.311510	-0.006774	0.003371	-0.000031
O	0.511030	11.699496	4.494905	-0.006775	-0.003372	-0.000029
O	1.942113	2.102105	1.871885	0.006774	0.003370	0.000031
O	0.525580	2.169271	5.472081	-0.000637	0.003735	-0.005103
O	1.927562	11.632329	0.894709	0.000634	-0.003742	0.005104
O	-0.226867	9.070071	4.078104	0.000635	0.003740	0.005103
O	2.680009	4.731529	2.288686	-0.000636	-0.003739	-0.005106
O	0.058846	0.698526	2.444964	-0.023678	-0.023650	-0.008292
O	2.394296	13.103075	3.921826	0.023698	0.023667	0.008299
O	4.548725	7.599326	0.738431	0.023688	-0.023657	0.008296
O	-2.095583	6.202275	5.628359	-0.023696	0.023667	-0.008298
O	-2.459230	13.184059	5.445139	-0.007009	0.015751	-0.013245
O	4.912372	0.617542	0.921651	0.007009	-0.015741	0.013239
O	2.757943	6.283259	4.105046	0.007008	0.015753	0.013244
O	-0.304801	7.518342	2.261744	-0.007012	-0.015744	-0.013243

O	-0.175430	2.374756	0.744070	0.000325	0.003722	-0.003346
O	2.628573	11.426844	5.622720	-0.000328	-0.003727	0.003354
O	4.783002	9.275557	2.439325	-0.000323	0.003720	0.003347
O	-2.329859	4.526044	3.927465	0.000330	-0.003729	-0.003354
O	-1.223866	12.517207	2.155216	-0.004257	-0.041051	0.013664
O	3.677009	1.284394	4.211574	0.004262	0.041074	-0.013665
O	5.831438	5.616407	1.028179	0.004259	-0.041061	-0.013662
O	-3.378295	8.185194	5.338611	-0.004260	0.041076	0.013670
H	-0.637445	12.195109	2.878812	-0.010050	-0.052032	0.007175
H	3.090587	1.606491	3.487978	0.010050	0.052053	-0.007174
H	5.245016	5.294309	0.304583	0.010054	-0.052041	-0.007175
H	-2.791874	8.507292	6.062207	-0.010058	0.052074	0.007175

13 f = 35.099473 THz 220.536495 2PiTHz 1170.792371 cm-1 145.159806 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000582	-0.011428	-0.010902
Li	-1.316675	4.156264	2.365404	0.000584	0.011427	0.010903
Li	-3.471104	2.744536	5.548798	-0.000586	0.011432	-0.010910
Li	5.924247	11.057064	0.817991	0.000580	-0.011424	0.010894
Na	2.049025	6.784862	1.629696	-0.000694	0.001193	-0.000641
Na	0.404117	7.016739	4.737094	0.000695	-0.001194	0.000637
Na	2.558546	13.685662	1.553699	-0.000693	-0.001193	-0.000638
Na	-0.105403	0.115939	4.813091	0.000697	0.001194	0.000640
B	4.155007	8.978944	1.168663	0.011929	-0.026409	0.026184
B	-1.701865	4.822656	5.198127	-0.011913	0.026398	-0.026226
B	0.452564	2.078144	2.014732	0.011893	0.026408	0.026194
B	2.000578	11.723457	4.352058	-0.011946	-0.026400	-0.026211
B	-2.733891	11.746082	5.839177	0.011231	-0.021440	0.008653
B	5.187034	2.055518	0.527613	-0.011241	0.021434	-0.008694
B	3.032605	4.845282	3.711007	0.011253	0.021425	0.008695
B	-0.579463	8.956318	2.655782	-0.011227	-0.021447	-0.008655
B	-0.983708	0.054306	1.827988	0.021705	0.009213	0.010718
B	3.436850	13.747295	4.538802	-0.021738	-0.009222	-0.010748
B	5.591279	6.955106	1.355407	0.021713	-0.009230	0.010719
B	-3.138137	6.846495	5.011383	-0.021726	0.009200	-0.010746

Si	0.631772	3.486686	4.508512	0.007424	0.018957	-0.005028
Si	1.821370	10.314915	1.858278	-0.007418	-0.018964	0.005047
Si	-0.333059	10.387486	5.041673	0.007429	-0.018957	-0.005040
Si	2.786201	3.414115	1.325117	-0.007412	0.018963	0.005035
O	0.061445	3.072947	3.041906	-0.000371	-0.012014	-0.015823
O	2.391697	10.728653	3.324884	0.000383	0.011992	0.015780
O	4.546126	9.973747	0.141489	-0.000383	0.011998	-0.015789
O	-2.092984	3.827853	6.225301	0.000371	-0.012008	0.015815
O	2.197450	3.933608	4.519003	-0.022716	-0.016560	0.010121
O	0.255692	9.867992	1.847787	0.022731	0.016570	-0.010133
O	-1.898737	10.834409	5.031182	-0.022735	0.016574	0.010138
O	4.351879	2.967192	1.335608	0.022708	-0.016555	-0.010118
O	-0.212316	4.798696	5.055280	0.005342	-0.011642	0.000519
O	2.665458	9.002905	1.311510	-0.005353	0.011669	-0.000512
O	0.511030	11.699496	4.494905	0.005339	0.011647	0.000521
O	1.942113	2.102105	1.871885	-0.005354	-0.011665	-0.000509
O	0.525580	2.169271	5.472081	0.002699	-0.020881	0.025657
O	1.927562	11.632329	0.894709	-0.002698	0.020894	-0.025661
O	-0.226867	9.070071	4.078104	0.002695	0.020888	0.025648
O	2.680009	4.731529	2.288686	-0.002703	-0.020887	-0.025670
O	0.058846	0.698526	2.444964	-0.021527	-0.022876	-0.009465
O	2.394296	13.103075	3.921826	0.021592	0.022927	0.009488
O	4.548725	7.599326	0.738431	-0.021544	0.022898	-0.009459
O	-2.095583	6.202275	5.628359	0.021571	-0.022901	0.009493
O	-2.459230	13.184059	5.445139	0.006100	-0.007912	0.008979
O	4.912372	0.617542	0.921651	-0.006103	0.007901	-0.008963
O	2.757943	6.283259	4.105046	0.006088	0.007919	0.008967
O	-0.304801	7.518342	2.261744	-0.006115	-0.007895	-0.008974
O	-0.175430	2.374756	0.744070	-0.009767	-0.003861	-0.005986
O	2.628573	11.426844	5.622720	0.009805	0.003857	0.006036
O	4.783002	9.275557	2.439325	-0.009790	0.003858	-0.006014
O	-2.329859	4.526044	3.927465	0.009779	-0.003859	0.006009
O	-1.223866	12.517207	2.155216	0.015936	0.019555	0.013229
O	3.677009	1.284394	4.211574	-0.015991	-0.019626	-0.013242
O	5.831438	5.616407	1.028179	0.015960	-0.019581	0.013225
O	-3.378295	8.185194	5.338611	-0.015965	0.019592	-0.013245

H	-0.637445	12.195109	2.878812	-0.092142	-0.338382	-0.073072
H	3.090587	1.606491	3.487978	0.092337	0.338991	0.073176
H	5.245016	5.294309	0.304583	-0.092182	0.338599	-0.073141
H	-2.791874	8.507292	6.062207	0.092276	-0.338732	0.073105

14 f = 34.680221 THz 217.902256 2PiTHz 1156.807621 cm-1 143.425917 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.006098	0.004232	0.008042
Li	-1.316675	4.156264	2.365404	0.006097	0.004235	0.008050
Li	-3.471104	2.744536	5.548798	0.006095	-0.004229	0.008038
Li	5.924247	11.057064	0.817991	0.006099	-0.004240	0.008056
Na	2.049025	6.784862	1.629696	-0.000311	0.000022	0.000970
Na	0.404117	7.016739	4.737094	-0.000309	0.000022	0.000971
Na	2.558546	13.685662	1.553699	-0.000310	-0.000022	0.000970
Na	-0.105403	0.115939	4.813091	-0.000311	-0.000021	0.000971
B	4.155007	8.978944	1.168663	0.011112	0.010162	0.017168
B	-1.701865	4.822656	5.198127	0.011099	0.010168	0.017133
B	0.452564	2.078144	2.014732	0.011119	-0.010147	0.017168
B	2.000578	11.723457	4.352058	0.011093	-0.010181	0.017131
B	-2.733891	11.746082	5.839177	0.010435	-0.016416	0.001346
B	5.187034	2.055518	0.527613	0.010407	-0.016378	0.001332
B	3.032605	4.845282	3.711007	0.010416	0.016390	0.001342
B	-0.579463	8.956318	2.655782	0.010420	0.016407	0.001336
B	-0.983708	0.054306	1.827988	0.022309	0.005962	0.010943
B	3.436850	13.747295	4.538802	0.022271	0.005966	0.010913
B	5.591279	6.955106	1.355407	0.022281	-0.005965	0.010921
B	-3.138137	6.846495	5.011383	0.022292	-0.005961	0.010931
Si	0.631772	3.486686	4.508512	-0.012256	0.003697	-0.006719
Si	1.821370	10.314915	1.858278	-0.012267	0.003687	-0.006711
Si	-0.333059	10.387486	5.041673	-0.012261	-0.003696	-0.006719
Si	2.786201	3.414115	1.325117	-0.012263	-0.003689	-0.006709
O	0.061445	3.072947	3.041906	0.001073	0.007246	0.009295
O	2.391697	10.728653	3.324884	0.001076	0.007256	0.009309
O	4.546126	9.973747	0.141489	0.001076	-0.007247	0.009299
O	-2.092984	3.827853	6.225301	0.001073	-0.007254	0.009302

O	2.197450	3.933608	4.519003	0.009405	0.001573	-0.000606
O	0.255692	9.867992	1.847787	0.009419	0.001573	-0.000613
O	-1.898737	10.834409	5.031182	0.009405	-0.001563	-0.000599
O	4.351879	2.967192	1.335608	0.009419	-0.001584	-0.000621
O	-0.212316	4.798696	5.055280	0.011491	-0.012896	-0.004319
O	2.665458	9.002905	1.311510	0.011500	-0.012901	-0.004328
O	0.511030	11.699496	4.494905	0.011498	0.012903	-0.004321
O	1.942113	2.102105	1.871885	0.011496	0.012897	-0.004327
O	0.525580	2.169271	5.472081	0.002372	-0.002809	0.009737
O	1.927562	11.632329	0.894709	0.002365	-0.002796	0.009700
O	-0.226867	9.070071	4.078104	0.002371	0.002805	0.009725
O	2.680009	4.731529	2.288686	0.002367	0.002798	0.009711
O	0.058846	0.698526	2.444964	-0.019579	-0.016667	-0.007236
O	2.394296	13.103075	3.921826	-0.019529	-0.016618	-0.007211
O	4.548725	7.599326	0.738431	-0.019558	0.016642	-0.007227
O	-2.095583	6.202275	5.628359	-0.019542	0.016635	-0.007218
O	-2.459230	13.184059	5.445139	-0.010878	0.020341	-0.016157
O	4.912372	0.617542	0.921651	-0.010885	0.020349	-0.016173
O	2.757943	6.283259	4.105046	-0.010890	-0.020342	-0.016171
O	-0.304801	7.518342	2.261744	-0.010871	-0.020347	-0.016156
O	-0.175430	2.374756	0.744070	-0.015534	0.004614	-0.014448
O	2.628573	11.426844	5.622720	-0.015528	0.004620	-0.014432
O	4.783002	9.275557	2.439325	-0.015542	-0.004618	-0.014450
O	-2.329859	4.526044	3.927465	-0.015518	-0.004617	-0.014430
O	-1.223866	12.517207	2.155216	0.018453	0.019805	0.015206
O	3.677009	1.284394	4.211574	0.018413	0.019748	0.015182
O	5.831438	5.616407	1.028179	0.018431	-0.019776	0.015194
O	-3.378295	8.185194	5.338611	0.018428	-0.019764	0.015192
H	-0.637445	12.195109	2.878812	-0.114977	-0.388579	-0.071468
H	3.090587	1.606491	3.487978	-0.114753	-0.387847	-0.071328
H	5.245016	5.294309	0.304583	-0.114845	0.388196	-0.071409
H	-2.791874	8.507292	6.062207	-0.114841	0.388131	-0.071380

15 f = 34.382652 THz 216.032573 2PiTHz 1146.881778 cm-1 142.195269
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.002174	-0.005093	-0.006170
Li	-1.316675	4.156264	2.365404	0.002178	0.005098	0.006180
Li	-3.471104	2.744536	5.548798	0.002178	-0.005096	0.006177
Li	5.924247	11.057064	0.817991	-0.002174	0.005092	-0.006170
Na	2.049025	6.784862	1.629696	-0.000762	0.001120	-0.000843
Na	0.404117	7.016739	4.737094	0.000762	-0.001119	0.000842
Na	2.558546	13.685662	1.553699	0.000762	0.001119	0.000842
Na	-0.105403	0.115939	4.813091	-0.000762	-0.001120	-0.000843
B	4.155007	8.978944	1.168663	0.008615	-0.021439	-0.000640
B	-1.701865	4.822656	5.198127	-0.008620	0.021463	0.000644
B	0.452564	2.078144	2.014732	-0.008621	-0.021463	0.000648
B	2.000578	11.723457	4.352058	0.008610	0.021435	-0.000646
B	-2.733891	11.746082	5.839177	-0.002209	0.032090	-0.004465
B	5.187034	2.055518	0.527613	0.002235	-0.032124	0.004483
B	3.032605	4.845282	3.711007	0.002237	0.032122	0.004485
B	-0.579463	8.956318	2.655782	-0.002213	-0.032096	-0.004468
B	-0.983708	0.054306	1.827988	-0.024648	0.005770	-0.017365
B	3.436850	13.747295	4.538802	0.024666	-0.005754	0.017371
B	5.591279	6.955106	1.355407	0.024670	0.005757	0.017373
B	-3.138137	6.846495	5.011383	-0.024644	-0.005772	-0.017364
Si	0.631772	3.486686	4.508512	-0.001639	-0.001941	0.001086
Si	1.821370	10.314915	1.858278	0.001630	0.001945	-0.001090
Si	-0.333059	10.387486	5.041673	0.001631	-0.001946	-0.001092
Si	2.786201	3.414115	1.325117	-0.001640	0.001944	0.001085
O	0.061445	3.072947	3.041906	0.000785	0.001303	0.002605
O	2.391697	10.728653	3.324884	-0.000786	-0.001292	-0.002591
O	4.546126	9.973747	0.141489	-0.000786	0.001293	-0.002591
O	-2.092984	3.827853	6.225301	0.000786	-0.001306	0.002612
O	2.197450	3.933608	4.519003	-0.007031	-0.010544	0.004349
O	0.255692	9.867992	1.847787	0.007029	0.010538	-0.004346
O	-1.898737	10.834409	5.031182	0.007025	-0.010536	-0.004346
O	4.351879	2.967192	1.335608	-0.007028	0.010542	0.004347
O	-0.212316	4.798696	5.055280	0.002759	-0.007273	-0.001369
O	2.665458	9.002905	1.311510	-0.002740	0.007259	0.001365
O	0.511030	11.699496	4.494905	-0.002740	-0.007260	0.001366
O	1.942113	2.102105	1.871885	0.002758	0.007270	-0.001368

O	0.525580	2.169271	5.472081	0.000485	0.012931	-0.011106
O	1.927562	11.632329	0.894709	-0.000486	-0.012926	0.011101
O	-0.226867	9.070071	4.078104	-0.000484	0.012931	0.011106
O	2.680009	4.731529	2.288686	0.000485	-0.012932	-0.011107
O	0.058846	0.698526	2.444964	0.023424	0.025612	0.007665
O	2.394296	13.103075	3.921826	-0.023429	-0.025614	-0.007666
O	4.548725	7.599326	0.738431	-0.023434	0.025621	-0.007666
O	-2.095583	6.202275	5.628359	0.023418	-0.025604	0.007665
O	-2.459230	13.184059	5.445139	-0.010778	0.007320	-0.012126
O	4.912372	0.617542	0.921651	0.010765	-0.007301	0.012107
O	2.757943	6.283259	4.105046	0.010763	0.007302	0.012106
O	-0.304801	7.518342	2.261744	-0.010781	-0.007321	-0.012127
O	-0.175430	2.374756	0.744070	0.005591	0.007037	-0.000819
O	2.628573	11.426844	5.622720	-0.005603	-0.007030	0.000807
O	4.783002	9.275557	2.439325	-0.005603	0.007029	0.000803
O	-2.329859	4.526044	3.927465	0.005593	-0.007039	-0.000821
O	-1.223866	12.517207	2.155216	-0.019977	-0.029287	-0.013579
O	3.677009	1.284394	4.211574	0.019984	0.029289	0.013592
O	5.831438	5.616407	1.028179	0.019989	-0.029294	0.013594
O	-3.378295	8.185194	5.338611	-0.019971	0.029277	-0.013579
H	-0.637445	12.195109	2.878812	0.111115	0.380597	0.078928
H	3.090587	1.606491	3.487978	-0.111184	-0.380861	-0.078985
H	5.245016	5.294309	0.304583	-0.111198	0.380945	-0.079012
H	-2.791874	8.507292	6.062207	0.111096	-0.380538	0.078918

16 f = 34.017288 THz 213.736923 2PiTHz 1134.694550 cm-1 140.684245 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000771	-0.000780	-0.010699
Li	-1.316675	4.156264	2.365404	-0.000769	-0.000783	-0.010684
Li	-3.471104	2.744536	5.548798	0.000769	-0.000783	0.010683
Li	5.924247	11.057064	0.817991	0.000769	-0.000778	0.010697
Na	2.049025	6.784862	1.629696	0.000316	0.000961	-0.001014
Na	0.404117	7.016739	4.737094	0.000316	0.000957	-0.001017
Na	2.558546	13.685662	1.553699	-0.000315	0.000961	0.001017
Na	-0.105403	0.115939	4.813091	-0.000316	0.000959	0.001014

B	4.155007	8.978944	1.168663	-0.010730	0.007920	0.012252
B	-1.701865	4.822656	5.198127	-0.010740	0.007909	0.012219
B	0.452564	2.078144	2.014732	0.010751	0.007910	-0.012207
B	2.000578	11.723457	4.352058	0.010730	0.007933	-0.012260
B	-2.733891	11.746082	5.839177	0.020474	0.017378	0.010057
B	5.187034	2.055518	0.527613	0.020451	0.017347	0.010052
B	3.032605	4.845282	3.711007	-0.020475	0.017346	-0.010060
B	-0.579463	8.956318	2.655782	-0.020470	0.017362	-0.010064
B	-0.983708	0.054306	1.827988	0.017484	-0.016275	0.016143
B	3.436850	13.747295	4.538802	0.017483	-0.016287	0.016148
B	5.591279	6.955106	1.355407	-0.017480	-0.016283	-0.016143
B	-3.138137	6.846495	5.011383	-0.017495	-0.016281	-0.016152
Si	0.631772	3.486686	4.508512	0.003659	-0.001065	-0.004452
Si	1.821370	10.314915	1.858278	0.003655	-0.001059	-0.004437
Si	-0.333059	10.387486	5.041673	-0.003655	-0.001059	0.004438
Si	2.786201	3.414115	1.325117	-0.003657	-0.001064	0.004454
O	0.061445	3.072947	3.041906	-0.000354	0.007274	0.014381
O	2.391697	10.728653	3.324884	-0.000351	0.007263	0.014373
O	4.546126	9.973747	0.141489	0.000352	0.007265	-0.014372
O	-2.092984	3.827853	6.225301	0.000350	0.007278	-0.014391
O	2.197450	3.933608	4.519003	-0.004263	-0.008041	0.001569
O	0.255692	9.867992	1.847787	-0.004262	-0.008044	0.001565
O	-1.898737	10.834409	5.031182	0.004264	-0.008047	-0.001565
O	4.351879	2.967192	1.335608	0.004270	-0.008043	-0.001570
O	-0.212316	4.798696	5.055280	-0.006467	0.005742	-0.000052
O	2.665458	9.002905	1.311510	-0.006448	0.005732	-0.000064
O	0.511030	11.699496	4.494905	0.006447	0.005728	0.000065
O	1.942113	2.102105	1.871885	0.006458	0.005740	0.000053
O	0.525580	2.169271	5.472081	-0.001726	-0.004148	0.000650
O	1.927562	11.632329	0.894709	-0.001731	-0.004145	0.000637
O	-0.226867	9.070071	4.078104	0.001730	-0.004141	-0.000634
O	2.680009	4.731529	2.288686	0.001729	-0.004148	-0.000645
O	0.058846	0.698526	2.444964	-0.020065	-0.022133	-0.003367
O	2.394296	13.103075	3.921826	-0.020057	-0.022129	-0.003361
O	4.548725	7.599326	0.738431	0.020051	-0.022122	0.003359
O	-2.095583	6.202275	5.628359	0.020070	-0.022138	0.003368

O	-2.459230	13.184059	5.445139	-0.012577	0.012423	-0.015615
O	4.912372	0.617542	0.921651	-0.012583	0.012439	-0.015625
O	2.757943	6.283259	4.105046	0.012589	0.012444	0.015631
O	-0.304801	7.518342	2.261744	0.012578	0.012428	0.015617
O	-0.175430	2.374756	0.744070	-0.014201	-0.005199	-0.004343
O	2.628573	11.426844	5.622720	-0.014195	-0.005210	-0.004315
O	4.783002	9.275557	2.439325	0.014192	-0.005204	0.004320
O	-2.329859	4.526044	3.927465	0.014209	-0.005201	0.004342
O	-1.223866	12.517207	2.155216	0.021265	0.032869	0.011467
O	3.677009	1.284394	4.211574	0.021250	0.032861	0.011456
O	5.831438	5.616407	1.028179	-0.021248	0.032853	-0.011457
O	-3.378295	8.185194	5.338611	-0.021268	0.032876	-0.011472
H	-0.637445	12.195109	2.878812	-0.113073	-0.383880	-0.075827
H	3.090587	1.606491	3.487978	-0.112982	-0.383557	-0.075774
H	5.245016	5.294309	0.304583	0.112964	-0.383548	0.075782
H	-2.791874	8.507292	6.062207	0.113105	-0.384000	0.075854

17 f = 33.518157 THz 210.600790 2PiTHz 1118.045330 cm-1 138.620004 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002749	-0.001742	-0.003448
Li	-1.316675	4.156264	2.365404	0.002745	-0.001743	-0.003442
Li	-3.471104	2.744536	5.548798	0.002744	0.001735	-0.003445
Li	5.924247	11.057064	0.817991	0.002747	0.001749	-0.003446
Na	2.049025	6.784862	1.629696	0.000025	-0.002926	0.000507
Na	0.404117	7.016739	4.737094	0.000026	-0.002926	0.000503
Na	2.558546	13.685662	1.553699	0.000027	0.002927	0.000503
Na	-0.105403	0.115939	4.813091	0.000025	0.002925	0.000506
B	4.155007	8.978944	1.168663	0.054488	-0.028185	0.053158
B	-1.701865	4.822656	5.198127	0.054388	-0.028200	0.053013
B	0.452564	2.078144	2.014732	0.054391	0.028180	0.053023
B	2.000578	11.723457	4.352058	0.054465	0.028207	0.053134
B	-2.733891	11.746082	5.839177	-0.068909	0.027598	-0.046782
B	5.187034	2.055518	0.527613	-0.068750	0.027559	-0.046680
B	3.032605	4.845282	3.711007	-0.068766	-0.027584	-0.046709
B	-0.579463	8.956318	2.655782	-0.068907	-0.027578	-0.046748

B	-0.983708	0.054306	1.827988	-0.003355	-0.000046	-0.000870
B	3.436850	13.747295	4.538802	-0.003342	-0.000011	-0.000864
B	5.591279	6.955106	1.355407	-0.003346	0.000018	-0.000867
B	-3.138137	6.846495	5.011383	-0.003347	0.000040	-0.000866
Si	0.631772	3.486686	4.508512	-0.004721	0.001384	0.000638
Si	1.821370	10.314915	1.858278	-0.004730	0.001387	0.000664
Si	-0.333059	10.387486	5.041673	-0.004719	-0.001382	0.000646
Si	2.786201	3.414115	1.325117	-0.004727	-0.001390	0.000652
O	0.061445	3.072947	3.041906	-0.008011	-0.013351	-0.030611
O	2.391697	10.728653	3.324884	-0.008039	-0.013386	-0.030705
O	4.546126	9.973747	0.141489	-0.008036	0.013367	-0.030677
O	-2.092984	3.827853	6.225301	-0.008015	0.013367	-0.030634
O	2.197450	3.933608	4.519003	0.037737	0.017486	-0.005587
O	0.255692	9.867992	1.847787	0.037828	0.017510	-0.005598
O	-1.898737	10.834409	5.031182	0.037792	-0.017507	-0.005596
O	4.351879	2.967192	1.335608	0.037756	-0.017480	-0.005585
O	-0.212316	4.798696	5.055280	-0.020765	0.010462	0.000457
O	2.665458	9.002905	1.311510	-0.020794	0.010463	0.000449
O	0.511030	11.699496	4.494905	-0.020801	-0.010475	0.000455
O	1.942113	2.102105	1.871885	-0.020755	-0.010451	0.000452
O	0.525580	2.169271	5.472081	0.008970	-0.017509	0.035786
O	1.927562	11.632329	0.894709	0.008994	-0.017509	0.035842
O	-0.226867	9.070071	4.078104	0.008992	0.017515	0.035841
O	2.680009	4.731529	2.288686	0.008975	0.017505	0.035789
O	0.058846	0.698526	2.444964	-0.012981	-0.008791	-0.009432
O	2.394296	13.103075	3.921826	-0.013005	-0.008793	-0.009464
O	4.548725	7.599326	0.738431	-0.013005	0.008795	-0.009462
O	-2.095583	6.202275	5.628359	-0.012988	0.008794	-0.009436
O	-2.459230	13.184059	5.445139	0.014121	-0.006011	0.011374
O	4.912372	0.617542	0.921651	0.014086	-0.005988	0.011348
O	2.757943	6.283259	4.105046	0.014095	0.006002	0.011359
O	-0.304801	7.518342	2.261744	0.014111	0.005991	0.011358
O	-0.175430	2.374756	0.744070	-0.000056	-0.000101	-0.004894
O	2.628573	11.426844	5.622720	-0.000018	-0.000098	-0.004886
O	4.783002	9.275557	2.439325	-0.000036	0.000086	-0.004913
O	-2.329859	4.526044	3.927465	-0.000044	0.000109	-0.004876

O	-1.223866	12.517207	2.155216	0.000562	0.003723	-0.001836
O	3.677009	1.284394	4.211574	0.000555	0.003707	-0.001833
O	5.831438	5.616407	1.028179	0.000568	-0.003718	-0.001825
O	-3.378295	8.185194	5.338611	0.000556	-0.003719	-0.001838
H	-0.637445	12.195109	2.878812	-0.008216	0.008996	0.011530
H	3.090587	1.606491	3.487978	-0.008185	0.009059	0.011529
H	5.245016	5.294309	0.304583	-0.008242	-0.008869	0.011498
H	-2.791874	8.507292	6.062207	-0.008199	-0.009071	0.011548

18 f = 33.270156 THz 209.042555 2PiTHz 1109.772913 cm-1 137.594354 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002689	0.001908	0.000973
Li	-1.316675	4.156264	2.365404	0.002698	-0.001914	-0.000986
Li	-3.471104	2.744536	5.548798	0.002693	0.001910	-0.000979
Li	5.924247	11.057064	0.817991	-0.002690	-0.001910	0.000979
Na	2.049025	6.784862	1.629696	0.000122	-0.000249	0.000220
Na	0.404117	7.016739	4.737094	-0.000121	0.000242	-0.000217
Na	2.558546	13.685662	1.553699	-0.000121	-0.000243	-0.000218
Na	-0.105403	0.115939	4.813091	0.000122	0.000248	0.000220
B	4.155007	8.978944	1.168663	-0.050836	0.002399	-0.067140
B	-1.701865	4.822656	5.198127	0.050960	-0.002468	0.067260
B	0.452564	2.078144	2.014732	0.050935	0.002472	0.067213
B	2.000578	11.723457	4.352058	-0.050848	-0.002402	-0.067163
B	-2.733891	11.746082	5.839177	0.078306	-0.003197	0.041181
B	5.187034	2.055518	0.527613	-0.078375	0.003263	-0.041252
B	3.032605	4.845282	3.711007	-0.078430	-0.003260	-0.041275
B	-0.579463	8.956318	2.655782	0.078287	0.003199	0.041161
B	-0.983708	0.054306	1.827988	-0.003833	0.015520	-0.005935
B	3.436850	13.747295	4.538802	0.003815	-0.015535	0.005933
B	5.591279	6.955106	1.355407	0.003820	0.015535	0.005934
B	-3.138137	6.846495	5.011383	-0.003832	-0.015530	-0.005938
Si	0.631772	3.486686	4.508512	-0.005074	0.001113	0.000690
Si	1.821370	10.314915	1.858278	0.005056	-0.001112	-0.000697
Si	-0.333059	10.387486	5.041673	0.005061	0.001108	-0.000697
Si	2.786201	3.414115	1.325117	-0.005068	-0.001118	0.000692

O	0.061445	3.072947	3.041906	-0.008620	-0.009734	-0.029732
O	2.391697	10.728653	3.324884	0.008622	0.009715	0.029710
O	4.546126	9.973747	0.141489	0.008618	-0.009710	0.029695
O	-2.092984	3.827853	6.225301	-0.008624	0.009743	-0.029755
O	2.197450	3.933608	4.519003	0.036938	0.013034	-0.004182
O	0.255692	9.867992	1.847787	-0.036861	-0.012992	0.004160
O	-1.898737	10.834409	5.031182	-0.036867	0.012995	0.004163
O	4.351879	2.967192	1.335608	0.036918	-0.013025	-0.004176
O	-0.212316	4.798696	5.055280	-0.018737	0.005305	-0.001303
O	2.665458	9.002905	1.311510	0.018694	-0.005292	0.001301
O	0.511030	11.699496	4.494905	0.018695	0.005290	0.001304
O	1.942113	2.102105	1.871885	-0.018727	-0.005306	-0.001299
O	0.525580	2.169271	5.472081	0.010576	-0.011693	0.032757
O	1.927562	11.632329	0.894709	-0.010567	0.011657	-0.032701
O	-0.226867	9.070071	4.078104	-0.010564	-0.011653	-0.032683
O	2.680009	4.731529	2.288686	0.010584	0.011699	0.032778
O	0.058846	0.698526	2.444964	-0.007731	0.002570	-0.010369
O	2.394296	13.103075	3.921826	0.007716	-0.002593	0.010359
O	4.548725	7.599326	0.738431	0.007706	0.002598	0.010354
O	-2.095583	6.202275	5.628359	-0.007739	-0.002572	-0.010377
O	-2.459230	13.184059	5.445139	-0.016209	-0.000196	-0.009780
O	4.912372	0.617542	0.921651	0.016238	0.000172	0.009807
O	2.757943	6.283259	4.105046	0.016245	-0.000180	0.009808
O	-0.304801	7.518342	2.261744	-0.016211	0.000184	-0.009784
O	-0.175430	2.374756	0.744070	0.003839	0.007113	-0.011816
O	2.628573	11.426844	5.622720	-0.003857	-0.007126	0.011815
O	4.783002	9.275557	2.439325	-0.003860	0.007126	0.011813
O	-2.329859	4.526044	3.927465	0.003843	-0.007119	-0.011824
O	-1.223866	12.517207	2.155216	-0.002153	-0.011003	0.001496
O	3.677009	1.284394	4.211574	0.002153	0.011016	-0.001507
O	5.831438	5.616407	1.028179	0.002159	-0.011021	-0.001500
O	-3.378295	8.185194	5.338611	-0.002152	0.011007	0.001500
H	-0.637445	12.195109	2.878812	0.017018	0.036420	0.003045
H	3.090587	1.606491	3.487978	-0.016981	-0.036263	-0.003010
H	5.245016	5.294309	0.304583	-0.017027	0.036412	-0.003035
H	-2.791874	8.507292	6.062207	0.016992	-0.036362	0.003044

19 f = 33.101190 THz 207.980912 2PiTHz 1104.136824 cm-1 136.895568

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001938	-0.004086	-0.015741
Li	-1.316675	4.156264	2.365404	0.001931	-0.004097	-0.015759
Li	-3.471104	2.744536	5.548798	-0.001933	-0.004098	0.015761
Li	5.924247	11.057064	0.817991	-0.001937	-0.004086	0.015739
Na	2.049025	6.784862	1.629696	0.000279	-0.000670	0.000644
Na	0.404117	7.016739	4.737094	0.000279	-0.000665	0.000642
Na	2.558546	13.685662	1.553699	-0.000279	-0.000665	-0.000642
Na	-0.105403	0.115939	4.813091	-0.000279	-0.000670	-0.000645
B	4.155007	8.978944	1.168663	0.023343	-0.000784	0.075549
B	-1.701865	4.822656	5.198127	0.023246	-0.000810	0.075603
B	0.452564	2.078144	2.014732	-0.023279	-0.000799	-0.075644
B	2.000578	11.723457	4.352058	-0.023320	-0.000804	-0.075515
B	-2.733891	11.746082	5.839177	0.067893	0.011046	0.056273
B	5.187034	2.055518	0.527613	0.068073	0.011080	0.056428
B	3.032605	4.845282	3.711007	-0.068026	0.011069	-0.056404
B	-0.579463	8.956318	2.655782	-0.067931	0.011064	-0.056287
B	-0.983708	0.054306	1.827988	-0.007360	-0.013429	0.000072
B	3.436850	13.747295	4.538802	-0.007358	-0.013377	0.000061
B	5.591279	6.955106	1.355407	0.007355	-0.013384	-0.000065
B	-3.138137	6.846495	5.011383	0.007364	-0.013422	-0.000066
Si	0.631772	3.486686	4.508512	-0.005452	-0.006620	-0.003234
Si	1.821370	10.314915	1.858278	-0.005472	-0.006605	-0.003204
Si	-0.333059	10.387486	5.041673	0.005469	-0.006606	0.003204
Si	2.786201	3.414115	1.325117	0.005455	-0.006619	0.003234
O	0.061445	3.072947	3.041906	0.003573	0.014875	0.041590
O	2.391697	10.728653	3.324884	0.003580	0.014823	0.041469
O	4.546126	9.973747	0.141489	-0.003581	0.014824	-0.041477
O	-2.092984	3.827853	6.225301	-0.003570	0.014871	-0.041574
O	2.197450	3.933608	4.519003	0.012837	0.003244	-0.001124
O	0.255692	9.867992	1.847787	0.012907	0.003267	-0.001148
O	-1.898737	10.834409	5.031182	-0.012894	0.003264	0.001148
O	4.351879	2.967192	1.335608	-0.012856	0.003250	0.001125

O	-0.212316	4.798696	5.055280	-0.006358	-0.006606	-0.009534
O	2.665458	9.002905	1.311510	-0.006366	-0.006587	-0.009520
O	0.511030	11.699496	4.494905	0.006361	-0.006586	0.009519
O	1.942113	2.102105	1.871885	0.006367	-0.006606	0.009535
O	0.525580	2.169271	5.472081	-0.010996	0.012895	-0.040448
O	1.927562	11.632329	0.894709	-0.010978	0.012865	-0.040374
O	-0.226867	9.070071	4.078104	0.010982	0.012869	0.040383
O	2.680009	4.731529	2.288686	0.010991	0.012890	0.040431
O	0.058846	0.698526	2.444964	0.010517	0.001003	0.013353
O	2.394296	13.103075	3.921826	0.010517	0.001030	0.013326
O	4.548725	7.599326	0.738431	-0.010523	0.001019	-0.013340
O	-2.095583	6.202275	5.628359	-0.010507	0.001011	-0.013338
O	-2.459230	13.184059	5.445139	-0.007497	-0.010044	-0.001928
O	4.912372	0.617542	0.921651	-0.007531	-0.010030	-0.001960
O	2.757943	6.283259	4.105046	0.007515	-0.010022	0.001952
O	-0.304801	7.518342	2.261744	0.007511	-0.010053	0.001933
O	-0.175430	2.374756	0.744070	-0.009986	-0.008452	0.008369
O	2.628573	11.426844	5.622720	-0.009894	-0.008427	0.008390
O	4.783002	9.275557	2.439325	0.009898	-0.008430	-0.008393
O	-2.329859	4.526044	3.927465	0.009982	-0.008452	-0.008367
O	-1.223866	12.517207	2.155216	-0.004801	0.004031	-0.007319
O	3.677009	1.284394	4.211574	-0.004823	0.004000	-0.007327
O	5.831438	5.616407	1.028179	0.004822	0.004012	0.007328
O	-3.378295	8.185194	5.338611	0.004801	0.004022	0.007318
H	-0.637445	12.195109	2.878812	0.043487	0.088516	-0.002516
H	3.090587	1.606491	3.487978	0.043613	0.088744	-0.002506
H	5.245016	5.294309	0.304583	-0.043601	0.088744	0.002501
H	-2.791874	8.507292	6.062207	-0.043495	0.088522	0.002516

20 f = 33.044669 THz 207.625779 2PiTHz 1102.251480 cm-1 136.661815 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000668	0.006834	0.010669
Li	-1.316675	4.156264	2.365404	0.000660	-0.006827	-0.010628
Li	-3.471104	2.744536	5.548798	-0.000667	-0.006826	0.010632
Li	5.924247	11.057064	0.817991	0.000663	0.006835	-0.010666

Na	2.049025	6.784862	1.629696	-0.000123	-0.001633	0.000093
Na	0.404117	7.016739	4.737094	0.000122	0.001635	-0.000087
Na	2.558546	13.685662	1.553699	-0.000123	0.001635	0.000087
Na	-0.105403	0.115939	4.813091	0.000123	-0.001633	-0.000093
B	4.155007	8.978944	1.168663	-0.000430	0.002562	-0.059428
B	-1.701865	4.822656	5.198127	0.000321	-0.002540	0.059226
B	0.452564	2.078144	2.014732	-0.000355	-0.002557	-0.059247
B	2.000578	11.723457	4.352058	0.000416	0.002552	0.059428
B	-2.733891	11.746082	5.839177	-0.068045	-0.008948	-0.060738
B	5.187034	2.055518	0.527613	0.067910	0.008914	0.060640
B	3.032605	4.845282	3.711007	-0.067893	0.008930	-0.060618
B	-0.579463	8.956318	2.655782	0.068043	-0.008938	0.060746
B	-0.983708	0.054306	1.827988	0.000609	-0.019665	0.004016
B	3.436850	13.747295	4.538802	-0.000612	0.019685	-0.004023
B	5.591279	6.955106	1.355407	0.000611	0.019690	0.004026
B	-3.138137	6.846495	5.011383	-0.000610	-0.019658	-0.004012
Si	0.631772	3.486686	4.508512	0.001478	-0.007281	-0.011296
Si	1.821370	10.314915	1.858278	-0.001460	0.007288	0.011282
Si	-0.333059	10.387486	5.041673	0.001464	0.007288	-0.011282
Si	2.786201	3.414115	1.325117	-0.001470	-0.007280	0.011296
O	0.061445	3.072947	3.041906	0.002147	0.021063	0.049125
O	2.391697	10.728653	3.324884	-0.002157	-0.021070	-0.049165
O	4.546126	9.973747	0.141489	0.002160	-0.021076	0.049174
O	-2.092984	3.827853	6.225301	-0.002141	0.021053	-0.049105
O	2.197450	3.933608	4.519003	-0.002977	-0.002935	0.004929
O	0.255692	9.867992	1.847787	0.002915	0.002916	-0.004918
O	-1.898737	10.834409	5.031182	-0.002935	0.002924	0.004922
O	4.351879	2.967192	1.335608	0.002941	-0.002920	-0.004924
O	-0.212316	4.798696	5.055280	-0.007632	-0.003056	-0.006341
O	2.665458	9.002905	1.311510	0.007643	0.003061	0.006363
O	0.511030	11.699496	4.494905	-0.007638	0.003065	-0.006368
O	1.942113	2.102105	1.871885	0.007643	-0.003049	0.006336
O	0.525580	2.169271	5.472081	-0.009509	0.010234	-0.031548
O	1.927562	11.632329	0.894709	0.009535	-0.010260	0.031623
O	-0.226867	9.070071	4.078104	-0.009533	-0.010263	-0.031630
O	2.680009	4.731529	2.288686	0.009508	0.010226	0.031527

O	0.058846	0.698526	2.444964	-0.000614	-0.010481	0.009622
O	2.394296	13.103075	3.921826	0.000594	0.010482	-0.009647
O	4.548725	7.599326	0.738431	-0.000595	0.010480	0.009645
O	-2.095583	6.202275	5.628359	0.000616	-0.010485	-0.009620
O	-2.459230	13.184059	5.445139	0.013901	-0.004937	0.011914
O	4.912372	0.617542	0.921651	-0.013875	0.004955	-0.011901
O	2.757943	6.283259	4.105046	0.013872	0.004954	0.011899
O	-0.304801	7.518342	2.261744	-0.013900	-0.004939	-0.011913
O	-0.175430	2.374756	0.744070	-0.025694	-0.006309	-0.004045
O	2.628573	11.426844	5.622720	0.025712	0.006329	0.003983
O	4.783002	9.275557	2.439325	-0.025694	0.006323	-0.003992
O	-2.329859	4.526044	3.927465	0.025715	-0.006316	0.004038
O	-1.223866	12.517207	2.155216	0.009953	0.016469	0.003925
O	3.677009	1.284394	4.211574	-0.009942	-0.016474	-0.003916
O	5.831438	5.616407	1.028179	0.009945	-0.016477	0.003917
O	-3.378295	8.185194	5.338611	-0.009950	0.016464	-0.003925
H	-0.637445	12.195109	2.878812	-0.053350	-0.116860	-0.011831
H	3.090587	1.606491	3.487978	0.053264	0.116830	0.011905
H	5.245016	5.294309	0.304583	-0.053275	0.116806	-0.011883
H	-2.791874	8.507292	6.062207	0.053333	-0.116900	0.011865

21 f = 32.639684 THz 205.081181 2PiTHz 1088.742620 cm-1 134.986929 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.012955	0.003056	0.000446
Li	-1.316675	4.156264	2.365404	-0.013037	0.003068	0.000463
Li	-3.471104	2.744536	5.548798	0.013038	0.003068	-0.000464
Li	5.924247	11.057064	0.817991	0.012955	0.003056	-0.000446
Na	2.049025	6.784862	1.629696	0.000582	-0.000428	0.000175
Na	0.404117	7.016739	4.737094	0.000575	-0.000414	0.000172
Na	2.558546	13.685662	1.553699	-0.000575	-0.000415	-0.000171
Na	-0.105403	0.115939	4.813091	-0.000582	-0.000428	-0.000175
B	4.155007	8.978944	1.168663	-0.057040	-0.021640	-0.028854
B	-1.701865	4.822656	5.198127	-0.057379	-0.021818	-0.029126
B	0.452564	2.078144	2.014732	0.057393	-0.021833	0.029151
B	2.000578	11.723457	4.352058	0.057038	-0.021622	0.028845

B	-2.733891	11.746082	5.839177	-0.024628	0.006393	0.067600
B	5.187034	2.055518	0.527613	-0.024948	0.006355	0.067898
B	3.032605	4.845282	3.711007	0.024932	0.006367	-0.067899
B	-0.579463	8.956318	2.655782	0.024624	0.006381	-0.067613
B	-0.983708	0.054306	1.827988	-0.011020	0.006453	-0.011094
B	3.436850	13.747295	4.538802	-0.010972	0.006386	-0.011062
B	5.591279	6.955106	1.355407	0.010974	0.006387	0.011065
B	-3.138137	6.846495	5.011383	0.011020	0.006452	0.011092
Si	0.631772	3.486686	4.508512	0.011141	0.005879	-0.012883
Si	1.821370	10.314915	1.858278	0.011096	0.005874	-0.012824
Si	-0.333059	10.387486	5.041673	-0.011092	0.005874	0.012826
Si	2.786201	3.414115	1.325117	-0.011142	0.005877	0.012883
O	0.061445	3.072947	3.041906	0.001080	0.010822	0.025744
O	2.391697	10.728653	3.324884	0.001075	0.010761	0.025645
O	4.546126	9.973747	0.141489	-0.001075	0.010766	-0.025653
O	-2.092984	3.827853	6.225301	-0.001084	0.010820	-0.025748
O	2.197450	3.933608	4.519003	-0.056698	-0.027623	0.024412
O	0.255692	9.867992	1.847787	-0.056404	-0.027487	0.024293
O	-1.898737	10.834409	5.031182	0.056396	-0.027486	-0.024293
O	4.351879	2.967192	1.335608	0.056702	-0.027623	-0.024415
O	-0.212316	4.798696	5.055280	0.019607	-0.007397	-0.003194
O	2.665458	9.002905	1.311510	0.019483	-0.007384	-0.003189
O	0.511030	11.699496	4.494905	-0.019487	-0.007389	0.003191
O	1.942113	2.102105	1.871885	-0.019607	-0.007393	0.003192
O	0.525580	2.169271	5.472081	0.004993	0.006626	-0.012798
O	1.927562	11.632329	0.894709	0.004937	0.006564	-0.012753
O	-0.226867	9.070071	4.078104	-0.004938	0.006569	0.012758
O	2.680009	4.731529	2.288686	-0.004989	0.006626	0.012805
O	0.058846	0.698526	2.444964	0.002152	0.006645	0.001751
O	2.394296	13.103075	3.921826	0.002126	0.006572	0.001768
O	4.548725	7.599326	0.738431	-0.002130	0.006578	-0.001768
O	-2.095583	6.202275	5.628359	-0.002151	0.006639	-0.001753
O	-2.459230	13.184059	5.445139	0.007889	0.005327	-0.002928
O	4.912372	0.617542	0.921651	0.007930	0.005394	-0.002961
O	2.757943	6.283259	4.105046	-0.007931	0.005387	0.002957
O	-0.304801	7.518342	2.261744	-0.007888	0.005333	0.002933

O	-0.175430	2.374756	0.744070	-0.026600	0.006360	-0.032021
O	2.628573	11.426844	5.622720	-0.026506	0.006286	-0.031814
O	4.783002	9.275557	2.439325	0.026512	0.006288	0.031824
O	-2.329859	4.526044	3.927465	0.026596	0.006357	0.032010
O	-1.223866	12.517207	2.155216	-0.005202	-0.007299	0.000956
O	3.677009	1.284394	4.211574	-0.005201	-0.007210	0.000956
O	5.831438	5.616407	1.028179	0.005201	-0.007214	-0.000957
O	-3.378295	8.185194	5.338611	0.005202	-0.007294	-0.000953
H	-0.637445	12.195109	2.878812	0.038680	0.024174	-0.012943
H	3.090587	1.606491	3.487978	0.038799	0.024019	-0.013123
H	5.245016	5.294309	0.304583	-0.038796	0.023995	0.013130
H	-2.791874	8.507292	6.062207	-0.038685	0.024216	0.012933

22 f = 32.555774 THz 204.553962 2PiTHz 1085.943701 cm-1 134.639908
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.014438	0.002058	0.000812
Li	-1.316675	4.156264	2.365404	0.014362	-0.002041	-0.000820
Li	-3.471104	2.744536	5.548798	-0.014361	-0.002040	0.000821
Li	5.924247	11.057064	0.817991	0.014440	0.002059	-0.000812
Na	2.049025	6.784862	1.629696	-0.000601	0.002577	-0.000840
Na	0.404117	7.016739	4.737094	0.000605	-0.002581	0.000836
Na	2.558546	13.685662	1.553699	-0.000605	-0.002579	-0.000835
Na	-0.105403	0.115939	4.813091	0.000601	0.002579	0.000841
B	4.155007	8.978944	1.168663	-0.058419	-0.031374	-0.043745
B	-1.701865	4.822656	5.198127	0.058098	0.031216	0.043623
B	0.452564	2.078144	2.014732	-0.058089	0.031252	-0.043643
B	2.000578	11.723457	4.352058	0.058440	-0.031338	0.043747
B	-2.733891	11.746082	5.839177	-0.045495	-0.001176	0.056932
B	5.187034	2.055518	0.527613	0.045387	0.001261	-0.056531
B	3.032605	4.845282	3.711007	-0.045378	0.001231	0.056514
B	-0.579463	8.956318	2.655782	0.045479	-0.001205	-0.056963
B	-0.983708	0.054306	1.827988	0.011223	-0.009299	0.006953
B	3.436850	13.747295	4.538802	-0.011301	0.009314	-0.007020
B	5.591279	6.955106	1.355407	0.011299	0.009320	0.007022
B	-3.138137	6.846495	5.011383	-0.011226	-0.009290	-0.006951

Si	0.631772	3.486686	4.508512	-0.007905	-0.001229	0.009827
Si	1.821370	10.314915	1.858278	0.007965	0.001258	-0.009902
Si	-0.333059	10.387486	5.041673	-0.007965	0.001256	0.009903
Si	2.786201	3.414115	1.325117	0.007900	-0.001230	-0.009827
O	0.061445	3.072947	3.041906	-0.001143	-0.010409	-0.019878
O	2.391697	10.728653	3.324884	0.001152	0.010470	0.020044
O	4.546126	9.973747	0.141489	-0.001153	0.010484	-0.020064
O	-2.092984	3.827853	6.225301	0.001146	-0.010399	0.019871
O	2.197450	3.933608	4.519003	0.050905	0.023654	-0.021466
O	0.255692	9.867992	1.847787	-0.051214	-0.023797	0.021599
O	-1.898737	10.834409	5.031182	0.051224	-0.023810	-0.021607
O	4.351879	2.967192	1.335608	-0.050891	0.023639	0.021460
O	-0.212316	4.798696	5.055280	-0.019997	0.003107	0.000897
O	2.665458	9.002905	1.311510	0.020097	-0.003147	-0.000913
O	0.511030	11.699496	4.494905	-0.020110	-0.003158	0.000919
O	1.942113	2.102105	1.871885	0.019989	0.003099	-0.000890
O	0.525580	2.169271	5.472081	-0.007860	-0.010906	0.012007
O	1.927562	11.632329	0.894709	0.007883	0.010941	-0.012091
O	-0.226867	9.070071	4.078104	-0.007882	0.010958	0.012116
O	2.680009	4.731529	2.288686	0.007858	-0.010895	-0.011993
O	0.058846	0.698526	2.444964	-0.004056	-0.011742	0.002265
O	2.394296	13.103075	3.921826	0.004062	0.011770	-0.002248
O	4.548725	7.599326	0.738431	-0.004068	0.011781	0.002247
O	-2.095583	6.202275	5.628359	0.004052	-0.011730	-0.002262
O	-2.459230	13.184059	5.445139	0.009419	0.007392	-0.002752
O	4.912372	0.617542	0.921651	-0.009376	-0.007377	0.002741
O	2.757943	6.283259	4.105046	0.009374	-0.007369	-0.002738
O	-0.304801	7.518342	2.261744	-0.009420	0.007397	0.002754
O	-0.175430	2.374756	0.744070	0.017521	-0.009728	0.032825
O	2.628573	11.426844	5.622720	-0.017682	0.009745	-0.032992
O	4.783002	9.275557	2.439325	0.017684	0.009752	0.033002
O	-2.329859	4.526044	3.927465	-0.017523	-0.009720	-0.032812
O	-1.223866	12.517207	2.155216	0.000997	0.014125	0.000901
O	3.677009	1.284394	4.211574	-0.001028	-0.014150	-0.000897
O	5.831438	5.616407	1.028179	0.001031	-0.014157	0.000897
O	-3.378295	8.185194	5.338611	-0.000994	0.014115	-0.000903

H	-0.637445	12.195109	2.878812	0.014299	-0.062679	-0.040885
H	3.090587	1.606491	3.487978	-0.014080	0.062789	0.040793
H	5.245016	5.294309	0.304583	0.014064	0.062832	-0.040802
H	-2.791874	8.507292	6.062207	-0.014316	-0.062653	0.040881

23 f = 31.896090 THz 200.409042 2PiTHz 1063.938999 cm-1 131.911671
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004644	0.012598	-0.010885
Li	-1.316675	4.156264	2.365404	0.004669	-0.012604	0.010900
Li	-3.471104	2.744536	5.548798	-0.004672	-0.012602	-0.010902
Li	5.924247	11.057064	0.817991	0.004640	0.012600	0.010882
Na	2.049025	6.784862	1.629696	-0.000312	0.000891	-0.000267
Na	0.404117	7.016739	4.737094	0.000310	-0.000894	0.000269
Na	2.558546	13.685662	1.553699	-0.000313	-0.000892	-0.000268
Na	-0.105403	0.115939	4.813091	0.000309	0.000892	0.000267
B	4.155007	8.978944	1.168663	0.014175	0.040331	0.045800
B	-1.701865	4.822656	5.198127	-0.014149	-0.040508	-0.046063
B	0.452564	2.078144	2.014732	0.014131	-0.040317	0.045874
B	2.000578	11.723457	4.352058	-0.014193	0.040525	-0.045995
B	-2.733891	11.746082	5.839177	0.013544	0.049827	0.028685
B	5.187034	2.055518	0.527613	-0.013305	-0.049701	-0.028762
B	3.032605	4.845282	3.711007	0.013462	-0.049864	0.028747
B	-0.579463	8.956318	2.655782	-0.013400	0.049660	-0.028717
B	-0.983708	0.054306	1.827988	-0.000821	-0.011860	0.004245
B	3.436850	13.747295	4.538802	0.000756	0.011778	-0.004248
B	5.591279	6.955106	1.355407	-0.000776	0.011861	0.004282
B	-3.138137	6.846495	5.011383	0.000795	-0.011778	-0.004217
Si	0.631772	3.486686	4.508512	-0.008213	-0.033811	-0.013375
Si	1.821370	10.314915	1.858278	0.008207	0.033813	0.013349
Si	-0.333059	10.387486	5.041673	-0.008207	0.033810	-0.013339
Si	2.786201	3.414115	1.325117	0.008202	-0.033815	0.013378
O	0.061445	3.072947	3.041906	0.000000	0.022788	0.022608
O	2.391697	10.728653	3.324884	-0.000014	-0.022792	-0.022576
O	4.546126	9.973747	0.141489	0.000019	-0.022774	0.022589
O	-2.092984	3.827853	6.225301	0.000007	0.022799	-0.022578

O	2.197450	3.933608	4.519003	0.033584	0.028470	-0.011741
O	0.255692	9.867992	1.847787	-0.033555	-0.028438	0.011738
O	-1.898737	10.834409	5.031182	0.033519	-0.028442	-0.011737
O	4.351879	2.967192	1.335608	-0.033605	0.028460	0.011741
O	-0.212316	4.798696	5.055280	-0.023031	0.028572	0.015508
O	2.665458	9.002905	1.311510	0.022984	-0.028553	-0.015473
O	0.511030	11.699496	4.494905	-0.022960	-0.028560	0.015482
O	1.942113	2.102105	1.871885	0.023063	0.028570	-0.015501
O	0.525580	2.169271	5.472081	0.003069	0.017558	0.000104
O	1.927562	11.632329	0.894709	-0.003101	-0.017599	-0.000068
O	-0.226867	9.070071	4.078104	0.003080	-0.017588	0.000047
O	2.680009	4.731529	2.288686	-0.003090	0.017568	-0.000126
O	0.058846	0.698526	2.444964	-0.001930	0.005511	-0.005105
O	2.394296	13.103075	3.921826	0.001870	-0.005619	0.005113
O	4.548725	7.599326	0.738431	-0.001959	-0.005512	-0.005135
O	-2.095583	6.202275	5.628359	0.001843	0.005619	0.005087
O	-2.459230	13.184059	5.445139	0.002436	-0.017440	0.008093
O	4.912372	0.617542	0.921651	-0.002385	0.017333	-0.008004
O	2.757943	6.283259	4.105046	0.002436	0.017416	0.008074
O	-0.304801	7.518342	2.261744	-0.002385	-0.017354	-0.008020
O	-0.175430	2.374756	0.744070	0.000591	0.013839	-0.022592
O	2.628573	11.426844	5.622720	-0.000682	-0.013893	0.022607
O	4.783002	9.275557	2.439325	0.000653	-0.013825	-0.022527
O	-2.329859	4.526044	3.927465	-0.000636	0.013906	0.022661
O	-1.223866	12.517207	2.155216	0.007669	0.006604	0.005231
O	3.677009	1.284394	4.211574	-0.007639	-0.006500	-0.005273
O	5.831438	5.616407	1.028179	0.007670	-0.006613	0.005250
O	-3.378295	8.185194	5.338611	-0.007635	0.006490	-0.005254
H	-0.637445	12.195109	2.878812	-0.026193	-0.155003	-0.041462
H	3.090587	1.606491	3.487978	0.026142	0.155405	0.041619
H	5.245016	5.294309	0.304583	-0.026204	0.155347	-0.041600
H	-2.791874	8.507292	6.062207	0.026129	-0.155067	0.041488

24 f = 31.781316 THz 199.687900 2PiTHz 1060.110570 cm-1 131.437006
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.003193	0.002227	-0.001805
Li	-1.316675	4.156264	2.365404	-0.003212	0.002191	-0.001808
Li	-3.471104	2.744536	5.548798	-0.003232	-0.002227	-0.001839
Li	5.924247	11.057064	0.817991	-0.003174	-0.002191	-0.001776
Na	2.049025	6.784862	1.629696	0.000279	0.001841	-0.000135
Na	0.404117	7.016739	4.737094	0.000281	0.001841	-0.000139
Na	2.558546	13.685662	1.553699	0.000279	-0.001845	-0.000140
Na	-0.105403	0.115939	4.813091	0.000281	-0.001837	-0.000134
B	4.155007	8.978944	1.168663	-0.005596	0.071700	0.051695
B	-1.701865	4.822656	5.198127	-0.005742	0.071648	0.051440
B	0.452564	2.078144	2.014732	-0.005724	-0.071736	0.051570
B	2.000578	11.723457	4.352058	-0.005621	-0.071608	0.051562
B	-2.733891	11.746082	5.839177	-0.058208	-0.056520	0.011734
B	5.187034	2.055518	0.527613	-0.058517	-0.056651	0.011492
B	3.032605	4.845282	3.711007	-0.058489	0.056508	0.011600
B	-0.579463	8.956318	2.655782	-0.058245	0.056660	0.011632
B	-0.983708	0.054306	1.827988	0.010472	0.024211	-0.001936
B	3.436850	13.747295	4.538802	0.010367	0.024240	-0.002035
B	5.591279	6.955106	1.355407	0.010370	-0.024199	-0.002017
B	-3.138137	6.846495	5.011383	0.010468	-0.024251	-0.001953
Si	0.631772	3.486686	4.508512	0.009254	-0.001761	0.004221
Si	1.821370	10.314915	1.858278	0.009162	-0.001626	0.004159
Si	-0.333059	10.387486	5.041673	0.009128	0.001730	0.004124
Si	2.786201	3.414115	1.325117	0.009283	0.001662	0.004254
O	0.061445	3.072947	3.041906	-0.004137	0.004750	-0.009305
O	2.391697	10.728653	3.324884	-0.004101	0.004753	-0.009196
O	4.546126	9.973747	0.141489	-0.004101	-0.004810	-0.009138
O	-2.092984	3.827853	6.225301	-0.004135	-0.004697	-0.009354
O	2.197450	3.933608	4.519003	-0.006227	-0.010042	0.003001
O	0.255692	9.867992	1.847787	-0.006220	-0.010090	0.003014
O	-1.898737	10.834409	5.031182	-0.006092	0.009995	0.002977
O	4.351879	2.967192	1.335608	-0.006351	0.010135	0.003040
O	-0.212316	4.798696	5.055280	-0.005979	-0.008271	-0.005862
O	2.665458	9.002905	1.311510	-0.005811	-0.008385	-0.005923
O	0.511030	11.699496	4.494905	-0.005889	0.008305	-0.005873
O	1.942113	2.102105	1.871885	-0.005898	0.008351	-0.005913

O	0.525580	2.169271	5.472081	0.005014	0.013788	-0.007939
O	1.927562	11.632329	0.894709	0.005006	0.013666	-0.007874
O	-0.226867	9.070071	4.078104	0.005017	-0.013727	-0.007873
O	2.680009	4.731529	2.288686	0.005004	-0.013731	-0.007947
O	0.058846	0.698526	2.444964	0.016238	0.032827	-0.004689
O	2.394296	13.103075	3.921826	0.016255	0.032797	-0.004654
O	4.548725	7.599326	0.738431	0.016248	-0.032804	-0.004666
O	-2.095583	6.202275	5.628359	0.016243	-0.032821	-0.004680
O	-2.459230	13.184059	5.445139	-0.003634	0.021809	-0.013811
O	4.912372	0.617542	0.921651	-0.003665	0.021818	-0.013840
O	2.757943	6.283259	4.105046	-0.003654	-0.021776	-0.013818
O	-0.304801	7.518342	2.261744	-0.003641	-0.021845	-0.013827
O	-0.175430	2.374756	0.744070	0.026864	0.021017	-0.016298
O	2.628573	11.426844	5.622720	0.026571	0.020961	-0.016392
O	4.783002	9.275557	2.439325	0.026588	-0.021001	-0.016467
O	-2.329859	4.526044	3.927465	0.026851	-0.020979	-0.016228
O	-1.223866	12.517207	2.155216	-0.007775	-0.028912	0.006700
O	3.677009	1.284394	4.211574	-0.007782	-0.028931	0.006691
O	5.831438	5.616407	1.028179	-0.007766	0.028912	0.006704
O	-3.378295	8.185194	5.338611	-0.007794	0.028930	0.006684
H	-0.637445	12.195109	2.878812	0.011161	0.005468	0.007789
H	3.090587	1.606491	3.487978	0.011219	0.006013	0.007972
H	5.245016	5.294309	0.304583	0.011171	-0.005602	0.007840
H	-2.791874	8.507292	6.062207	0.011233	-0.005911	0.007913

25 f = 31.530527 THz 198.112145 2PiTHz 1051.745144 cm-1 130.399825
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.007973	-0.000452	-0.006691
Li	-1.316675	4.156264	2.365404	0.007956	0.000462	0.006678
Li	-3.471104	2.744536	5.548798	0.007957	-0.000459	0.006683
Li	5.924247	11.057064	0.817991	-0.007974	0.000451	-0.006690
Na	2.049025	6.784862	1.629696	-0.000052	0.000820	-0.000463
Na	0.404117	7.016739	4.737094	0.000054	-0.000812	0.000460
Na	2.558546	13.685662	1.553699	0.000054	0.000813	0.000460
Na	-0.105403	0.115939	4.813091	-0.000052	-0.000820	-0.000463

B	4.155007	8.978944	1.168663	-0.026693	0.002234	-0.033548
B	-1.701865	4.822656	5.198127	0.026659	-0.001922	0.033732
B	0.452564	2.078144	2.014732	0.026638	0.001919	0.033728
B	2.000578	11.723457	4.352058	-0.026711	-0.002249	-0.033547
B	-2.733891	11.746082	5.839177	-0.051980	0.004115	-0.027208
B	5.187034	2.055518	0.527613	0.051694	-0.004380	0.027254
B	3.032605	4.845282	3.711007	0.051702	0.004382	0.027239
B	-0.579463	8.956318	2.655782	-0.051964	-0.004129	-0.027205
B	-0.983708	0.054306	1.827988	-0.021801	-0.001785	-0.017233
B	3.436850	13.747295	4.538802	0.021870	0.001884	0.017241
B	5.591279	6.955106	1.355407	0.021865	-0.001888	0.017236
B	-3.138137	6.846495	5.011383	-0.021804	0.001784	-0.017235
Si	0.631772	3.486686	4.508512	-0.027111	0.008588	-0.021895
Si	1.821370	10.314915	1.858278	0.027163	-0.008595	0.021927
Si	-0.333059	10.387486	5.041673	0.027170	0.008590	0.021924
Si	2.786201	3.414115	1.325117	-0.027104	-0.008581	-0.021897
O	0.061445	3.072947	3.041906	0.006607	0.013317	0.034303
O	2.391697	10.728653	3.324884	-0.006625	-0.013306	-0.034363
O	4.546126	9.973747	0.141489	-0.006627	0.013308	-0.034362
O	-2.092984	3.827853	6.225301	0.006604	-0.013322	0.034306
O	2.197450	3.933608	4.519003	0.028856	0.012224	-0.008373
O	0.255692	9.867992	1.847787	-0.028897	-0.012280	0.008392
O	-1.898737	10.834409	5.031182	-0.028913	0.012289	0.008399
O	4.351879	2.967192	1.335608	0.028849	-0.012225	-0.008375
O	-0.212316	4.798696	5.055280	0.020010	-0.009780	-0.003378
O	2.665458	9.002905	1.311510	-0.020041	0.009756	0.003359
O	0.511030	11.699496	4.494905	-0.020039	-0.009749	0.003356
O	1.942113	2.102105	1.871885	0.020008	0.009777	-0.003378
O	0.525580	2.169271	5.472081	0.002100	-0.014921	0.020716
O	1.927562	11.632329	0.894709	-0.002083	0.014982	-0.020765
O	-0.226867	9.070071	4.078104	-0.002083	-0.014980	-0.020762
O	2.680009	4.731529	2.288686	0.002100	0.014914	0.020718
O	0.058846	0.698526	2.444964	0.004964	-0.003981	0.006903
O	2.394296	13.103075	3.921826	-0.004887	0.004139	-0.006923
O	4.548725	7.599326	0.738431	-0.004888	-0.004134	-0.006922
O	-2.095583	6.202275	5.628359	0.004959	0.003986	0.006902

O	-2.459230	13.184059	5.445139	-0.002731	-0.008209	0.001411
O	4.912372	0.617542	0.921651	0.002693	0.008322	-0.001499
O	2.757943	6.283259	4.105046	0.002697	-0.008320	-0.001492
O	-0.304801	7.518342	2.261744	-0.002726	0.008218	0.001419
O	-0.175430	2.374756	0.744070	-0.059326	-0.000435	-0.043243
O	2.628573	11.426844	5.622720	0.059496	0.000524	0.043213
O	4.783002	9.275557	2.439325	0.059475	-0.000520	0.043209
O	-2.329859	4.526044	3.927465	-0.059341	0.000433	-0.043242
O	-1.223866	12.517207	2.155216	0.002804	-0.001119	0.002078
O	3.677009	1.284394	4.211574	-0.002832	0.000995	-0.002038
O	5.831438	5.616407	1.028179	-0.002834	-0.000994	-0.002042
O	-3.378295	8.185194	5.338611	0.002805	0.001116	0.002077
H	-0.637445	12.195109	2.878812	-0.004901	0.008304	0.009408
H	3.090587	1.606491	3.487978	0.004942	-0.008474	-0.009444
H	5.245016	5.294309	0.304583	0.004947	0.008407	-0.009422
H	-2.791874	8.507292	6.062207	-0.004902	-0.008311	0.009411

26 f = 31.234252 THz 196.250593 2PiTHz 1041.862465 cm-1 129.174529 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.005213	-0.001513	0.003180
Li	-1.316675	4.156264	2.365404	0.005223	-0.001531	0.003198
Li	-3.471104	2.744536	5.548798	0.005213	0.001521	0.003186
Li	5.924247	11.057064	0.817991	0.005208	0.001522	0.003185
Na	2.049025	6.784862	1.629696	-0.000223	0.000463	-0.000699
Na	0.404117	7.016739	4.737094	-0.000222	0.000461	-0.000701
Na	2.558546	13.685662	1.553699	-0.000222	-0.000462	-0.000701
Na	-0.105403	0.115939	4.813091	-0.000223	-0.000462	-0.000699
B	4.155007	8.978944	1.168663	0.024070	0.012270	0.044018
B	-1.701865	4.822656	5.198127	0.024104	0.012138	0.043948
B	0.452564	2.078144	2.014732	0.024083	-0.012169	0.043997
B	2.000578	11.723457	4.352058	0.024099	-0.012225	0.044020
B	-2.733891	11.746082	5.839177	0.039046	-0.005736	0.034826
B	5.187034	2.055518	0.527613	0.039105	-0.005724	0.034808
B	3.032605	4.845282	3.711007	0.039077	0.005673	0.034818
B	-0.579463	8.956318	2.655782	0.038994	0.005772	0.034838

B	-0.983708	0.054306	1.827988	-0.023706	0.003109	-0.019660
B	3.436850	13.747295	4.538802	-0.023700	0.003118	-0.019657
B	5.591279	6.955106	1.355407	-0.023677	-0.003111	-0.019637
B	-3.138137	6.846495	5.011383	-0.023703	-0.003121	-0.019660
Si	0.631772	3.486686	4.508512	-0.021904	0.007952	-0.020547
Si	1.821370	10.314915	1.858278	-0.021851	0.007974	-0.020517
Si	-0.333059	10.387486	5.041673	-0.021873	-0.007956	-0.020506
Si	2.786201	3.414115	1.325117	-0.021891	-0.007968	-0.020524
O	0.061445	3.072947	3.041906	0.005646	0.012378	0.030786
O	2.391697	10.728653	3.324884	0.005624	0.012362	0.030731
O	4.546126	9.973747	0.141489	0.005631	-0.012368	0.030736
O	-2.092984	3.827853	6.225301	0.005640	-0.012363	0.030760
O	2.197450	3.933608	4.519003	0.027428	0.011715	-0.009204
O	0.255692	9.867992	1.847787	0.027339	0.011669	-0.009188
O	-1.898737	10.834409	5.031182	0.027372	-0.011689	-0.009198
O	4.351879	2.967192	1.335608	0.027381	-0.011687	-0.009196
O	-0.212316	4.798696	5.055280	0.014845	-0.007176	-0.002944
O	2.665458	9.002905	1.311510	0.014842	-0.007208	-0.002962
O	0.511030	11.699496	4.494905	0.014851	0.007206	-0.002962
O	1.942113	2.102105	1.871885	0.014877	0.007193	-0.002958
O	0.525580	2.169271	5.472081	0.002103	-0.014071	0.017366
O	1.927562	11.632329	0.894709	0.002104	-0.014067	0.017351
O	-0.226867	9.070071	4.078104	0.002106	0.014041	0.017314
O	2.680009	4.731529	2.288686	0.002104	0.014067	0.017352
O	0.058846	0.698526	2.444964	0.014903	0.009834	0.008470
O	2.394296	13.103075	3.921826	0.014909	0.009861	0.008467
O	4.548725	7.599326	0.738431	0.014922	-0.009877	0.008469
O	-2.095583	6.202275	5.628359	0.014881	-0.009819	0.008461
O	-2.459230	13.184059	5.445139	0.004931	0.005151	-0.000518
O	4.912372	0.617542	0.921651	0.004936	0.005139	-0.000504
O	2.757943	6.283259	4.105046	0.004955	-0.005116	-0.000481
O	-0.304801	7.518342	2.261744	0.004910	-0.005167	-0.000542
O	-0.175430	2.374756	0.744070	-0.053642	0.002091	-0.046415
O	2.628573	11.426844	5.622720	-0.053609	0.002106	-0.046409
O	4.783002	9.275557	2.439325	-0.053557	-0.002121	-0.046399
O	-2.329859	4.526044	3.927465	-0.053632	-0.002082	-0.046379

O	-1.223866	12.517207	2.155216	-0.008805	-0.014376	-0.003282
O	3.677009	1.284394	4.211574	-0.008807	-0.014389	-0.003280
O	5.831438	5.616407	1.028179	-0.008803	0.014393	-0.003274
O	-3.378295	8.185194	5.338611	-0.008808	0.014366	-0.003287
H	-0.637445	12.195109	2.878812	0.038076	0.114452	0.022968
H	3.090587	1.606491	3.487978	0.038070	0.114440	0.022979
H	5.245016	5.294309	0.304583	0.038048	-0.114254	0.022926
H	-2.791874	8.507292	6.062207	0.038115	-0.114584	0.022981

27 f = 31.153251 THz 195.741651 2PiTHz 1039.160575 cm-1 128.839537 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.013094	0.001434	-0.006709
Li	-1.316675	4.156264	2.365404	-0.013076	0.001422	-0.006704
Li	-3.471104	2.744536	5.548798	0.013076	0.001420	0.006701
Li	5.924247	11.057064	0.817991	0.013100	0.001438	0.006715
Na	2.049025	6.784862	1.629696	0.000124	0.000357	-0.000264
Na	0.404117	7.016739	4.737094	0.000126	0.000357	-0.000268
Na	2.558546	13.685662	1.553699	-0.000126	0.000356	0.000267
Na	-0.105403	0.115939	4.813091	-0.000124	0.000357	0.000264
B	4.155007	8.978944	1.168663	0.007905	-0.019664	0.028355
B	-1.701865	4.822656	5.198127	0.007846	-0.019647	0.028262
B	0.452564	2.078144	2.014732	-0.007839	-0.019687	-0.028229
B	2.000578	11.723457	4.352058	-0.007883	-0.019642	-0.028331
B	-2.733891	11.746082	5.839177	-0.073945	0.006865	0.027810
B	5.187034	2.055518	0.527613	-0.073884	0.006809	0.027762
B	3.032605	4.845282	3.711007	0.073885	0.006837	-0.027740
B	-0.579463	8.956318	2.655782	0.073984	0.006847	-0.027787
B	-0.983708	0.054306	1.827988	0.021726	0.001623	0.017934
B	3.436850	13.747295	4.538802	0.021758	0.001645	0.017950
B	5.591279	6.955106	1.355407	-0.021779	0.001648	-0.017964
B	-3.138137	6.846495	5.011383	-0.021732	0.001615	-0.017943
Si	0.631772	3.486686	4.508512	-0.014967	-0.004093	0.024762
Si	1.821370	10.314915	1.858278	-0.014973	-0.004041	0.024816
Si	-0.333059	10.387486	5.041673	0.014953	-0.004046	-0.024831
Si	2.786201	3.414115	1.325117	0.014962	-0.004097	-0.024771

O	0.061445	3.072947	3.041906	0.003348	-0.004990	-0.011473
O	2.391697	10.728653	3.324884	0.003353	-0.005042	-0.011543
O	4.546126	9.973747	0.141489	-0.003352	-0.005050	0.011564
O	-2.092984	3.827853	6.225301	-0.003342	-0.004997	0.011489
O	2.197450	3.933608	4.519003	-0.002722	-0.003050	0.000769
O	0.255692	9.867992	1.847787	-0.002776	-0.003092	0.000781
O	-1.898737	10.834409	5.031182	0.002800	-0.003103	-0.000788
O	4.351879	2.967192	1.335608	0.002732	-0.003054	-0.000773
O	-0.212316	4.798696	5.055280	0.030616	-0.011877	-0.009643
O	2.665458	9.002905	1.311510	0.030707	-0.011932	-0.009676
O	0.511030	11.699496	4.494905	-0.030692	-0.011929	0.009675
O	1.942113	2.102105	1.871885	-0.030614	-0.011873	0.009641
O	0.525580	2.169271	5.472081	0.003350	0.026062	-0.044984
O	1.927562	11.632329	0.894709	0.003351	0.026066	-0.045021
O	-0.226867	9.070071	4.078104	-0.003348	0.026073	0.045030
O	2.680009	4.731529	2.288686	-0.003350	0.026070	0.044993
O	0.058846	0.698526	2.444964	-0.003001	0.007041	-0.006550
O	2.394296	13.103075	3.921826	-0.003007	0.007039	-0.006553
O	4.548725	7.599326	0.738431	0.003006	0.007051	0.006558
O	-2.095583	6.202275	5.628359	0.003021	0.007019	0.006555
O	-2.459230	13.184059	5.445139	-0.004035	-0.000615	-0.007180
O	4.912372	0.617542	0.921651	-0.004030	-0.000602	-0.007185
O	2.757943	6.283259	4.105046	0.004025	-0.000624	0.007170
O	-0.304801	7.518342	2.261744	0.004047	-0.000600	0.007192
O	-0.175430	2.374756	0.744070	0.053400	0.004769	0.027102
O	2.628573	11.426844	5.622720	0.053473	0.004754	0.027187
O	4.783002	9.275557	2.439325	-0.053515	0.004757	-0.027218
O	-2.329859	4.526044	3.927465	-0.053419	0.004759	-0.027124
O	-1.223866	12.517207	2.155216	-0.001032	0.000912	0.003148
O	3.677009	1.284394	4.211574	-0.001031	0.000905	0.003144
O	5.831438	5.616407	1.028179	0.001028	0.000899	-0.003150
O	-3.378295	8.185194	5.338611	0.001025	0.000935	-0.003145
H	-0.637445	12.195109	2.878812	0.022009	-0.073432	-0.049950
H	3.090587	1.606491	3.487978	0.021989	-0.073301	-0.049860
H	5.245016	5.294309	0.304583	-0.021959	-0.073428	0.049883
H	-2.791874	8.507292	6.062207	-0.021998	-0.073437	0.049957

28 f = 30.994260 THz 194.742682 2PiTHz 1033.857214 cm-1 128.182004
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.011037	-0.001073	-0.002069
Li	-1.316675	4.156264	2.365404	0.011053	0.001076	0.002084
Li	-3.471104	2.744536	5.548798	-0.011052	0.001077	-0.002083
Li	5.924247	11.057064	0.817991	0.011040	-0.001071	0.002072
Na	2.049025	6.784862	1.629696	-0.000464	0.000455	0.000677
Na	0.404117	7.016739	4.737094	0.000463	-0.000455	-0.000679
Na	2.558546	13.685662	1.553699	-0.000463	-0.000455	0.000679
Na	-0.105403	0.115939	4.813091	0.000465	0.000455	-0.000677
B	4.155007	8.978944	1.168663	0.002878	-0.014616	0.035224
B	-1.701865	4.822656	5.198127	-0.002904	0.014655	-0.035241
B	0.452564	2.078144	2.014732	0.002896	0.014643	0.035240
B	2.000578	11.723457	4.352058	-0.002882	-0.014615	-0.035226
B	-2.733891	11.746082	5.839177	-0.068952	0.003437	0.020253
B	5.187034	2.055518	0.527613	0.069068	-0.003446	-0.020278
B	3.032605	4.845282	3.711007	-0.069047	-0.003437	0.020296
B	-0.579463	8.956318	2.655782	0.068979	0.003441	-0.020232
B	-0.983708	0.054306	1.827988	-0.023002	0.004292	-0.021022
B	3.436850	13.747295	4.538802	0.022980	-0.004269	0.020992
B	5.591279	6.955106	1.355407	-0.022984	-0.004271	-0.020999
B	-3.138137	6.846495	5.011383	0.023003	0.004291	0.021019
Si	0.631772	3.486686	4.508512	0.015499	0.010437	-0.022238
Si	1.821370	10.314915	1.858278	-0.015464	-0.010405	0.022213
Si	-0.333059	10.387486	5.041673	0.015456	-0.010405	-0.022219
Si	2.786201	3.414115	1.325117	-0.015502	0.010436	0.022235
O	0.061445	3.072947	3.041906	-0.002766	0.000453	0.004735
O	2.391697	10.728653	3.324884	0.002747	-0.000456	-0.004750
O	4.546126	9.973747	0.141489	-0.002747	-0.000458	0.004755
O	-2.092984	3.827853	6.225301	0.002765	0.000453	-0.004734
O	2.197450	3.933608	4.519003	-0.002740	-0.002608	0.001539
O	0.255692	9.867992	1.847787	0.002710	0.002591	-0.001529
O	-1.898737	10.834409	5.031182	-0.002694	0.002585	0.001528
O	4.351879	2.967192	1.335608	0.002746	-0.002609	-0.001538

O	-0.212316	4.798696	5.055280	-0.027413	0.009896	0.008387
O	2.665458	9.002905	1.311510	0.027388	-0.009890	-0.008381
O	0.511030	11.699496	4.494905	-0.027386	-0.009898	0.008384
O	1.942113	2.102105	1.871885	0.027414	0.009889	-0.008384
O	0.525580	2.169271	5.472081	-0.002117	-0.029794	0.047074
O	1.927562	11.632329	0.894709	0.002112	0.029738	-0.046992
O	-0.226867	9.070071	4.078104	-0.002112	0.029745	0.046992
O	2.680009	4.731529	2.288686	0.002116	-0.029788	-0.047075
O	0.058846	0.698526	2.444964	0.009686	0.001278	0.008126
O	2.394296	13.103075	3.921826	-0.009684	-0.001282	-0.008113
O	4.548725	7.599326	0.738431	0.009689	-0.001287	0.008119
O	-2.095583	6.202275	5.628359	-0.009676	0.001264	-0.008121
O	-2.459230	13.184059	5.445139	-0.004556	0.000281	-0.006277
O	4.912372	0.617542	0.921651	0.004562	-0.000272	0.006287
O	2.757943	6.283259	4.105046	-0.004570	-0.000279	-0.006293
O	-0.304801	7.518342	2.261744	0.004553	0.000278	0.006276
O	-0.175430	2.374756	0.744070	-0.052842	-0.004282	-0.029620
O	2.628573	11.426844	5.622720	0.052747	0.004269	0.029597
O	4.783002	9.275557	2.439325	-0.052762	0.004269	-0.029605
O	-2.329859	4.526044	3.927465	0.052833	-0.004280	0.029611
O	-1.223866	12.517207	2.155216	-0.007649	-0.009024	-0.001848
O	3.677009	1.284394	4.211574	0.007645	0.009015	0.001842
O	5.831438	5.616407	1.028179	-0.007648	0.009020	-0.001845
O	-3.378295	8.185194	5.338611	0.007645	-0.009016	0.001848
H	-0.637445	12.195109	2.878812	0.060948	0.096127	-0.008353
H	3.090587	1.606491	3.487978	-0.060952	-0.095994	0.008420
H	5.245016	5.294309	0.304583	0.060967	-0.096042	-0.008410
H	-2.791874	8.507292	6.062207	-0.060936	0.096130	0.008346

29 f = 30.726296 THz 193.059013 2PiTHz 1024.918887 cm-1 127.073792 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000462	0.005335	0.000200
Li	-1.316675	4.156264	2.365404	0.000511	0.005192	0.000312
Li	-3.471104	2.744536	5.548798	-0.000458	0.005331	-0.000190
Li	5.924247	11.057064	0.817991	-0.000513	0.005196	-0.000320

Na	2.049025	6.784862	1.629696	-0.000003	-0.001814	-0.000045
Na	0.404117	7.016739	4.737094	-0.000006	-0.001812	-0.000039
Na	2.558546	13.685662	1.553699	0.000004	-0.001813	0.000036
Na	-0.105403	0.115939	4.813091	0.000006	-0.001813	0.000048
B	4.155007	8.978944	1.168663	0.044820	-0.007078	0.025705
B	-1.701865	4.822656	5.198127	0.044902	-0.008570	0.024853
B	0.452564	2.078144	2.014732	-0.044772	-0.007051	-0.025740
B	2.000578	11.723457	4.352058	-0.044944	-0.008585	-0.024824
B	-2.733891	11.746082	5.839177	0.032381	-0.008712	0.023163
B	5.187034	2.055518	0.527613	0.032921	-0.007675	0.022399
B	3.032605	4.845282	3.711007	-0.032351	-0.008688	-0.023163
B	-0.579463	8.956318	2.655782	-0.032931	-0.007702	-0.022404
B	-0.983708	0.054306	1.827988	0.006167	0.018093	-0.005121
B	3.436850	13.747295	4.538802	0.006227	0.018085	-0.005012
B	5.591279	6.955106	1.355407	-0.006164	0.018122	0.005133
B	-3.138137	6.846495	5.011383	-0.006234	0.018057	0.004998
Si	0.631772	3.486686	4.508512	0.018537	0.036491	0.014458
Si	1.821370	10.314915	1.858278	0.018749	0.036581	0.014488
Si	-0.333059	10.387486	5.041673	-0.018556	0.036518	-0.014461
Si	2.786201	3.414115	1.325117	-0.018729	0.036549	-0.014487
O	0.061445	3.072947	3.041906	-0.005009	-0.024244	-0.042584
O	2.391697	10.728653	3.324884	-0.005038	-0.024101	-0.042553
O	4.546126	9.973747	0.141489	0.005004	-0.024269	0.042624
O	-2.092984	3.827853	6.225301	0.005044	-0.024074	0.042511
O	2.197450	3.933608	4.519003	-0.033534	-0.020723	0.009154
O	0.255692	9.867992	1.847787	-0.033857	-0.020935	0.009181
O	-1.898737	10.834409	5.031182	0.033556	-0.020738	-0.009168
O	4.351879	2.967192	1.335608	0.033826	-0.020915	-0.009168
O	-0.212316	4.798696	5.055280	0.009796	-0.015251	-0.008598
O	2.665458	9.002905	1.311510	0.009783	-0.015508	-0.008739
O	0.511030	11.699496	4.494905	-0.009790	-0.015252	0.008596
O	1.942113	2.102105	1.871885	-0.009789	-0.015510	0.008744
O	0.525580	2.169271	5.472081	-0.004438	-0.022722	0.018966
O	1.927562	11.632329	0.894709	-0.004403	-0.022537	0.018733
O	-0.226867	9.070071	4.078104	0.004440	-0.022745	-0.019002
O	2.680009	4.731529	2.288686	0.004400	-0.022506	-0.018688

O	0.058846	0.698526	2.444964	0.023081	0.022137	0.010493
O	2.394296	13.103075	3.921826	0.023577	0.022859	0.010529
O	4.548725	7.599326	0.738431	-0.023115	0.022172	-0.010503
O	-2.095583	6.202275	5.628359	-0.023544	0.022827	-0.010517
O	-2.459230	13.184059	5.445139	-0.019760	0.023223	-0.022646
O	4.912372	0.617542	0.921651	-0.019411	0.022523	-0.021991
O	2.757943	6.283259	4.105046	0.019746	0.023198	0.022626
O	-0.304801	7.518342	2.261744	0.019425	0.022545	0.022008
O	-0.175430	2.374756	0.744070	-0.005554	-0.000939	0.017889
O	2.628573	11.426844	5.622720	-0.005345	-0.000576	0.017388
O	4.783002	9.275557	2.439325	0.005568	-0.000932	-0.017884
O	-2.329859	4.526044	3.927465	0.005320	-0.000580	-0.017395
O	-1.223866	12.517207	2.155216	-0.000608	-0.023724	0.008290
O	3.677009	1.284394	4.211574	-0.000556	-0.024082	0.008446
O	5.831438	5.616407	1.028179	0.000619	-0.023759	-0.008292
O	-3.378295	8.185194	5.338611	0.000546	-0.024049	-0.008444
H	-0.637445	12.195109	2.878812	-0.014524	-0.045694	0.005061
H	3.090587	1.606491	3.487978	-0.015182	-0.048640	0.004726
H	5.245016	5.294309	0.304583	0.014483	-0.045652	-0.005069
H	-2.791874	8.507292	6.062207	0.015223	-0.048674	-0.004720

30 f = 30.721734 THz 193.030350 2PiTHz 1024.766722 cm-1 127.054926 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002594	0.006630	-0.005863
Li	-1.316675	4.156264	2.365404	0.002561	-0.006740	0.005863
Li	-3.471104	2.744536	5.548798	0.002587	0.006633	0.005863
Li	5.924247	11.057064	0.817991	-0.002567	-0.006738	-0.005863
Na	2.049025	6.784862	1.629696	0.000138	-0.000045	0.000135
Na	0.404117	7.016739	4.737094	-0.000138	0.000083	-0.000138
Na	2.558546	13.685662	1.553699	-0.000139	-0.000044	-0.000138
Na	-0.105403	0.115939	4.813091	0.000136	0.000083	0.000135
B	4.155007	8.978944	1.168663	-0.006756	0.073010	0.042524
B	-1.701865	4.822656	5.198127	0.005689	-0.072797	-0.042969
B	0.452564	2.078144	2.014732	0.006729	0.073016	-0.042545
B	2.000578	11.723457	4.352058	-0.005728	-0.072795	0.042937

B	-2.733891	11.746082	5.839177	-0.027732	-0.048494	0.036554
B	5.187034	2.055518	0.527613	0.026951	0.048723	-0.037111
B	3.032605	4.845282	3.711007	0.027656	-0.048472	-0.036574
B	-0.579463	8.956318	2.655782	-0.027017	0.048739	0.037091
B	-0.983708	0.054306	1.827988	-0.003280	0.001372	-0.005837
B	3.436850	13.747295	4.538802	0.003189	-0.001746	0.005974
B	5.591279	6.955106	1.355407	0.003305	0.001380	0.005863
B	-3.138137	6.846495	5.011383	-0.003158	-0.001741	-0.005946
Si	0.631772	3.486686	4.508512	-0.009605	-0.003389	-0.001400
Si	1.821370	10.314915	1.858278	0.009295	0.002628	0.001160
Si	-0.333059	10.387486	5.041673	0.009639	-0.003378	0.001419
Si	2.786201	3.414115	1.325117	-0.009261	0.002637	-0.001132
O	0.061445	3.072947	3.041906	0.001634	-0.007805	-0.002957
O	2.391697	10.728653	3.324884	-0.001554	0.008280	0.003766
O	4.546126	9.973747	0.141489	-0.001636	-0.007791	0.002922
O	-2.092984	3.827853	6.225301	0.001551	0.008298	-0.003810
O	2.197450	3.933608	4.519003	0.014637	0.009503	-0.000654
O	0.255692	9.867992	1.847787	-0.014083	-0.009131	0.000489
O	-1.898737	10.834409	5.031182	-0.014685	0.009527	0.000671
O	4.351879	2.967192	1.335608	0.014032	-0.009107	-0.000474
O	-0.212316	4.798696	5.055280	0.000541	0.012331	0.006952
O	2.665458	9.002905	1.311510	-0.000716	-0.012018	-0.006790
O	0.511030	11.699496	4.494905	-0.000566	0.012322	-0.006948
O	1.942113	2.102105	1.871885	0.000696	-0.012026	0.006793
O	0.525580	2.169271	5.472081	-0.001768	-0.009622	0.012674
O	1.927562	11.632329	0.894709	0.001863	0.010140	-0.013100
O	-0.226867	9.070071	4.078104	0.001769	-0.009650	-0.012702
O	2.680009	4.731529	2.288686	-0.001862	0.010109	0.013066
O	0.058846	0.698526	2.444964	-0.022979	-0.033732	-0.001571
O	2.394296	13.103075	3.921826	0.022430	0.033225	0.001329
O	4.548725	7.599326	0.738431	0.022967	-0.033727	0.001557
O	-2.095583	6.202275	5.628359	-0.022439	0.033227	-0.001341
O	-2.459230	13.184059	5.445139	-0.016335	0.032515	-0.030876
O	4.912372	0.617542	0.921651	0.016761	-0.033015	0.031373
O	2.757943	6.283259	4.105046	0.016322	0.032500	0.030859
O	-0.304801	7.518342	2.261744	-0.016769	-0.033023	-0.031382

O	-0.175430	2.374756	0.744070	-0.011151	-0.017340	0.023786
O	2.628573	11.426844	5.622720	0.011330	0.017335	-0.024022
O	4.783002	9.275557	2.439325	0.011228	-0.017343	-0.023747
O	-2.329859	4.526044	3.927465	-0.011241	0.017330	0.024073
O	-1.223866	12.517207	2.155216	-0.002967	0.016122	-0.007605
O	3.677009	1.284394	4.211574	0.002993	-0.015590	0.007427
O	5.831438	5.616407	1.028179	0.002977	0.016111	0.007610
O	-3.378295	8.185194	5.338611	-0.002982	-0.015600	-0.007419
H	-0.637445	12.195109	2.878812	0.033933	0.145490	0.016719
H	3.090587	1.606491	3.487978	-0.033663	-0.144614	-0.016854
H	5.245016	5.294309	0.304583	-0.033972	0.145657	-0.016762
H	-2.791874	8.507292	6.062207	0.033619	-0.144419	0.016807

31 f = 30.434227 THz 191.223891 2PiTHz 1015.176524 cm-1 125.865893
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.003122	0.001548	-0.001919
Li	-1.316675	4.156264	2.365404	0.003131	0.001535	-0.001912
Li	-3.471104	2.744536	5.548798	-0.003129	0.001549	0.001922
Li	5.924247	11.057064	0.817991	-0.003127	0.001534	0.001907
Na	2.049025	6.784862	1.629696	-0.000714	-0.000173	0.000141
Na	0.404117	7.016739	4.737094	-0.000714	-0.000173	0.000144
Na	2.558546	13.685662	1.553699	0.000714	-0.000173	-0.000144
Na	-0.105403	0.115939	4.813091	0.000715	-0.000173	-0.000140
B	4.155007	8.978944	1.168663	0.048340	-0.030955	-0.056576
B	-1.701865	4.822656	5.198127	0.048396	-0.031096	-0.056658
B	0.452564	2.078144	2.014732	-0.048400	-0.030952	0.056538
B	2.000578	11.723457	4.352058	-0.048349	-0.031096	0.056674
B	-2.733891	11.746082	5.839177	-0.005907	-0.034727	0.043299
B	5.187034	2.055518	0.527613	-0.005820	-0.034641	0.043218
B	3.032605	4.845282	3.711007	0.005863	-0.034732	-0.043309
B	-0.579463	8.956318	2.655782	0.005843	-0.034637	-0.043213
B	-0.983708	0.054306	1.827988	0.000369	-0.000385	-0.000222
B	3.436850	13.747295	4.538802	0.000372	-0.000403	-0.000203
B	5.591279	6.955106	1.355407	-0.000371	-0.000393	0.000218
B	-3.138137	6.846495	5.011383	-0.000363	-0.000396	0.000212

Si	0.631772	3.486686	4.508512	-0.024564	-0.000973	-0.016296
Si	1.821370	10.314915	1.858278	-0.024565	-0.001000	-0.016302
Si	-0.333059	10.387486	5.041673	0.024580	-0.001001	0.016301
Si	2.786201	3.414115	1.325117	0.024547	-0.000963	0.016302
O	0.061445	3.072947	3.041906	0.013421	0.002741	0.015621
O	2.391697	10.728653	3.324884	0.013430	0.002770	0.015666
O	4.546126	9.973747	0.141489	-0.013430	0.002746	-0.015644
O	-2.092984	3.827853	6.225301	-0.013419	0.002764	-0.015640
O	2.197450	3.933608	4.519003	0.041700	0.012880	0.000042
O	0.255692	9.867992	1.847787	0.041696	0.012873	0.000039
O	-1.898737	10.834409	5.031182	-0.041719	0.012891	-0.000038
O	4.351879	2.967192	1.335608	-0.041662	0.012857	-0.000043
O	-0.212316	4.798696	5.055280	-0.016183	0.003434	0.008618
O	2.665458	9.002905	1.311510	-0.016163	0.003412	0.008607
O	0.511030	11.699496	4.494905	0.016164	0.003439	-0.008623
O	1.942113	2.102105	1.871885	0.016176	0.003404	-0.008602
O	0.525580	2.169271	5.472081	0.001455	-0.007153	-0.002844
O	1.927562	11.632329	0.894709	0.001464	-0.007097	-0.002916
O	-0.226867	9.070071	4.078104	-0.001463	-0.007123	0.002876
O	2.680009	4.731529	2.288686	-0.001460	-0.007135	0.002873
O	0.058846	0.698526	2.444964	0.026960	0.022078	0.004415
O	2.394296	13.103075	3.921826	0.026982	0.022139	0.004399
O	4.548725	7.599326	0.738431	-0.026946	0.022079	-0.004404
O	-2.095583	6.202275	5.628359	-0.026997	0.022139	-0.004410
O	-2.459230	13.184059	5.445139	-0.015861	0.021836	-0.027394
O	4.912372	0.617542	0.921651	-0.015835	0.021787	-0.027342
O	2.757943	6.283259	4.105046	0.015857	0.021840	0.027393
O	-0.304801	7.518342	2.261744	0.015836	0.021781	0.027339
O	-0.175430	2.374756	0.744070	0.013115	0.010058	-0.034650
O	2.628573	11.426844	5.622720	0.013150	0.010093	-0.034704
O	4.783002	9.275557	2.439325	-0.013124	0.010056	0.034648
O	-2.329859	4.526044	3.927465	-0.013120	0.010096	0.034723
O	-1.223866	12.517207	2.155216	-0.002253	-0.015502	0.008348
O	3.677009	1.284394	4.211574	-0.002239	-0.015509	0.008364
O	5.831438	5.616407	1.028179	0.002248	-0.015494	-0.008351
O	-3.378295	8.185194	5.338611	0.002246	-0.015520	-0.008359

H	-0.637445	12.195109	2.878812	0.002947	-0.070954	-0.020686
H	3.090587	1.606491	3.487978	0.002826	-0.071355	-0.020746
H	5.245016	5.294309	0.304583	-0.002905	-0.071064	0.020713
H	-2.791874	8.507292	6.062207	-0.002885	-0.071209	0.020716

32 f = 30.282151 THz 190.268369 2PiTHz 1010.103815 cm-1 125.236957 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000348	0.002491	-0.005873
Li	-1.316675	4.156264	2.365404	0.000339	-0.002494	0.005874
Li	-3.471104	2.744536	5.548798	-0.000342	-0.002489	-0.005868
Li	5.924247	11.057064	0.817991	0.000345	0.002495	0.005878
Na	2.049025	6.784862	1.629696	0.000138	0.000668	0.000109
Na	0.404117	7.016739	4.737094	-0.000140	-0.000672	-0.000121
Na	2.558546	13.685662	1.553699	0.000140	-0.000670	0.000121
Na	-0.105403	0.115939	4.813091	-0.000137	0.000670	-0.000108
B	4.155007	8.978944	1.168663	-0.054247	0.041711	0.005026
B	-1.701865	4.822656	5.198127	0.054256	-0.041710	-0.004972
B	0.452564	2.078144	2.014732	-0.054278	-0.041705	0.004944
B	2.000578	11.723457	4.352058	0.054225	0.041700	-0.005040
B	-2.733891	11.746082	5.839177	-0.017092	0.040257	-0.034266
B	5.187034	2.055518	0.527613	0.017073	-0.040263	0.034287
B	3.032605	4.845282	3.711007	-0.017083	-0.040245	-0.034290
B	-0.579463	8.956318	2.655782	0.017075	0.040281	0.034268
B	-0.983708	0.054306	1.827988	0.005494	0.010105	0.000347
B	3.436850	13.747295	4.538802	-0.005472	-0.010102	-0.000331
B	5.591279	6.955106	1.355407	0.005479	-0.010084	0.000344
B	-3.138137	6.846495	5.011383	-0.005487	0.010120	-0.000337
Si	0.631772	3.486686	4.508512	0.004223	0.019350	0.007560
Si	1.821370	10.314915	1.858278	-0.004203	-0.019326	-0.007518
Si	-0.333059	10.387486	5.041673	0.004212	-0.019327	0.007523
Si	2.786201	3.414115	1.325117	-0.004215	0.019349	-0.007553
O	0.061445	3.072947	3.041906	-0.000441	-0.013898	-0.027230
O	2.391697	10.728653	3.324884	0.000423	0.013871	0.027164
O	4.546126	9.973747	0.141489	-0.000427	0.013871	-0.027174
O	-2.092984	3.827853	6.225301	0.000438	-0.013895	0.027217

O	2.197450	3.933608	4.519003	-0.004824	-0.004027	0.004224
O	0.255692	9.867992	1.847787	0.004782	0.004001	-0.004212
O	-1.898737	10.834409	5.031182	-0.004798	0.004012	0.004219
O	4.351879	2.967192	1.335608	0.004812	-0.004017	-0.004218
O	-0.212316	4.798696	5.055280	0.001555	-0.005409	-0.001197
O	2.665458	9.002905	1.311510	-0.001526	0.005398	0.001188
O	0.511030	11.699496	4.494905	0.001531	0.005399	-0.001187
O	1.942113	2.102105	1.871885	-0.001552	-0.005412	0.001201
O	0.525580	2.169271	5.472081	-0.003081	-0.010503	0.005454
O	1.927562	11.632329	0.894709	0.003075	0.010503	-0.005476
O	-0.226867	9.070071	4.078104	-0.003076	0.010504	0.005469
O	2.680009	4.731529	2.288686	0.003078	-0.010499	-0.005460
O	0.058846	0.698526	2.444964	0.039324	0.039927	0.012372
O	2.394296	13.103075	3.921826	-0.039318	-0.039915	-0.012365
O	4.548725	7.599326	0.738431	0.039312	-0.039917	0.012361
O	-2.095583	6.202275	5.628359	-0.039330	0.039931	-0.012374
O	-2.459230	13.184059	5.445139	0.028861	-0.034914	0.037182
O	4.912372	0.617542	0.921651	-0.028881	0.034935	-0.037202
O	2.757943	6.283259	4.105046	0.028875	0.034918	0.037191
O	-0.304801	7.518342	2.261744	-0.028868	-0.034931	-0.037193
O	-0.175430	2.374756	0.744070	0.007355	0.009371	0.001323
O	2.628573	11.426844	5.622720	-0.007305	-0.009372	-0.001266
O	4.783002	9.275557	2.439325	0.007330	-0.009376	0.001275
O	-2.329859	4.526044	3.927465	-0.007332	0.009370	-0.001307
O	-1.223866	12.517207	2.155216	-0.004691	-0.030511	0.007453
O	3.677009	1.284394	4.211574	0.004699	0.030505	-0.007444
O	5.831438	5.616407	1.028179	-0.004690	0.030490	0.007447
O	-3.378295	8.185194	5.338611	0.004699	-0.030526	-0.007450
H	-0.637445	12.195109	2.878812	-0.004129	-0.080642	-0.006261
H	3.090587	1.606491	3.487978	0.004122	0.080530	0.006235
H	5.245016	5.294309	0.304583	-0.004150	0.080626	-0.006249
H	-2.791874	8.507292	6.062207	0.004107	-0.080556	0.006247

33 f = 29.449967 THz 185.039603 2PiTHz 982.345144 cm-1 121.795319
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.000523	-0.000049	-0.002560
Li	-1.316675	4.156264	2.365404	-0.000530	0.000054	0.002563
Li	-3.471104	2.744536	5.548798	0.000529	0.000052	-0.002563
Li	5.924247	11.057064	0.817991	-0.000528	-0.000051	0.002557
Na	2.049025	6.784862	1.629696	-0.000941	-0.000513	-0.000776
Na	0.404117	7.016739	4.737094	0.000941	0.000515	0.000780
Na	2.558546	13.685662	1.553699	-0.000942	0.000513	-0.000780
Na	-0.105403	0.115939	4.813091	0.000939	-0.000515	0.000776
B	4.155007	8.978944	1.168663	0.044228	0.033405	-0.044628
B	-1.701865	4.822656	5.198127	-0.044179	-0.033390	0.044701
B	0.452564	2.078144	2.014732	0.044236	-0.033412	-0.044625
B	2.000578	11.723457	4.352058	-0.044182	0.033371	0.044691
B	-2.733891	11.746082	5.839177	-0.019893	0.023086	0.052986
B	5.187034	2.055518	0.527613	0.019856	-0.023094	-0.052974
B	3.032605	4.845282	3.711007	-0.019845	-0.023091	0.053015
B	-0.579463	8.956318	2.655782	0.019876	0.023088	-0.052932
B	-0.983708	0.054306	1.827988	0.004895	0.003653	-0.003788
B	3.436850	13.747295	4.538802	-0.004901	-0.003656	0.003797
B	5.591279	6.955106	1.355407	0.004890	-0.003641	-0.003788
B	-3.138137	6.846495	5.011383	-0.004909	0.003668	0.003794
Si	0.631772	3.486686	4.508512	0.038330	-0.011460	0.024078
Si	1.821370	10.314915	1.858278	-0.038317	0.011478	-0.024064
Si	-0.333059	10.387486	5.041673	0.038327	0.011470	0.024074
Si	2.786201	3.414115	1.325117	-0.038311	-0.011481	-0.024066
O	0.061445	3.072947	3.041906	-0.022602	0.004768	-0.021555
O	2.391697	10.728653	3.324884	0.022593	-0.004759	0.021554
O	4.546126	9.973747	0.141489	-0.022605	-0.004773	-0.021543
O	-2.092984	3.827853	6.225301	0.022587	0.004762	0.021546
O	2.197450	3.933608	4.519003	-0.044699	-0.005359	-0.008426
O	0.255692	9.867992	1.847787	0.044641	0.005322	0.008440
O	-1.898737	10.834409	5.031182	-0.044676	0.005346	-0.008431
O	4.351879	2.967192	1.335608	0.044634	-0.005319	0.008440
O	-0.212316	4.798696	5.055280	-0.001295	0.017231	-0.002828
O	2.665458	9.002905	1.311510	0.001339	-0.017262	0.002812
O	0.511030	11.699496	4.494905	-0.001314	-0.017226	-0.002832
O	1.942113	2.102105	1.871885	0.001327	0.017270	0.002809

O	0.525580	2.169271	5.472081	-0.001997	0.022706	-0.002560
O	1.927562	11.632329	0.894709	0.001999	-0.022688	0.002523
O	-0.226867	9.070071	4.078104	-0.002001	-0.022716	-0.002580
O	2.680009	4.731529	2.288686	0.002000	0.022690	0.002519
O	0.058846	0.698526	2.444964	-0.007577	0.009404	0.002652
O	2.394296	13.103075	3.921826	0.007538	-0.009417	-0.002672
O	4.548725	7.599326	0.738431	-0.007581	-0.009395	0.002645
O	-2.095583	6.202275	5.628359	0.007531	0.009430	-0.002677
O	-2.459230	13.184059	5.445139	0.001342	-0.011475	-0.006769
O	4.912372	0.617542	0.921651	-0.001310	0.011439	0.006798
O	2.757943	6.283259	4.105046	0.001353	0.011476	-0.006763
O	-0.304801	7.518342	2.261744	-0.001300	-0.011439	0.006804
O	-0.175430	2.374756	0.744070	-0.021530	0.003178	0.028539
O	2.628573	11.426844	5.622720	0.021527	-0.003172	-0.028561
O	4.783002	9.275557	2.439325	-0.021533	-0.003181	0.028519
O	-2.329859	4.526044	3.927465	0.021504	0.003171	-0.028591
O	-1.223866	12.517207	2.155216	-0.001735	-0.003794	0.005030
O	3.677009	1.284394	4.211574	0.001746	0.003829	-0.005038
O	5.831438	5.616407	1.028179	-0.001738	0.003790	0.005026
O	-3.378295	8.185194	5.338611	0.001743	-0.003834	-0.005039
H	-0.637445	12.195109	2.878812	0.031656	-0.034164	-0.037912
H	3.090587	1.606491	3.487978	-0.031690	0.034195	0.037933
H	5.245016	5.294309	0.304583	0.031660	0.034113	-0.037893
H	-2.791874	8.507292	6.062207	-0.031682	-0.034255	0.037952

34 f = 29.090305 THz 182.779777 2PiTHz 970.348100 cm-1 120.307875
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.001019	-0.000575	-0.000657
Li	-1.316675	4.156264	2.365404	-0.001017	-0.000581	-0.000649
Li	-3.471104	2.744536	5.548798	-0.001015	0.000581	-0.000655
Li	5.924247	11.057064	0.817991	-0.001018	0.000577	-0.000652
Na	2.049025	6.784862	1.629696	0.000341	-0.000221	0.000113
Na	0.404117	7.016739	4.737094	0.000343	-0.000222	0.000107
Na	2.558546	13.685662	1.553699	0.000342	0.000223	0.000106
Na	-0.105403	0.115939	4.813091	0.000342	0.000220	0.000114

B	4.155007	8.978944	1.168663	-0.048906	0.001057	-0.046501
B	-1.701865	4.822656	5.198127	-0.048917	0.000975	-0.046444
B	0.452564	2.078144	2.014732	-0.048837	-0.001025	-0.046480
B	2.000578	11.723457	4.352058	-0.048963	-0.001008	-0.046489
B	-2.733891	11.746082	5.839177	-0.030471	-0.000908	-0.021973
B	5.187034	2.055518	0.527613	-0.030384	-0.000935	-0.021992
B	3.032605	4.845282	3.711007	-0.030407	0.000891	-0.021928
B	-0.579463	8.956318	2.655782	-0.030444	0.000952	-0.022019
B	-0.983708	0.054306	1.827988	0.000023	0.007091	-0.004336
B	3.436850	13.747295	4.538802	0.000012	0.007085	-0.004337
B	5.591279	6.955106	1.355407	0.000019	-0.007086	-0.004338
B	-3.138137	6.846495	5.011383	0.000017	-0.007088	-0.004333
Si	0.631772	3.486686	4.508512	-0.021729	-0.008096	-0.021239
Si	1.821370	10.314915	1.858278	-0.021798	-0.008081	-0.021301
Si	-0.333059	10.387486	5.041673	-0.021763	0.008114	-0.021272
Si	2.786201	3.414115	1.325117	-0.021767	0.008068	-0.021266
O	0.061445	3.072947	3.041906	0.010735	0.015638	0.036319
O	2.391697	10.728653	3.324884	0.010781	0.015671	0.036421
O	4.546126	9.973747	0.141489	0.010753	-0.015680	0.036399
O	-2.092984	3.827853	6.225301	0.010764	-0.015623	0.036332
O	2.197450	3.933608	4.519003	0.046807	0.027002	-0.012839
O	0.255692	9.867992	1.847787	0.046884	0.027019	-0.012832
O	-1.898737	10.834409	5.031182	0.046860	-0.027026	-0.012850
O	4.351879	2.967192	1.335608	0.046840	-0.026998	-0.012825
O	-0.212316	4.798696	5.055280	0.002701	0.008097	-0.000025
O	2.665458	9.002905	1.311510	0.002731	0.008065	-0.000038
O	0.511030	11.699496	4.494905	0.002717	-0.008095	-0.000034
O	1.942113	2.102105	1.871885	0.002703	-0.008074	-0.000022
O	0.525580	2.169271	5.472081	-0.002991	-0.018516	0.033473
O	1.927562	11.632329	0.894709	-0.002991	-0.018570	0.033524
O	-0.226867	9.070071	4.078104	-0.002992	0.018520	0.033492
O	2.680009	4.731529	2.288686	-0.002990	0.018560	0.033492
O	0.058846	0.698526	2.444964	0.022552	0.012212	0.009089
O	2.394296	13.103075	3.921826	0.022571	0.012197	0.009089
O	4.548725	7.599326	0.738431	0.022562	-0.012213	0.009088
O	-2.095583	6.202275	5.628359	0.022562	-0.012196	0.009088

O	-2.459230	13.184059	5.445139	-0.012610	0.020063	-0.014408
O	4.912372	0.617542	0.921651	-0.012616	0.020072	-0.014406
O	2.757943	6.283259	4.105046	-0.012616	-0.020049	-0.014410
O	-0.304801	7.518342	2.261744	-0.012613	-0.020080	-0.014403
O	-0.175430	2.374756	0.744070	0.026282	-0.002885	0.028739
O	2.628573	11.426844	5.622720	0.026352	-0.002887	0.028729
O	4.783002	9.275557	2.439325	0.026323	0.002880	0.028746
O	-2.329859	4.526044	3.927465	0.026315	0.002892	0.028710
O	-1.223866	12.517207	2.155216	-0.001709	-0.019998	0.005744
O	3.677009	1.284394	4.211574	-0.001707	-0.019987	0.005737
O	5.831438	5.616407	1.028179	-0.001707	0.019994	0.005745
O	-3.378295	8.185194	5.338611	-0.001706	0.019987	0.005736
H	-0.637445	12.195109	2.878812	-0.002696	-0.013867	0.007776
H	3.090587	1.606491	3.487978	-0.002724	-0.013853	0.007803
H	5.245016	5.294309	0.304583	-0.002680	0.013904	0.007752
H	-2.791874	8.507292	6.062207	-0.002745	0.013829	0.007824

35 f = 29.039522 THz 182.460697 2PiTHz 968.654153 cm-1 120.097852 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001141	-0.001999	0.001704
Li	-1.316675	4.156264	2.365404	-0.001141	0.001995	-0.001701
Li	-3.471104	2.744536	5.548798	-0.001142	-0.001993	-0.001701
Li	5.924247	11.057064	0.817991	0.001137	0.001998	0.001703
Na	2.049025	6.784862	1.629696	-0.000019	-0.001056	0.000505
Na	0.404117	7.016739	4.737094	0.000022	0.001056	-0.000495
Na	2.558546	13.685662	1.553699	0.000021	-0.001056	-0.000495
Na	-0.105403	0.115939	4.813091	-0.000019	0.001056	0.000505
B	4.155007	8.978944	1.168663	0.045648	-0.007275	0.048331
B	-1.701865	4.822656	5.198127	-0.045741	0.007237	-0.048398
B	0.452564	2.078144	2.014732	-0.045702	-0.007246	-0.048407
B	2.000578	11.723457	4.352058	0.045657	0.007274	0.048355
B	-2.733891	11.746082	5.839177	0.032983	0.004582	0.021106
B	5.187034	2.055518	0.527613	-0.033007	-0.004580	-0.021116
B	3.032605	4.845282	3.711007	-0.033027	0.004572	-0.021091
B	-0.579463	8.956318	2.655782	0.032954	-0.004586	0.021101

B	-0.983708	0.054306	1.827988	0.001063	0.006554	-0.004637
B	3.436850	13.747295	4.538802	-0.001061	-0.006559	0.004641
B	5.591279	6.955106	1.355407	-0.001060	0.006552	0.004638
B	-3.138137	6.846495	5.011383	0.001064	-0.006556	-0.004635
Si	0.631772	3.486686	4.508512	-0.022462	-0.007585	-0.020218
Si	1.821370	10.314915	1.858278	0.022453	0.007555	0.020199
Si	-0.333059	10.387486	5.041673	0.022447	-0.007567	0.020186
Si	2.786201	3.414115	1.325117	-0.022477	0.007576	-0.020231
O	0.061445	3.072947	3.041906	0.010064	0.017744	0.038866
O	2.391697	10.728653	3.324884	-0.010058	-0.017727	-0.038825
O	4.546126	9.973747	0.141489	-0.010050	0.017717	-0.038802
O	-2.092984	3.827853	6.225301	0.010076	-0.017743	0.038876
O	2.197450	3.933608	4.519003	0.047142	0.026150	-0.012535
O	0.255692	9.867992	1.847787	-0.047103	-0.026119	0.012517
O	-1.898737	10.834409	5.031182	-0.047107	0.026125	0.012526
O	4.351879	2.967192	1.335608	0.047154	-0.026147	-0.012529
O	-0.212316	4.798696	5.055280	0.002999	0.005180	-0.001271
O	2.665458	9.002905	1.311510	-0.003009	-0.005144	0.001278
O	0.511030	11.699496	4.494905	-0.002998	0.005155	0.001273
O	1.942113	2.102105	1.871885	0.003000	-0.005172	-0.001269
O	0.525580	2.169271	5.472081	-0.003109	-0.016626	0.030745
O	1.927562	11.632329	0.894709	0.003103	0.016629	-0.030742
O	-0.226867	9.070071	4.078104	0.003105	-0.016611	-0.030719
O	2.680009	4.731529	2.288686	-0.003108	0.016641	0.030751
O	0.058846	0.698526	2.444964	0.022082	0.012546	0.009667
O	2.394296	13.103075	3.921826	-0.022068	-0.012553	-0.009657
O	4.548725	7.599326	0.738431	-0.022061	0.012551	-0.009654
O	-2.095583	6.202275	5.628359	0.022089	-0.012546	0.009665
O	-2.459230	13.184059	5.445139	0.012762	-0.020476	0.014521
O	4.912372	0.617542	0.921651	-0.012779	0.020485	-0.014531
O	2.757943	6.283259	4.105046	-0.012780	-0.020483	-0.014537
O	-0.304801	7.518342	2.261744	0.012762	0.020466	0.014513
O	-0.175430	2.374756	0.744070	0.027856	-0.001069	0.028726
O	2.628573	11.426844	5.622720	-0.027817	0.001074	-0.028704
O	4.783002	9.275557	2.439325	-0.027800	-0.001071	-0.028692
O	-2.329859	4.526044	3.927465	0.027879	0.001073	0.028721

O	-1.223866	12.517207	2.155216	-0.003296	-0.018582	0.004923
O	3.677009	1.284394	4.211574	0.003299	0.018576	-0.004922
O	5.831438	5.616407	1.028179	0.003298	-0.018567	-0.004916
O	-3.378295	8.185194	5.338611	-0.003296	0.018582	0.004925
H	-0.637445	12.195109	2.878812	0.005429	-0.020779	0.001448
H	3.090587	1.606491	3.487978	-0.005472	0.020761	-0.001420
H	5.245016	5.294309	0.304583	-0.005450	-0.020744	-0.001439
H	-2.791874	8.507292	6.062207	0.005436	0.020795	0.001437

36 f = 28.791484 THz 180.902228 2PiTHz 960.380495 cm-1 119.072049 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002032	0.004485	-0.000686
Li	-1.316675	4.156264	2.365404	-0.002042	0.004540	-0.000675
Li	-3.471104	2.744536	5.548798	-0.002043	-0.004540	-0.000671
Li	5.924247	11.057064	0.817991	-0.002026	-0.004483	-0.000690
Na	2.049025	6.784862	1.629696	-0.000088	0.000523	-0.000159
Na	0.404117	7.016739	4.737094	-0.000095	0.000530	-0.000151
Na	2.558546	13.685662	1.553699	-0.000094	-0.000530	-0.000150
Na	-0.105403	0.115939	4.813091	-0.000089	-0.000522	-0.000159
B	4.155007	8.978944	1.168663	0.010685	0.010760	0.006961
B	-1.701865	4.822656	5.198127	0.010834	0.010990	0.007052
B	0.452564	2.078144	2.014732	0.010768	-0.010947	0.007053
B	2.000578	11.723457	4.352058	0.010740	-0.010805	0.006926
B	-2.733891	11.746082	5.839177	-0.030326	-0.021037	-0.038508
B	5.187034	2.055518	0.527613	-0.030590	-0.021304	-0.039133
B	3.032605	4.845282	3.711007	-0.030565	0.021351	-0.039161
B	-0.579463	8.956318	2.655782	-0.030319	0.021001	-0.038466
B	-0.983708	0.054306	1.827988	-0.002904	-0.010669	0.002616
B	3.436850	13.747295	4.538802	-0.002841	-0.010514	0.002605
B	5.591279	6.955106	1.355407	-0.002848	0.010520	0.002606
B	-3.138137	6.846495	5.011383	-0.002895	0.010669	0.002618
Si	0.631772	3.486686	4.508512	-0.011158	-0.016443	-0.015451
Si	1.821370	10.314915	1.858278	-0.011138	-0.016454	-0.015235
Si	-0.333059	10.387486	5.041673	-0.011150	0.016436	-0.015235
Si	2.786201	3.414115	1.325117	-0.011143	0.016476	-0.015432

O	0.061445	3.072947	3.041906	0.008642	0.035203	0.063483
O	2.391697	10.728653	3.324884	0.008551	0.034845	0.062876
O	4.546126	9.973747	0.141489	0.008560	-0.034816	0.062837
O	-2.092984	3.827853	6.225301	0.008625	-0.035215	0.063486
O	2.197450	3.933608	4.519003	-0.009264	-0.012667	0.011974
O	0.255692	9.867992	1.847787	-0.008814	-0.012389	0.011769
O	-1.898737	10.834409	5.031182	-0.008807	0.012397	0.011782
O	4.351879	2.967192	1.335608	-0.009259	0.012649	0.011955
O	-0.212316	4.798696	5.055280	0.014977	-0.007298	-0.011094
O	2.665458	9.002905	1.311510	0.014734	-0.007131	-0.010946
O	0.511030	11.699496	4.494905	0.014730	0.007139	-0.010944
O	1.942113	2.102105	1.871885	0.014975	0.007278	-0.011092
O	0.525580	2.169271	5.472081	0.005908	0.027184	-0.016146
O	1.927562	11.632329	0.894709	0.005809	0.027126	-0.016285
O	-0.226867	9.070071	4.078104	0.005810	-0.027109	-0.016277
O	2.680009	4.731529	2.288686	0.005903	-0.027230	-0.016189
O	0.058846	0.698526	2.444964	-0.027567	-0.026138	-0.015492
O	2.394296	13.103075	3.921826	-0.027316	-0.025889	-0.015362
O	4.548725	7.599326	0.738431	-0.027316	0.025905	-0.015365
O	-2.095583	6.202275	5.628359	-0.027574	0.026122	-0.015492
O	-2.459230	13.184059	5.445139	0.023925	-0.020574	0.032034
O	4.912372	0.617542	0.921651	0.024137	-0.020727	0.032279
O	2.757943	6.283259	4.105046	0.024129	0.020711	0.032276
O	-0.304801	7.518342	2.261744	0.023933	0.020593	0.032040
O	-0.175430	2.374756	0.744070	0.016315	0.005939	-0.009617
O	2.628573	11.426844	5.622720	0.016135	0.005888	-0.009470
O	4.783002	9.275557	2.439325	0.016138	-0.005883	-0.009486
O	-2.329859	4.526044	3.927465	0.016296	-0.005947	-0.009616
O	-1.223866	12.517207	2.155216	0.003380	0.027086	-0.008754
O	3.677009	1.284394	4.211574	0.003323	0.026788	-0.008698
O	5.831438	5.616407	1.028179	0.003325	-0.026804	-0.008705
O	-3.378295	8.185194	5.338611	0.003378	-0.027078	-0.008748
H	-0.637445	12.195109	2.878812	-0.008833	0.063873	0.014986
H	3.090587	1.606491	3.487978	-0.008907	0.063946	0.015224
H	5.245016	5.294309	0.304583	-0.008945	-0.063973	0.015259
H	-2.791874	8.507292	6.062207	-0.008797	-0.063832	0.014943

37 f = 28.773679 THz 180.790358 2PiTHz 959.786596 cm-1 118.998414
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001306	-0.004463	-0.001172
Li	-1.316675	4.156264	2.365404	-0.001285	0.004404	0.001175
Li	-3.471104	2.744536	5.548798	-0.001286	-0.004406	0.001174
Li	5.924247	11.057064	0.817991	0.001302	0.004460	-0.001173
Na	2.049025	6.784862	1.629696	0.000193	-0.000708	0.000420
Na	0.404117	7.016739	4.737094	-0.000196	0.000701	-0.000423
Na	2.558546	13.685662	1.553699	-0.000196	-0.000703	-0.000423
Na	-0.105403	0.115939	4.813091	0.000193	0.000707	0.000420
B	4.155007	8.978944	1.168663	-0.005485	-0.014215	-0.012172
B	-1.701865	4.822656	5.198127	0.005407	0.014114	0.012022
B	0.452564	2.078144	2.014732	0.005358	-0.014092	0.012031
B	2.000578	11.723457	4.352058	-0.005519	0.014252	-0.012134
B	-2.733891	11.746082	5.839177	0.028111	0.028761	0.054295
B	5.187034	2.055518	0.527613	-0.027829	-0.028471	-0.053696
B	3.032605	4.845282	3.711007	-0.027822	0.028488	-0.053730
B	-0.579463	8.956318	2.655782	0.028091	-0.028743	0.054238
B	-0.983708	0.054306	1.827988	-0.004277	-0.014680	0.002757
B	3.436850	13.747295	4.538802	0.004315	0.014798	-0.002778
B	5.591279	6.955106	1.355407	0.004315	-0.014799	-0.002781
B	-3.138137	6.846495	5.011383	-0.004276	0.014683	0.002757
Si	0.631772	3.486686	4.508512	-0.001755	-0.004661	-0.019307
Si	1.821370	10.314915	1.858278	0.001844	0.004817	0.019472
Si	-0.333059	10.387486	5.041673	0.001853	-0.004809	0.019468
Si	2.786201	3.414115	1.325117	-0.001748	0.004675	-0.019296
O	0.061445	3.072947	3.041906	0.008675	0.034095	0.058364
O	2.391697	10.728653	3.324884	-0.008768	-0.034491	-0.059039
O	4.546126	9.973747	0.141489	-0.008772	0.034465	-0.059008
O	-2.092984	3.827853	6.225301	0.008666	-0.034103	0.058363
O	2.197450	3.933608	4.519003	-0.035787	-0.022555	0.016577
O	0.255692	9.867992	1.847787	0.036007	0.022743	-0.016732
O	-1.898737	10.834409	5.031182	0.035991	-0.022746	-0.016744
O	4.351879	2.967192	1.335608	-0.035789	0.022546	0.016568

O	-0.212316	4.798696	5.055280	0.020364	-0.011649	-0.013014
O	2.665458	9.002905	1.311510	-0.020574	0.011745	0.013150
O	0.511030	11.699496	4.494905	-0.020570	-0.011752	0.013145
O	1.942113	2.102105	1.871885	0.020371	0.011643	-0.013018
O	0.525580	2.169271	5.472081	0.008329	0.011844	0.004620
O	1.927562	11.632329	0.894709	-0.008413	-0.012121	-0.004527
O	-0.226867	9.070071	4.078104	-0.008410	0.012124	-0.004505
O	2.680009	4.731529	2.288686	0.008330	-0.011859	0.004615
O	0.058846	0.698526	2.444964	-0.023737	-0.022360	-0.013086
O	2.394296	13.103075	3.921826	0.024039	0.022627	0.013255
O	4.548725	7.599326	0.738431	0.024047	-0.022642	0.013261
O	-2.095583	6.202275	5.628359	-0.023739	0.022351	-0.013083
O	-2.459230	13.184059	5.445139	-0.019653	0.013113	-0.022771
O	4.912372	0.617542	0.921651	0.019386	-0.012899	0.022413
O	2.757943	6.283259	4.105046	0.019382	0.012889	0.022411
O	-0.304801	7.518342	2.261744	-0.019659	-0.013130	-0.022778
O	-0.175430	2.374756	0.744070	0.018628	0.005444	-0.011900
O	2.628573	11.426844	5.622720	-0.018765	-0.005507	0.012014
O	4.783002	9.275557	2.439325	-0.018766	0.005508	0.012032
O	-2.329859	4.526044	3.927465	0.018612	-0.005445	-0.011898
O	-1.223866	12.517207	2.155216	0.005283	0.027560	-0.004815
O	3.677009	1.284394	4.211574	-0.005315	-0.027841	0.004912
O	5.831438	5.616407	1.028179	-0.005317	0.027856	0.004913
O	-3.378295	8.185194	5.338611	0.005282	-0.027555	-0.004815
H	-0.637445	12.195109	2.878812	0.009917	-0.008555	-0.025063
H	3.090587	1.606491	3.487978	-0.009804	0.007805	0.024856
H	5.245016	5.294309	0.304583	-0.009817	-0.007806	0.024879
H	-2.791874	8.507292	6.062207	0.009908	0.008557	-0.025051

38 f = 28.699607 THz 180.324950 2PiTHz 957.315821 cm-1 118.692077 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002932	-0.002400	-0.002912
Li	-1.316675	4.156264	2.365404	0.002914	0.002384	0.002887
Li	-3.471104	2.744536	5.548798	0.002917	-0.002383	0.002891
Li	5.924247	11.057064	0.817991	-0.002926	0.002405	-0.002909

Na	2.049025	6.784862	1.629696	0.000506	-0.000769	0.000262
Na	0.404117	7.016739	4.737094	-0.000506	0.000775	-0.000252
Na	2.558546	13.685662	1.553699	-0.000506	-0.000774	-0.000251
Na	-0.105403	0.115939	4.813091	0.000506	0.000771	0.000262
B	4.155007	8.978944	1.168663	0.012610	-0.000047	0.004565
B	-1.701865	4.822656	5.198127	-0.012564	-0.000032	-0.004547
B	0.452564	2.078144	2.014732	-0.012545	0.000002	-0.004599
B	2.000578	11.723457	4.352058	0.012667	0.000004	0.004501
B	-2.733891	11.746082	5.839177	-0.030108	0.006712	0.056300
B	5.187034	2.055518	0.527613	0.030029	-0.006600	-0.055815
B	3.032605	4.845282	3.711007	0.030062	0.006595	-0.055763
B	-0.579463	8.956318	2.655782	-0.030094	-0.006721	0.056366
B	-0.983708	0.054306	1.827988	-0.002222	0.006698	-0.008168
B	3.436850	13.747295	4.538802	0.002256	-0.006700	0.008203
B	5.591279	6.955106	1.355407	0.002257	0.006705	0.008210
B	-3.138137	6.846495	5.011383	-0.002219	-0.006699	-0.008163
Si	0.631772	3.486686	4.508512	0.015385	0.028847	-0.004563
Si	1.821370	10.314915	1.858278	-0.015490	-0.029015	0.004673
Si	-0.333059	10.387486	5.041673	-0.015497	0.029019	0.004683
Si	2.786201	3.414115	1.325117	0.015390	-0.028846	-0.004539
O	0.061445	3.072947	3.041906	-0.002438	-0.007810	-0.023112
O	2.391697	10.728653	3.324884	0.002412	0.007767	0.023082
O	4.546126	9.973747	0.141489	0.002419	-0.007732	0.023036
O	-2.092984	3.827853	6.225301	-0.002442	0.007846	-0.023173
O	2.197450	3.933608	4.519003	-0.047730	-0.017708	0.010064
O	0.255692	9.867992	1.847787	0.048170	0.017906	-0.010193
O	-1.898737	10.834409	5.031182	0.048185	-0.017904	-0.010188
O	4.351879	2.967192	1.335608	-0.047725	0.017710	0.010071
O	-0.212316	4.798696	5.055280	0.013812	-0.005791	-0.001067
O	2.665458	9.002905	1.311510	-0.013949	0.005846	0.001108
O	0.511030	11.699496	4.494905	-0.013969	-0.005853	0.001123
O	1.942113	2.102105	1.871885	0.013805	0.005788	-0.001060
O	0.525580	2.169271	5.472081	0.005424	-0.042411	0.063077
O	1.927562	11.632329	0.894709	-0.005489	0.042645	-0.063479
O	-0.226867	9.070071	4.078104	-0.005493	-0.042664	-0.063522
O	2.680009	4.731529	2.288686	0.005421	0.042387	0.063036

O	0.058846	0.698526	2.444964	0.015038	0.013010	0.009452
O	2.394296	13.103075	3.921826	-0.015055	-0.013009	-0.009451
O	4.548725	7.599326	0.738431	-0.015063	0.013024	-0.009460
O	-2.095583	6.202275	5.628359	0.015028	-0.013003	0.009444
O	-2.459230	13.184059	5.445139	0.011177	-0.010857	0.013347
O	4.912372	0.617542	0.921651	-0.011193	0.010872	-0.013360
O	2.757943	6.283259	4.105046	-0.011188	-0.010861	-0.013352
O	-0.304801	7.518342	2.261744	0.011184	0.010873	0.013352
O	-0.175430	2.374756	0.744070	-0.008874	-0.004141	0.003060
O	2.628573	11.426844	5.622720	0.008852	0.004153	-0.003014
O	4.783002	9.275557	2.439325	0.008856	-0.004153	-0.003031
O	-2.329859	4.526044	3.927465	-0.008891	0.004140	0.003049
O	-1.223866	12.517207	2.155216	-0.002803	-0.016804	0.004642
O	3.677009	1.284394	4.211574	0.002809	0.016818	-0.004635
O	5.831438	5.616407	1.028179	0.002813	-0.016836	-0.004637
O	-3.378295	8.185194	5.338611	-0.002801	0.016794	0.004641
H	-0.637445	12.195109	2.878812	0.004491	-0.011976	0.001903
H	3.090587	1.606491	3.487978	-0.004457	0.011814	-0.001992
H	5.245016	5.294309	0.304583	-0.004466	-0.011813	-0.001997
H	-2.791874	8.507292	6.062207	0.004492	0.011967	0.001897

39 f = 28.694290 THz 180.291542 2PiTHz 957.138461 cm-1 118.670087 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002109	-0.002411	-0.003015
Li	-1.316675	4.156264	2.365404	-0.002124	-0.002436	-0.003037
Li	-3.471104	2.744536	5.548798	-0.002131	0.002436	-0.003041
Li	5.924247	11.057064	0.817991	-0.002101	0.002413	-0.003012
Na	2.049025	6.784862	1.629696	-0.000229	0.000582	-0.000172
Na	0.404117	7.016739	4.737094	-0.000226	0.000575	-0.000164
Na	2.558546	13.685662	1.553699	-0.000226	-0.000575	-0.000163
Na	-0.105403	0.115939	4.813091	-0.000229	-0.000582	-0.000173
B	4.155007	8.978944	1.168663	0.010316	-0.003978	-0.003837
B	-1.701865	4.822656	5.198127	0.010449	-0.003945	-0.003877
B	0.452564	2.078144	2.014732	0.010430	0.003979	-0.003812
B	2.000578	11.723457	4.352058	0.010365	0.003948	-0.003905

B	-2.733891	11.746082	5.839177	-0.016865	0.012813	0.067622
B	5.187034	2.055518	0.527613	-0.016995	0.012925	0.068202
B	3.032605	4.845282	3.711007	-0.017055	-0.012922	0.068128
B	-0.579463	8.956318	2.655782	-0.016825	-0.012815	0.067692
B	-0.983708	0.054306	1.827988	0.004933	-0.001880	0.006079
B	3.436850	13.747295	4.538802	0.004912	-0.001841	0.006014
B	5.591279	6.955106	1.355407	0.004912	0.001855	0.006024
B	-3.138137	6.846495	5.011383	0.004932	0.001870	0.006070
Si	0.631772	3.486686	4.508512	-0.015409	-0.025373	0.013446
Si	1.821370	10.314915	1.858278	-0.015310	-0.025160	0.013341
Si	-0.333059	10.387486	5.041673	-0.015302	0.025174	0.013368
Si	2.786201	3.414115	1.325117	-0.015422	0.025366	0.013407
O	0.061445	3.072947	3.041906	-0.001744	-0.005431	-0.001538
O	2.391697	10.728653	3.324884	-0.001738	-0.005391	-0.001536
O	4.546126	9.973747	0.141489	-0.001741	0.005429	-0.001599
O	-2.092984	3.827853	6.225301	-0.001733	0.005384	-0.001455
O	2.197450	3.933608	4.519003	0.059772	0.025189	-0.015062
O	0.255692	9.867992	1.847787	0.059353	0.025020	-0.014962
O	-1.898737	10.834409	5.031182	0.059357	-0.025019	-0.014962
O	4.351879	2.967192	1.335608	0.059769	-0.025189	-0.015068
O	-0.212316	4.798696	5.055280	-0.019331	0.007775	0.005281
O	2.665458	9.002905	1.311510	-0.019173	0.007710	0.005242
O	0.511030	11.699496	4.494905	-0.019206	-0.007728	0.005259
O	1.942113	2.102105	1.871885	-0.019316	-0.007767	0.005271
O	0.525580	2.169271	5.472081	-0.008229	0.036974	-0.060943
O	1.927562	11.632329	0.894709	-0.008168	0.036641	-0.060393
O	-0.226867	9.070071	4.078104	-0.008174	-0.036681	-0.060461
O	2.680009	4.731529	2.288686	-0.008224	-0.036931	-0.060872
O	0.058846	0.698526	2.444964	-0.006698	-0.004526	-0.003639
O	2.394296	13.103075	3.921826	-0.006602	-0.004455	-0.003576
O	4.548725	7.599326	0.738431	-0.006615	0.004469	-0.003586
O	-2.095583	6.202275	5.628359	-0.006681	0.004513	-0.003630
O	-2.459230	13.184059	5.445139	0.001928	-0.002572	0.003199
O	4.912372	0.617542	0.921651	0.001996	-0.002665	0.003285
O	2.757943	6.283259	4.105046	0.001989	0.002643	0.003272
O	-0.304801	7.518342	2.261744	0.001935	0.002594	0.003212

O	-0.175430	2.374756	0.744070	0.001757	0.002544	0.004175
O	2.628573	11.426844	5.622720	0.001751	0.002514	0.004213
O	4.783002	9.275557	2.439325	0.001741	-0.002519	0.004190
O	-2.329859	4.526044	3.927465	0.001784	-0.002540	0.004197
O	-1.223866	12.517207	2.155216	0.001694	0.007537	-0.000464
O	3.677009	1.284394	4.211574	0.001680	0.007423	-0.000428
O	5.831438	5.616407	1.028179	0.001681	-0.007450	-0.000434
O	-3.378295	8.185194	5.338611	0.001692	-0.007512	-0.000457
H	-0.637445	12.195109	2.878812	0.002913	-0.015023	-0.011804
H	3.090587	1.606491	3.487978	0.002947	-0.015124	-0.011795
H	5.245016	5.294309	0.304583	0.002964	0.015135	-0.011831
H	-2.791874	8.507292	6.062207	0.002901	0.015021	-0.011778

40 f = 28.593174 THz 179.656213 2PiTHz 953.765607 cm-1 118.251907 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004325	0.000615	-0.002534
Li	-1.316675	4.156264	2.365404	-0.004651	0.000681	-0.002733
Li	-3.471104	2.744536	5.548798	0.004649	0.000687	0.002730
Li	5.924247	11.057064	0.817991	0.004328	0.000614	0.002537
Na	2.049025	6.784862	1.629696	-0.000106	0.000717	-0.000486
Na	0.404117	7.016739	4.737094	-0.000090	0.000721	-0.000444
Na	2.558546	13.685662	1.553699	0.000090	0.000721	0.000444
Na	-0.105403	0.115939	4.813091	0.000106	0.000717	0.000486
B	4.155007	8.978944	1.168663	0.003977	-0.002266	0.045945
B	-1.701865	4.822656	5.198127	0.003362	-0.003502	0.049495
B	0.452564	2.078144	2.014732	-0.003372	-0.003495	-0.049492
B	2.000578	11.723457	4.352058	-0.003957	-0.002260	-0.045940
B	-2.733891	11.746082	5.839177	-0.039189	0.009715	-0.026229
B	5.187034	2.055518	0.527613	-0.041684	0.009625	-0.028952
B	3.032605	4.845282	3.711007	0.041641	0.009614	0.029022
B	-0.579463	8.956318	2.655782	0.039249	0.009705	0.026214
B	-0.983708	0.054306	1.827988	-0.001742	0.006443	-0.005407
B	3.436850	13.747295	4.538802	-0.001724	0.006074	-0.005066
B	5.591279	6.955106	1.355407	0.001724	0.006068	0.005059
B	-3.138137	6.846495	5.011383	0.001745	0.006446	0.005415

Si	0.631772	3.486686	4.508512	-0.012879	0.017904	-0.031754
Si	1.821370	10.314915	1.858278	-0.012450	0.017188	-0.030025
Si	-0.333059	10.387486	5.041673	0.012471	0.017157	0.030043
Si	2.786201	3.414115	1.325117	0.012870	0.017928	0.031749
O	0.061445	3.072947	3.041906	0.013121	0.027151	0.057467
O	2.391697	10.728653	3.324884	0.012605	0.025167	0.053794
O	4.546126	9.973747	0.141489	-0.012616	0.025197	-0.053859
O	-2.092984	3.827853	6.225301	-0.013117	0.027147	-0.057446
O	2.197450	3.933608	4.519003	-0.004479	-0.003819	0.003644
O	0.255692	9.867992	1.847787	-0.003994	-0.003706	0.003699
O	-1.898737	10.834409	5.031182	0.003954	-0.003692	-0.003694
O	4.351879	2.967192	1.335608	0.004526	-0.003840	-0.003659
O	-0.212316	4.798696	5.055280	0.017748	-0.017595	-0.010423
O	2.665458	9.002905	1.311510	0.016742	-0.016854	-0.009754
O	0.511030	11.699496	4.494905	-0.016745	-0.016851	0.009761
O	1.942113	2.102105	1.871885	-0.017769	-0.017611	0.010428
O	0.525580	2.169271	5.472081	0.002738	-0.040214	0.050835
O	1.927562	11.632329	0.894709	0.002568	-0.038123	0.047760
O	-0.226867	9.070071	4.078104	-0.002568	-0.038091	-0.047726
O	2.680009	4.731529	2.288686	-0.002745	-0.040238	-0.050880
O	0.058846	0.698526	2.444964	0.008626	0.000697	0.004530
O	2.394296	13.103075	3.921826	0.007832	0.000191	0.004099
O	4.548725	7.599326	0.738431	-0.007821	0.000176	-0.004089
O	-2.095583	6.202275	5.628359	-0.008622	0.000699	-0.004533
O	-2.459230	13.184059	5.445139	-0.000137	0.005943	-0.006496
O	4.912372	0.617542	0.921651	-0.000459	0.006866	-0.007160
O	2.757943	6.283259	4.105046	0.000458	0.006864	0.007153
O	-0.304801	7.518342	2.261744	0.000124	0.005935	0.006481
O	-0.175430	2.374756	0.744070	0.024882	-0.005182	0.015813
O	2.628573	11.426844	5.622720	0.023572	-0.004970	0.014593
O	4.783002	9.275557	2.439325	-0.023606	-0.004965	-0.014596
O	-2.329859	4.526044	3.927465	-0.024863	-0.005187	-0.015810
O	-1.223866	12.517207	2.155216	-0.002479	-0.009128	0.003165
O	3.677009	1.284394	4.211574	-0.002401	-0.008084	0.002896
O	5.831438	5.616407	1.028179	0.002399	-0.008068	-0.002890
O	-3.378295	8.185194	5.338611	0.002478	-0.009131	-0.003165

H	-0.637445	12.195109	2.878812	0.023273	-0.001964	-0.013742
H	3.090587	1.606491	3.487978	0.023964	-0.001990	-0.014977
H	5.245016	5.294309	0.304583	-0.023954	-0.001954	0.014964
H	-2.791874	8.507292	6.062207	-0.023264	-0.001939	0.013725

41 f = 28.589604 THz 179.633780 2PiTHz 953.646509 cm-1 118.237140 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.005043	-0.001076	0.003120
Li	-1.316675	4.156264	2.365404	-0.004751	0.001018	-0.002945
Li	-3.471104	2.744536	5.548798	0.004749	0.001030	0.002946
Li	5.924247	11.057064	0.817991	-0.005047	-0.001068	-0.003118
Na	2.049025	6.784862	1.629696	-0.000267	-0.000095	-0.000485
Na	0.404117	7.016739	4.737094	0.000273	0.000045	0.000508
Na	2.558546	13.685662	1.553699	-0.000272	0.000047	-0.000508
Na	-0.105403	0.115939	4.813091	0.000268	-0.000094	0.000485
B	4.155007	8.978944	1.168663	0.008947	0.018925	-0.056249
B	-1.701865	4.822656	5.198127	-0.009164	-0.018699	0.053131
B	0.452564	2.078144	2.014732	0.009165	-0.018675	-0.053119
B	2.000578	11.723457	4.352058	-0.008966	0.018931	0.056247
B	-2.733891	11.746082	5.839177	0.038605	0.001125	0.043378
B	5.187034	2.055518	0.527613	-0.036015	-0.001729	-0.041455
B	3.032605	4.845282	3.711007	0.035985	-0.001742	0.041573
B	-0.579463	8.956318	2.655782	-0.038662	0.001130	-0.043299
B	-0.983708	0.054306	1.827988	-0.000299	0.005475	-0.005228
B	3.436850	13.747295	4.538802	0.000422	-0.005887	0.005586
B	5.591279	6.955106	1.355407	-0.000416	-0.005874	-0.005574
B	-3.138137	6.846495	5.011383	0.000307	0.005481	0.005240
Si	0.631772	3.486686	4.508512	-0.005658	0.010750	-0.025305
Si	1.821370	10.314915	1.858278	0.006453	-0.011922	0.027327
Si	-0.333059	10.387486	5.041673	-0.006483	-0.011880	-0.027328
Si	2.786201	3.414115	1.325117	0.005641	0.010787	0.025320
O	0.061445	3.072947	3.041906	0.007332	0.029301	0.053726
O	2.391697	10.728653	3.324884	-0.008156	-0.031032	-0.057359
O	4.546126	9.973747	0.141489	0.008163	-0.031041	0.057392
O	-2.092984	3.827853	6.225301	-0.007332	0.029315	-0.053737

O	2.197450	3.933608	4.519003	-0.008312	-0.002043	-0.000747
O	0.255692	9.867992	1.847787	0.008673	0.002320	0.000492
O	-1.898737	10.834409	5.031182	-0.008593	0.002286	-0.000509
O	4.351879	2.967192	1.335608	0.008393	-0.002078	0.000723
O	-0.212316	4.798696	5.055280	0.014770	-0.010744	-0.009813
O	2.665458	9.002905	1.311510	-0.015907	0.011876	0.010479
O	0.511030	11.699496	4.494905	0.015897	0.011866	-0.010478
O	1.942113	2.102105	1.871885	-0.014800	-0.010766	0.009825
O	0.525580	2.169271	5.472081	0.002538	-0.031039	0.046099
O	1.927562	11.632329	0.894709	-0.002723	0.033634	-0.049404
O	-0.226867	9.070071	4.078104	0.002715	0.033585	0.049329
O	2.680009	4.731529	2.288686	-0.002550	-0.031088	-0.046187
O	0.058846	0.698526	2.444964	0.011910	0.007683	0.006657
O	2.394296	13.103075	3.921826	-0.012464	-0.007744	-0.006952
O	4.548725	7.599326	0.738431	0.012459	-0.007733	0.006946
O	-2.095583	6.202275	5.628359	-0.011909	0.007689	-0.006660
O	-2.459230	13.184059	5.445139	0.005007	-0.014369	0.010361
O	4.912372	0.617542	0.921651	-0.004981	0.013936	-0.009908
O	2.757943	6.283259	4.105046	0.004975	0.013928	0.009898
O	-0.304801	7.518342	2.261744	-0.005008	-0.014374	-0.010361
O	-0.175430	2.374756	0.744070	0.018886	-0.003142	0.018285
O	2.628573	11.426844	5.622720	-0.020427	0.003477	-0.019274
O	4.783002	9.275557	2.439325	0.020459	0.003469	0.019279
O	-2.329859	4.526044	3.927465	-0.018879	-0.003148	-0.018283
O	-1.223866	12.517207	2.155216	-0.001076	-0.015749	0.004069
O	3.677009	1.284394	4.211574	0.001243	0.016336	-0.004269
O	5.831438	5.616407	1.028179	-0.001237	0.016321	0.004269
O	-3.378295	8.185194	5.338611	0.001079	-0.015753	-0.004067
H	-0.637445	12.195109	2.878812	-0.011242	0.001050	0.019617
H	3.090587	1.606491	3.487978	0.009702	-0.000959	-0.018709
H	5.245016	5.294309	0.304583	-0.009708	-0.000891	0.018686
H	-2.791874	8.507292	6.062207	0.011228	0.001101	-0.019623

42 f = 28.309707 THz 177.875134 2PiTHz 944.310145 cm-1 117.079578
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.002093	0.005349	-0.002334
Li	-1.316675	4.156264	2.365404	-0.002102	0.005357	-0.002335
Li	-3.471104	2.744536	5.548798	0.002099	0.005356	0.002335
Li	5.924247	11.057064	0.817991	0.002096	0.005349	0.002335
Na	2.049025	6.784862	1.629696	0.000295	0.001841	-0.000203
Na	0.404117	7.016739	4.737094	0.000295	0.001840	-0.000199
Na	2.558546	13.685662	1.553699	-0.000295	0.001842	0.000200
Na	-0.105403	0.115939	4.813091	-0.000295	0.001839	0.000203
B	4.155007	8.978944	1.168663	-0.044841	-0.070430	0.025693
B	-1.701865	4.822656	5.198127	-0.044811	-0.070443	0.025736
B	0.452564	2.078144	2.014732	0.044843	-0.070442	-0.025716
B	2.000578	11.723457	4.352058	0.044819	-0.070425	-0.025710
B	-2.733891	11.746082	5.839177	0.007822	-0.035690	-0.053427
B	5.187034	2.055518	0.527613	0.007776	-0.035689	-0.053447
B	3.032605	4.845282	3.711007	-0.007794	-0.035681	0.053435
B	-0.579463	8.956318	2.655782	-0.007792	-0.035684	0.053416
B	-0.983708	0.054306	1.827988	0.002309	-0.003186	0.000496
B	3.436850	13.747295	4.538802	0.002311	-0.003181	0.000492
B	5.591279	6.955106	1.355407	-0.002310	-0.003192	-0.000497
B	-3.138137	6.846495	5.011383	-0.002309	-0.003176	-0.000491
Si	0.631772	3.486686	4.508512	0.015467	-0.021620	0.011708
Si	1.821370	10.314915	1.858278	0.015482	-0.021609	0.011738
Si	-0.333059	10.387486	5.041673	-0.015481	-0.021629	-0.011726
Si	2.786201	3.414115	1.325117	-0.015472	-0.021598	-0.011711
O	0.061445	3.072947	3.041906	-0.015018	0.021641	0.014702
O	2.391697	10.728653	3.324884	-0.015038	0.021603	0.014611
O	4.546126	9.973747	0.141489	0.015029	0.021625	-0.014660
O	-2.092984	3.827853	6.225301	0.015024	0.021622	-0.014664
O	2.197450	3.933608	4.519003	-0.005959	0.010528	-0.016942
O	0.255692	9.867992	1.847787	-0.005966	0.010540	-0.016956
O	-1.898737	10.834409	5.031182	0.005971	0.010535	0.016955
O	4.351879	2.967192	1.335608	0.005953	0.010540	0.016951
O	-0.212316	4.798696	5.055280	-0.003414	0.017059	-0.002486
O	2.665458	9.002905	1.311510	-0.003411	0.017059	-0.002481
O	0.511030	11.699496	4.494905	0.003419	0.017066	0.002484
O	1.942113	2.102105	1.871885	0.003411	0.017057	0.002483

O	0.525580	2.169271	5.472081	-0.000268	0.019851	-0.004595
O	1.927562	11.632329	0.894709	-0.000278	0.019834	-0.004596
O	-0.226867	9.070071	4.078104	0.000278	0.019858	0.004630
O	2.680009	4.731529	2.288686	0.000271	0.019816	0.004557
O	0.058846	0.698526	2.444964	0.020457	0.034430	0.010608
O	2.394296	13.103075	3.921826	0.020469	0.034439	0.010622
O	4.548725	7.599326	0.738431	-0.020449	0.034421	-0.010609
O	-2.095583	6.202275	5.628359	-0.020481	0.034450	-0.010622
O	-2.459230	13.184059	5.445139	-0.017688	0.024537	-0.015915
O	4.912372	0.617542	0.921651	-0.017669	0.024528	-0.015903
O	2.757943	6.283259	4.105046	0.017687	0.024544	0.015926
O	-0.304801	7.518342	2.261744	0.017673	0.024516	0.015894
O	-0.175430	2.374756	0.744070	-0.013083	0.006574	0.009802
O	2.628573	11.426844	5.622720	-0.013097	0.006588	0.009808
O	4.783002	9.275557	2.439325	0.013083	0.006590	-0.009793
O	-2.329859	4.526044	3.927465	0.013087	0.006571	-0.009814
O	-1.223866	12.517207	2.155216	-0.002594	-0.024869	0.003128
O	3.677009	1.284394	4.211574	-0.002595	-0.024880	0.003132
O	5.831438	5.616407	1.028179	0.002590	-0.024855	-0.003128
O	-3.378295	8.185194	5.338611	0.002598	-0.024896	-0.003133
H	-0.637445	12.195109	2.878812	-0.031067	-0.046287	0.022906
H	3.090587	1.606491	3.487978	-0.031062	-0.046315	0.022901
H	5.245016	5.294309	0.304583	0.031052	-0.046318	-0.022877
H	-2.791874	8.507292	6.062207	0.031077	-0.046293	-0.022927

43 f = 27.901443 THz 175.309938 2PiTHz 930.691935 cm-1 115.391135 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.001449	0.012014	-0.000172
Li	-1.316675	4.156264	2.365404	0.001428	-0.011854	0.000184
Li	-3.471104	2.744536	5.548798	0.001431	0.011856	0.000182
Li	5.924247	11.057064	0.817991	-0.001444	-0.012012	-0.000173
Na	2.049025	6.784862	1.629696	-0.000923	0.000159	-0.000614
Na	0.404117	7.016739	4.737094	0.000918	-0.000143	0.000620
Na	2.558546	13.685662	1.553699	0.000918	0.000143	0.000620
Na	-0.105403	0.115939	4.813091	-0.000922	-0.000159	-0.000614

B	4.155007	8.978944	1.168663	0.030786	0.028848	-0.025584
B	-1.701865	4.822656	5.198127	-0.030464	-0.028362	0.025196
B	0.452564	2.078144	2.014732	-0.030466	0.028357	0.025226
B	2.000578	11.723457	4.352058	0.030796	-0.028852	-0.025559
B	-2.733891	11.746082	5.839177	0.038046	-0.039432	-0.073644
B	5.187034	2.055518	0.527613	-0.037392	0.038978	0.072452
B	3.032605	4.845282	3.711007	-0.037389	-0.038970	0.072442
B	-0.579463	8.956318	2.655782	0.038050	0.039437	-0.073656
B	-0.983708	0.054306	1.827988	-0.005611	0.005640	0.002301
B	3.436850	13.747295	4.538802	0.005652	-0.005538	-0.002333
B	5.591279	6.955106	1.355407	0.005652	0.005539	-0.002335
B	-3.138137	6.846495	5.011383	-0.005609	-0.005641	0.002299
Si	0.631772	3.486686	4.508512	0.024230	0.011918	-0.031548
Si	1.821370	10.314915	1.858278	-0.024619	-0.012079	0.032029
Si	-0.333059	10.387486	5.041673	-0.024606	0.012077	0.032024
Si	2.786201	3.414115	1.325117	0.024240	-0.011922	-0.031554
O	0.061445	3.072947	3.041906	0.011428	0.000811	0.017836
O	2.391697	10.728653	3.324884	-0.011598	-0.000863	-0.018189
O	4.546126	9.973747	0.141489	-0.011603	0.000856	-0.018184
O	-2.092984	3.827853	6.225301	0.011422	-0.000820	0.017844
O	2.197450	3.933608	4.519003	-0.024674	-0.001892	-0.011366
O	0.255692	9.867992	1.847787	0.025114	0.001956	0.011520
O	-1.898737	10.834409	5.031182	0.025100	-0.001950	0.011522
O	4.351879	2.967192	1.335608	-0.024684	0.001895	-0.011364
O	-0.212316	4.798696	5.055280	-0.013030	0.019131	0.004128
O	2.665458	9.002905	1.311510	0.013270	-0.019411	-0.004179
O	0.511030	11.699496	4.494905	0.013261	0.019413	-0.004179
O	1.942113	2.102105	1.871885	-0.013034	-0.019125	0.004124
O	0.525580	2.169271	5.472081	-0.002889	-0.037573	0.010575
O	1.927562	11.632329	0.894709	0.002937	0.038072	-0.010623
O	-0.226867	9.070071	4.078104	0.002934	-0.038071	-0.010613
O	2.680009	4.731529	2.288686	-0.002889	0.037575	0.010588
O	0.058846	0.698526	2.444964	0.005735	-0.010182	-0.002728
O	2.394296	13.103075	3.921826	-0.005739	0.010441	0.002750
O	4.548725	7.599326	0.738431	-0.005737	-0.010435	0.002756
O	-2.095583	6.202275	5.628359	0.005736	0.010190	-0.002720

O	-2.459230	13.184059	5.445139	-0.006194	0.017503	0.005833
O	4.912372	0.617542	0.921651	0.006166	-0.017393	-0.005649
O	2.757943	6.283259	4.105046	0.006161	0.017392	-0.005649
O	-0.304801	7.518342	2.261744	-0.006198	-0.017500	0.005835
O	-0.175430	2.374756	0.744070	0.024862	-0.005085	-0.020563
O	2.628573	11.426844	5.622720	-0.025318	0.005134	0.020888
O	4.783002	9.275557	2.439325	-0.025304	-0.005141	0.020890
O	-2.329859	4.526044	3.927465	0.024873	0.005079	-0.020562
O	-1.223866	12.517207	2.155216	-0.002585	0.003385	-0.005298
O	3.677009	1.284394	4.211574	0.002511	-0.003540	0.005271
O	5.831438	5.616407	1.028179	0.002511	0.003540	0.005269
O	-3.378295	8.185194	5.338611	-0.002585	-0.003385	-0.005299
H	-0.637445	12.195109	2.878812	0.001727	0.058640	0.017613
H	3.090587	1.606491	3.487978	-0.001656	-0.058223	-0.017469
H	5.245016	5.294309	0.304583	-0.001661	0.058217	-0.017464
H	-2.791874	8.507292	6.062207	0.001715	-0.058649	0.017627

44 f = 27.864286 THz 175.076473 2PiTHz 929.452512 cm-1 115.237466 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000705	0.009630	0.001309
Li	-1.316675	4.156264	2.365404	-0.000726	0.009817	0.001315
Li	-3.471104	2.744536	5.548798	-0.000721	-0.009811	0.001315
Li	5.924247	11.057064	0.817991	-0.000707	-0.009637	0.001310
Na	2.049025	6.784862	1.629696	-0.000337	0.000950	-0.000086
Na	0.404117	7.016739	4.737094	-0.000350	0.000955	-0.000093
Na	2.558546	13.685662	1.553699	-0.000351	-0.000954	-0.000093
Na	-0.105403	0.115939	4.813091	-0.000336	-0.000952	-0.000086
B	4.155007	8.978944	1.168663	0.017273	0.026862	-0.018068
B	-1.701865	4.822656	5.198127	0.017619	0.027220	-0.018398
B	0.452564	2.078144	2.014732	0.017695	-0.027231	-0.018418
B	2.000578	11.723457	4.352058	0.017209	-0.026833	-0.018047
B	-2.733891	11.746082	5.839177	0.045460	-0.032090	-0.079480
B	5.187034	2.055518	0.527613	0.046067	-0.032726	-0.080668
B	3.032605	4.845282	3.711007	0.046034	0.032721	-0.080646
B	-0.579463	8.956318	2.655782	0.045489	0.032107	-0.079514

B	-0.983708	0.054306	1.827988	0.003258	0.006632	-0.001762
B	3.436850	13.747295	4.538802	0.003164	0.006715	-0.001724
B	5.591279	6.955106	1.355407	0.003169	-0.006718	-0.001726
B	-3.138137	6.846495	5.011383	0.003250	-0.006626	-0.001761
Si	0.631772	3.486686	4.508512	-0.024887	-0.013244	0.030522
Si	1.821370	10.314915	1.858278	-0.024482	-0.013021	0.030050
Si	-0.333059	10.387486	5.041673	-0.024487	0.013026	0.030061
Si	2.786201	3.414115	1.325117	-0.024868	0.013251	0.030513
O	0.061445	3.072947	3.041906	-0.010243	-0.004607	-0.024473
O	2.391697	10.728653	3.324884	-0.010077	-0.004610	-0.024239
O	4.546126	9.973747	0.141489	-0.010089	0.004602	-0.024230
O	-2.092984	3.827853	6.225301	-0.010234	0.004611	-0.024481
O	2.197450	3.933608	4.519003	0.027682	0.003604	0.011176
O	0.255692	9.867992	1.847787	0.027258	0.003552	0.011004
O	-1.898737	10.834409	5.031182	0.027284	-0.003562	0.010998
O	4.351879	2.967192	1.335608	0.027643	-0.003587	0.011179
O	-0.212316	4.798696	5.055280	0.014531	-0.014800	-0.002369
O	2.665458	9.002905	1.311510	0.014286	-0.014508	-0.002289
O	0.511030	11.699496	4.494905	0.014312	0.014522	-0.002301
O	1.942113	2.102105	1.871885	0.014482	0.014767	-0.002348
O	0.525580	2.169271	5.472081	0.003616	0.034488	-0.002414
O	1.927562	11.632329	0.894709	0.003567	0.033870	-0.002253
O	-0.226867	9.070071	4.078104	0.003563	-0.033884	-0.002260
O	2.680009	4.731529	2.288686	0.003618	-0.034485	-0.002415
O	0.058846	0.698526	2.444964	0.001567	0.016747	0.001899
O	2.394296	13.103075	3.921826	0.001636	0.016591	0.001849
O	4.548725	7.599326	0.738431	0.001651	-0.016613	0.001859
O	-2.095583	6.202275	5.628359	0.001557	-0.016732	0.001892
O	-2.459230	13.184059	5.445139	-0.003582	0.008153	0.010860
O	4.912372	0.617542	0.921651	-0.003699	0.008431	0.010934
O	2.757943	6.283259	4.105046	-0.003684	-0.008421	0.010949
O	-0.304801	7.518342	2.261744	-0.003600	-0.008168	0.010844
O	-0.175430	2.374756	0.744070	-0.029463	0.003710	0.020061
O	2.628573	11.426844	5.622720	-0.029088	0.003634	0.019746
O	4.783002	9.275557	2.439325	-0.029107	-0.003630	0.019752
O	-2.329859	4.526044	3.927465	-0.029443	-0.003719	0.020060

O	-1.223866	12.517207	2.155216	-0.004869	-0.011370	-0.001421
O	3.677009	1.284394	4.211574	-0.004905	-0.011300	-0.001509
O	5.831438	5.616407	1.028179	-0.004907	0.011321	-0.001503
O	-3.378295	8.185194	5.338611	-0.004866	0.011353	-0.001428
H	-0.637445	12.195109	2.878812	0.002194	0.025059	0.011155
H	3.090587	1.606491	3.487978	0.002197	0.025974	0.011438
H	5.245016	5.294309	0.304583	0.002180	-0.025958	0.011455
H	-2.791874	8.507292	6.062207	0.002189	-0.025077	0.011158

45 f = 27.602827 THz 173.433678 2PiTHz 920.731179 cm-1 114.156158 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.004335	-0.003175	0.002229
Li	-1.316675	4.156264	2.365404	-0.004423	0.003180	-0.002278
Li	-3.471104	2.744536	5.548798	0.004427	0.003190	0.002282
Li	5.924247	11.057064	0.817991	-0.004332	-0.003166	-0.002226
Na	2.049025	6.784862	1.629696	-0.000508	-0.000956	-0.000014
Na	0.404117	7.016739	4.737094	0.000517	0.000970	0.000005
Na	2.558546	13.685662	1.553699	-0.000516	0.000971	-0.000005
Na	-0.105403	0.115939	4.813091	0.000509	-0.000953	0.000014
B	4.155007	8.978944	1.168663	0.071004	0.013945	0.005904
B	-1.701865	4.822656	5.198127	-0.072138	-0.014068	-0.006103
B	0.452564	2.078144	2.014732	0.072125	-0.013999	0.006166
B	2.000578	11.723457	4.352058	-0.070982	0.014004	-0.005870
B	-2.733891	11.746082	5.839177	-0.035331	-0.004073	0.014064
B	5.187034	2.055518	0.527613	0.035951	0.004354	-0.014085
B	3.032605	4.845282	3.711007	-0.035977	0.004365	0.014115
B	-0.579463	8.956318	2.655782	0.035297	-0.004075	-0.014012
B	-0.983708	0.054306	1.827988	0.008634	0.006075	0.002207
B	3.436850	13.747295	4.538802	-0.008503	-0.005952	-0.002141
B	5.591279	6.955106	1.355407	0.008507	-0.005945	0.002148
B	-3.138137	6.846495	5.011383	-0.008629	0.006084	-0.002200
Si	0.631772	3.486686	4.508512	-0.026286	0.010631	0.016440
Si	1.821370	10.314915	1.858278	0.025738	-0.010348	-0.016224
Si	-0.333059	10.387486	5.041673	-0.025723	-0.010327	0.016193
Si	2.786201	3.414115	1.325117	0.026307	0.010654	-0.016479

O	0.061445	3.072947	3.041906	-0.007514	-0.002533	-0.010164
O	2.391697	10.728653	3.324884	0.007474	0.002403	0.009934
O	4.546126	9.973747	0.141489	-0.007458	0.002403	-0.009904
O	-2.092984	3.827853	6.225301	0.007537	-0.002532	0.010191
O	2.197450	3.933608	4.519003	0.043290	0.024958	-0.012141
O	0.255692	9.867992	1.847787	-0.042486	-0.024548	0.011992
O	-1.898737	10.834409	5.031182	0.042471	-0.024541	-0.011999
O	4.351879	2.967192	1.335608	-0.043326	0.024977	0.012148
O	-0.212316	4.798696	5.055280	0.056789	-0.035774	-0.022969
O	2.665458	9.002905	1.311510	-0.055724	0.035109	0.022560
O	0.511030	11.699496	4.494905	0.055677	0.035064	-0.022543
O	1.942113	2.102105	1.871885	-0.056826	-0.035826	0.022984
O	0.525580	2.169271	5.472081	-0.002147	-0.003392	0.000016
O	1.927562	11.632329	0.894709	0.002124	0.003204	0.000054
O	-0.226867	9.070071	4.078104	-0.002121	0.003199	-0.000072
O	2.680009	4.731529	2.288686	0.002154	-0.003393	-0.000021
O	0.058846	0.698526	2.444964	0.004712	0.014821	0.000012
O	2.394296	13.103075	3.921826	-0.004673	-0.014635	-0.000066
O	4.548725	7.599326	0.738431	0.004670	-0.014610	0.000064
O	-2.095583	6.202275	5.628359	-0.004713	0.014849	-0.000016
O	-2.459230	13.184059	5.445139	0.007526	0.000177	0.007542
O	4.912372	0.617542	0.921651	-0.007580	-0.000308	-0.007642
O	2.757943	6.283259	4.105046	0.007575	-0.000303	0.007633
O	-0.304801	7.518342	2.261744	-0.007530	0.000178	-0.007553
O	-0.175430	2.374756	0.744070	-0.025522	-0.004767	-0.010105
O	2.628573	11.426844	5.622720	0.025095	0.004639	0.009856
O	4.783002	9.275557	2.439325	-0.025075	0.004640	-0.009877
O	-2.329859	4.526044	3.927465	0.025548	-0.004764	0.010070
O	-1.223866	12.517207	2.155216	-0.000985	-0.011984	0.002837
O	3.677009	1.284394	4.211574	0.000907	0.011877	-0.002808
O	5.831438	5.616407	1.028179	-0.000902	0.011868	0.002809
O	-3.378295	8.185194	5.338611	0.000989	-0.011998	-0.002837
H	-0.637445	12.195109	2.878812	-0.024475	-0.016831	0.017806
H	3.090587	1.606491	3.487978	0.025050	0.016238	-0.018515
H	5.245016	5.294309	0.304583	-0.025054	0.016268	0.018503
H	-2.791874	8.507292	6.062207	0.024483	-0.016788	-0.017833

46 f = 27.593395 THz 173.374416 2PiTHz 920.416568 cm-1 114.117151
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004861	0.000670	-0.003156
Li	-1.316675	4.156264	2.365404	-0.004780	0.000614	-0.003113
Li	-3.471104	2.744536	5.548798	0.004779	0.000613	0.003113
Li	5.924247	11.057064	0.817991	0.004865	0.000676	0.003158
Na	2.049025	6.784862	1.629696	0.000476	0.000874	-0.000368
Na	0.404117	7.016739	4.737094	0.000465	0.000856	-0.000360
Na	2.558546	13.685662	1.553699	-0.000465	0.000857	0.000360
Na	-0.105403	0.115939	4.813091	-0.000475	0.000874	0.000368
B	4.155007	8.978944	1.168663	-0.061327	-0.003858	-0.010663
B	-1.701865	4.822656	5.198127	-0.059991	-0.003552	-0.010564
B	0.452564	2.078144	2.014732	0.059981	-0.003552	0.010587
B	2.000578	11.723457	4.352058	0.061292	-0.003812	0.010693
B	-2.733891	11.746082	5.839177	0.035043	0.015653	-0.003808
B	5.187034	2.055518	0.527613	0.034377	0.015569	-0.003554
B	3.032605	4.845282	3.711007	-0.034365	0.015570	0.003537
B	-0.579463	8.956318	2.655782	-0.035043	0.015668	0.003811
B	-0.983708	0.054306	1.827988	0.006643	0.006903	0.002939
B	3.436850	13.747295	4.538802	0.006803	0.007019	0.002980
B	5.591279	6.955106	1.355407	-0.006801	0.007020	-0.002977
B	-3.138137	6.846495	5.011383	-0.006641	0.006905	-0.002938
Si	0.631772	3.486686	4.508512	-0.029696	0.016814	0.013295
Si	1.821370	10.314915	1.858278	-0.030184	0.017021	0.013602
Si	-0.333059	10.387486	5.041673	0.030193	0.017029	-0.013621
Si	2.786201	3.414115	1.325117	0.029701	0.016825	-0.013301
O	0.061445	3.072947	3.041906	-0.003856	-0.006145	-0.013159
O	2.391697	10.728653	3.324884	-0.003995	-0.006193	-0.013352
O	4.546126	9.973747	0.141489	0.004007	-0.006186	0.013352
O	-2.092984	3.827853	6.225301	0.003864	-0.006146	0.013166
O	2.197450	3.933608	4.519003	0.043207	0.022172	-0.007838
O	0.255692	9.867992	1.847787	0.044008	0.022632	-0.008065
O	-1.898737	10.834409	5.031182	-0.044027	0.022644	0.008074
O	4.351879	2.967192	1.335608	-0.043220	0.022179	0.007846

O	-0.212316	4.798696	5.055280	0.058605	-0.038691	-0.022876
O	2.665458	9.002905	1.311510	0.059659	-0.039354	-0.023307
O	0.511030	11.699496	4.494905	-0.059663	-0.039380	0.023312
O	1.942113	2.102105	1.871885	-0.058611	-0.038705	0.022882
O	0.525580	2.169271	5.472081	-0.001742	-0.010930	0.005030
O	1.927562	11.632329	0.894709	-0.001782	-0.011007	0.005034
O	-0.226867	9.070071	4.078104	0.001787	-0.011001	-0.005026
O	2.680009	4.731529	2.288686	0.001745	-0.010938	-0.005028
O	0.058846	0.698526	2.444964	0.002289	0.010722	-0.002142
O	2.394296	13.103075	3.921826	0.002376	0.010994	-0.002143
O	4.548725	7.599326	0.738431	-0.002371	0.011006	0.002141
O	-2.095583	6.202275	5.628359	-0.002286	0.010719	0.002139
O	-2.459230	13.184059	5.445139	-0.003010	-0.007577	-0.004669
O	4.912372	0.617542	0.921651	-0.002874	-0.007565	-0.004532
O	2.757943	6.283259	4.105046	0.002872	-0.007559	0.004535
O	-0.304801	7.518342	2.261744	0.003007	-0.007583	0.004662
O	-0.175430	2.374756	0.744070	-0.023062	-0.005943	-0.011905
O	2.628573	11.426844	5.622720	-0.023534	-0.006029	-0.012096
O	4.783002	9.275557	2.439325	0.023544	-0.006025	0.012088
O	-2.329859	4.526044	3.927465	0.023060	-0.005941	0.011891
O	-1.223866	12.517207	2.155216	-0.004411	-0.005769	0.001250
O	3.677009	1.284394	4.211574	-0.004428	-0.005988	0.001298
O	5.831438	5.616407	1.028179	0.004430	-0.005985	-0.001296
O	-3.378295	8.185194	5.338611	0.004410	-0.005772	-0.001250
H	-0.637445	12.195109	2.878812	0.032016	-0.026738	-0.036914
H	3.090587	1.606491	3.487978	0.031537	-0.027019	-0.036549
H	5.245016	5.294309	0.304583	-0.031544	-0.027027	0.036562
H	-2.791874	8.507292	6.062207	-0.032018	-0.026707	0.036897

47 f = 27.469876 THz 172.598319 2PiTHz 916.296394 cm-1 113.606315 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.003321	-0.003614	0.002510
Li	-1.316675	4.156264	2.365404	0.003357	-0.003639	0.002528
Li	-3.471104	2.744536	5.548798	0.003349	0.003635	0.002523
Li	5.924247	11.057064	0.817991	0.003324	0.003616	0.002513

Na	2.049025	6.784862	1.629696	0.000653	-0.000549	0.000007
Na	0.404117	7.016739	4.737094	0.000655	-0.000542	0.000003
Na	2.558546	13.685662	1.553699	0.000655	0.000542	0.000003
Na	-0.105403	0.115939	4.813091	0.000653	0.000549	0.000008
B	4.155007	8.978944	1.168663	-0.027320	-0.057655	0.048258
B	-1.701865	4.822656	5.198127	-0.027484	-0.058078	0.048608
B	0.452564	2.078144	2.014732	-0.027524	0.058098	0.048606
B	2.000578	11.723457	4.352058	-0.027328	0.057647	0.048256
B	-2.733891	11.746082	5.839177	0.026842	-0.028897	-0.025664
B	5.187034	2.055518	0.527613	0.026966	-0.029166	-0.025794
B	3.032605	4.845282	3.711007	0.027002	0.029129	-0.025787
B	-0.579463	8.956318	2.655782	0.026831	0.028916	-0.025676
B	-0.983708	0.054306	1.827988	0.007372	0.002358	0.006024
B	3.436850	13.747295	4.538802	0.007312	0.002329	0.005997
B	5.591279	6.955106	1.355407	0.007314	-0.002325	0.005994
B	-3.138137	6.846495	5.011383	0.007376	-0.002367	0.006029
Si	0.631772	3.486686	4.508512	0.003877	-0.039673	-0.017986
Si	1.821370	10.314915	1.858278	0.003795	-0.039372	-0.017813
Si	-0.333059	10.387486	5.041673	0.003814	0.039398	-0.017810
Si	2.786201	3.414115	1.325117	0.003836	0.039633	-0.017978
O	0.061445	3.072947	3.041906	0.019091	-0.011711	0.003252
O	2.391697	10.728653	3.324884	0.018947	-0.011642	0.003194
O	4.546126	9.973747	0.141489	0.018942	0.011637	0.003193
O	-2.092984	3.827853	6.225301	0.019094	0.011717	0.003244
O	2.197450	3.933608	4.519003	-0.010406	-0.009943	0.012752
O	0.255692	9.867992	1.847787	-0.010267	-0.009841	0.012663
O	-1.898737	10.834409	5.031182	-0.010280	0.009844	0.012658
O	4.351879	2.967192	1.335608	-0.010359	0.009926	0.012754
O	-0.212316	4.798696	5.055280	-0.025215	0.053079	0.018126
O	2.665458	9.002905	1.311510	-0.024934	0.052627	0.017961
O	0.511030	11.699496	4.494905	-0.024967	-0.052653	0.017972
O	1.942113	2.102105	1.871885	-0.025136	-0.053026	0.018095
O	0.525580	2.169271	5.472081	0.006824	0.022600	-0.004271
O	1.927562	11.632329	0.894709	0.006774	0.022451	-0.004231
O	-0.226867	9.070071	4.078104	0.006773	-0.022472	-0.004251
O	2.680009	4.731529	2.288686	0.006823	-0.022568	-0.004244

O	0.058846	0.698526	2.444964	0.015792	-0.001539	-0.001848
O	2.394296	13.103075	3.921826	0.015677	-0.001518	-0.001854
O	4.548725	7.599326	0.738431	0.015680	0.001517	-0.001845
O	-2.095583	6.202275	5.628359	0.015795	0.001527	-0.001858
O	-2.459230	13.184059	5.445139	-0.013484	0.013695	-0.010101
O	4.912372	0.617542	0.921651	-0.013580	0.013822	-0.010196
O	2.757943	6.283259	4.105046	-0.013576	-0.013799	-0.010194
O	-0.304801	7.518342	2.261744	-0.013492	-0.013713	-0.010107
O	-0.175430	2.374756	0.744070	-0.006090	-0.005209	-0.012121
O	2.628573	11.426844	5.622720	-0.006092	-0.005179	-0.012035
O	4.783002	9.275557	2.439325	-0.006090	0.005175	-0.012027
O	-2.329859	4.526044	3.927465	-0.006112	0.005214	-0.012134
O	-1.223866	12.517207	2.155216	0.000457	-0.013191	0.004665
O	3.677009	1.284394	4.211574	0.000478	-0.013084	0.004628
O	5.831438	5.616407	1.028179	0.000475	0.013097	0.004637
O	-3.378295	8.185194	5.338611	0.000457	0.013187	0.004658
H	-0.637445	12.195109	2.878812	-0.011665	-0.015330	0.009955
H	3.090587	1.606491	3.487978	-0.011849	-0.015233	0.010039
H	5.245016	5.294309	0.304583	-0.011774	0.015251	0.009981
H	-2.791874	8.507292	6.062207	-0.011723	0.015334	0.009993

48 f = 27.355795 THz 171.881531 2PiTHz 912.491084 cm-1 113.134516 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002821	-0.000965	0.001413
Li	-1.316675	4.156264	2.365404	-0.002807	0.000949	-0.001398
Li	-3.471104	2.744536	5.548798	-0.002806	-0.000948	-0.001398
Li	5.924247	11.057064	0.817991	0.002820	0.000965	0.001413
Na	2.049025	6.784862	1.629696	0.000234	0.001035	-0.000312
Na	0.404117	7.016739	4.737094	-0.000232	-0.001039	0.000314
Na	2.558546	13.685662	1.553699	-0.000233	0.001039	0.000315
Na	-0.105403	0.115939	4.813091	0.000234	-0.001035	-0.000311
B	4.155007	8.978944	1.168663	-0.019733	-0.052448	0.041828
B	-1.701865	4.822656	5.198127	0.019558	0.052066	-0.041485
B	0.452564	2.078144	2.014732	0.019557	-0.052079	-0.041494
B	2.000578	11.723457	4.352058	-0.019753	0.052444	0.041824

B	-2.733891	11.746082	5.839177	0.027933	-0.032899	-0.031501
B	5.187034	2.055518	0.527613	-0.027680	0.032709	0.031230
B	3.032605	4.845282	3.711007	-0.027678	-0.032707	0.031239
B	-0.579463	8.956318	2.655782	0.027938	0.032893	-0.031498
B	-0.983708	0.054306	1.827988	-0.009819	-0.004726	-0.003708
B	3.436850	13.747295	4.538802	0.009880	0.004754	0.003752
B	5.591279	6.955106	1.355407	0.009880	-0.004754	0.003751
B	-3.138137	6.846495	5.011383	-0.009821	0.004728	-0.003710
Si	0.631772	3.486686	4.508512	-0.003136	0.040091	0.017770
Si	1.821370	10.314915	1.858278	0.003162	-0.040392	-0.017882
Si	-0.333059	10.387486	5.041673	0.003157	0.040390	-0.017880
Si	2.786201	3.414115	1.325117	-0.003135	-0.040091	0.017770
O	0.061445	3.072947	3.041906	-0.018580	0.009989	-0.006047
O	2.391697	10.728653	3.324884	0.018716	-0.010073	0.006064
O	4.546126	9.973747	0.141489	0.018716	0.010077	0.006059
O	-2.092984	3.827853	6.225301	-0.018580	-0.009983	-0.006051
O	2.197450	3.933608	4.519003	0.008763	0.010518	-0.013306
O	0.255692	9.867992	1.847787	-0.008827	-0.010589	0.013401
O	-1.898737	10.834409	5.031182	-0.008818	0.010586	0.013402
O	4.351879	2.967192	1.335608	0.008762	-0.010520	-0.013307
O	-0.212316	4.798696	5.055280	0.030039	-0.053731	-0.019267
O	2.665458	9.002905	1.311510	-0.030239	0.054117	0.019403
O	0.511030	11.699496	4.494905	-0.030227	-0.054114	0.019399
O	1.942113	2.102105	1.871885	0.030037	0.053728	-0.019265
O	0.525580	2.169271	5.472081	-0.006848	-0.022032	0.003368
O	1.927562	11.632329	0.894709	0.006893	0.022198	-0.003384
O	-0.226867	9.070071	4.078104	0.006892	-0.022193	-0.003381
O	2.680009	4.731529	2.288686	-0.006848	0.022033	0.003365
O	0.058846	0.698526	2.444964	-0.017285	-0.001500	-0.001207
O	2.394296	13.103075	3.921826	0.017429	0.001530	0.001203
O	4.548725	7.599326	0.738431	0.017425	-0.001529	0.001203
O	-2.095583	6.202275	5.628359	-0.017294	0.001509	-0.001208
O	-2.459230	13.184059	5.445139	-0.014566	0.014991	-0.011370
O	4.912372	0.617542	0.921651	0.014450	-0.014888	0.011292
O	2.757943	6.283259	4.105046	0.014453	0.014893	0.011296
O	-0.304801	7.518342	2.261744	-0.014567	-0.014988	-0.011368

O	-0.175430	2.374756	0.744070	0.006387	0.004297	0.009429
O	2.628573	11.426844	5.622720	-0.006468	-0.004333	-0.009503
O	4.783002	9.275557	2.439325	-0.006474	0.004333	-0.009506
O	-2.329859	4.526044	3.927465	0.006388	-0.004297	0.009424
O	-1.223866	12.517207	2.155216	0.003208	0.014695	-0.004963
O	3.677009	1.284394	4.211574	-0.003210	-0.014815	0.005002
O	5.831438	5.616407	1.028179	-0.003209	0.014815	0.005001
O	-3.378295	8.185194	5.338611	0.003210	-0.014703	-0.004965
H	-0.637445	12.195109	2.878812	-0.018929	0.021613	0.010621
H	3.090587	1.606491	3.487978	0.018830	-0.021755	-0.010539
H	5.245016	5.294309	0.304583	0.018817	0.021748	-0.010526
H	-2.791874	8.507292	6.062207	-0.018934	-0.021626	0.010627

49 f = 26.968990 THz 169.451162 2PiTHz 899.588648 cm-1 111.534817 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.007281	0.005090	-0.003834
Li	-1.316675	4.156264	2.365404	0.007299	-0.005106	0.003842
Li	-3.471104	2.744536	5.548798	0.007299	0.005107	0.003840
Li	5.924247	11.057064	0.817991	-0.007281	-0.005088	-0.003837
Na	2.049025	6.784862	1.629696	-0.000951	-0.001422	0.000255
Na	0.404117	7.016739	4.737094	0.000952	0.001427	-0.000261
Na	2.558546	13.685662	1.553699	0.000952	-0.001427	-0.000261
Na	-0.105403	0.115939	4.813091	-0.000951	0.001422	0.000256
B	4.155007	8.978944	1.168663	0.084142	0.041650	-0.044207
B	-1.701865	4.822656	5.198127	-0.084399	-0.041752	0.044310
B	0.452564	2.078144	2.014732	-0.084384	0.041768	0.044304
B	2.000578	11.723457	4.352058	0.084169	-0.041648	-0.044205
B	-2.733891	11.746082	5.839177	0.008017	0.030127	-0.008383
B	5.187034	2.055518	0.527613	-0.008078	-0.030192	0.008451
B	3.032605	4.845282	3.711007	-0.008075	0.030164	0.008444
B	-0.579463	8.956318	2.655782	0.008009	-0.030149	-0.008384
B	-0.983708	0.054306	1.827988	-0.005013	-0.005297	0.001292
B	3.436850	13.747295	4.538802	0.004993	0.005281	-0.001299
B	5.591279	6.955106	1.355407	0.004992	-0.005281	-0.001301
B	-3.138137	6.846495	5.011383	-0.005012	0.005296	0.001292

Si	0.631772	3.486686	4.508512	-0.017331	0.005223	0.006700
Si	1.821370	10.314915	1.858278	0.017290	-0.005191	-0.006693
Si	-0.333059	10.387486	5.041673	0.017293	0.005191	-0.006698
Si	2.786201	3.414115	1.325117	-0.017335	-0.005225	0.006704
O	0.061445	3.072947	3.041906	0.003276	-0.018707	-0.034540
O	2.391697	10.728653	3.324884	-0.003280	0.018674	0.034463
O	4.546126	9.973747	0.141489	-0.003274	-0.018675	0.034468
O	-2.092984	3.827853	6.225301	0.003278	0.018704	-0.034537
O	2.197450	3.933608	4.519003	0.012110	0.006592	0.003013
O	0.255692	9.867992	1.847787	-0.012066	-0.006558	-0.003017
O	-1.898737	10.834409	5.031182	-0.012077	0.006568	-0.003012
O	4.351879	2.967192	1.335608	0.012107	-0.006587	0.003013
O	-0.212316	4.798696	5.055280	0.058253	-0.022876	-0.014445
O	2.665458	9.002905	1.311510	-0.058061	0.022805	0.014401
O	0.511030	11.699496	4.494905	-0.058077	-0.022812	0.014401
O	1.942113	2.102105	1.871885	0.058248	0.022878	-0.014450
O	0.525580	2.169271	5.472081	0.002409	0.011764	0.001104
O	1.927562	11.632329	0.894709	-0.002406	-0.011752	-0.001092
O	-0.226867	9.070071	4.078104	-0.002402	0.011757	-0.001085
O	2.680009	4.731529	2.288686	0.002413	-0.011762	0.001106
O	0.058846	0.698526	2.444964	-0.005335	-0.017796	-0.003276
O	2.394296	13.103075	3.921826	0.005299	0.017723	0.003266
O	4.548725	7.599326	0.738431	0.005297	-0.017717	0.003267
O	-2.095583	6.202275	5.628359	-0.005336	0.017797	-0.003278
O	-2.459230	13.184059	5.445139	-0.004164	-0.004807	-0.003085
O	4.912372	0.617542	0.921651	0.004191	0.004804	0.003107
O	2.757943	6.283259	4.105046	0.004195	-0.004786	0.003119
O	-0.304801	7.518342	2.261744	-0.004160	0.004820	-0.003075
O	-0.175430	2.374756	0.744070	0.013021	0.005590	-0.004646
O	2.628573	11.426844	5.622720	-0.012971	-0.005573	0.004625
O	4.783002	9.275557	2.439325	-0.012967	0.005571	0.004618
O	-2.329859	4.526044	3.927465	0.013017	-0.005593	-0.004658
O	-1.223866	12.517207	2.155216	0.003232	0.013773	-0.000779
O	3.677009	1.284394	4.211574	-0.003219	-0.013729	0.000769
O	5.831438	5.616407	1.028179	-0.003217	0.013721	0.000766
O	-3.378295	8.185194	5.338611	0.003232	-0.013783	-0.000782

H	-0.637445	12.195109	2.878812	0.021644	-0.002409	-0.019662
H	3.090587	1.606491	3.487978	-0.021695	0.002554	0.019735
H	5.245016	5.294309	0.304583	-0.021697	-0.002576	0.019740
H	-2.791874	8.507292	6.062207	0.021644	0.002403	-0.019668

50 f = 26.955709 THz 169.367714 2PiTHz 899.145636 cm-1 111.479891 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.006036	-0.006386	0.002054
Li	-1.316675	4.156264	2.365404	0.006018	-0.006374	0.002042
Li	-3.471104	2.744536	5.548798	0.006017	0.006374	0.002044
Li	5.924247	11.057064	0.817991	0.006036	0.006388	0.002051
Na	2.049025	6.784862	1.629696	0.000535	0.001444	-0.000589
Na	0.404117	7.016739	4.737094	0.000532	0.001438	-0.000580
Na	2.558546	13.685662	1.553699	0.000533	-0.001438	-0.000581
Na	-0.105403	0.115939	4.813091	0.000535	-0.001444	-0.000588
B	4.155007	8.978944	1.168663	-0.086308	-0.037130	0.043523
B	-1.701865	4.822656	5.198127	-0.086069	-0.036962	0.043382
B	0.452564	2.078144	2.014732	-0.086064	0.037008	0.043384
B	2.000578	11.723457	4.352058	-0.086317	0.037097	0.043511
B	-2.733891	11.746082	5.839177	-0.008711	-0.015458	0.011441
B	5.187034	2.055518	0.527613	-0.008717	-0.015379	0.011473
B	3.032605	4.845282	3.711007	-0.008715	0.015365	0.011448
B	-0.579463	8.956318	2.655782	-0.008704	0.015465	0.011460
B	-0.983708	0.054306	1.827988	-0.005462	-0.004624	-0.000559
B	3.436850	13.747295	4.538802	-0.005466	-0.004632	-0.000554
B	5.591279	6.955106	1.355407	-0.005465	0.004634	-0.000551
B	-3.138137	6.846495	5.011383	-0.005462	0.004622	-0.000561
Si	0.631772	3.486686	4.508512	-0.015298	0.008022	0.006782
Si	1.821370	10.314915	1.858278	-0.015346	0.008002	0.006811
Si	-0.333059	10.387486	5.041673	-0.015355	-0.008015	0.006815
Si	2.786201	3.414115	1.325117	-0.015292	-0.008009	0.006785
O	0.061445	3.072947	3.041906	0.002021	-0.016856	-0.033672
O	2.391697	10.728653	3.324884	0.002033	-0.016912	-0.033761
O	4.546126	9.973747	0.141489	0.002032	0.016921	-0.033780
O	-2.092984	3.827853	6.225301	0.002019	0.016845	-0.033656

O	2.197450	3.933608	4.519003	0.012083	0.008437	0.001090
O	0.255692	9.867992	1.847787	0.012120	0.008451	0.001105
O	-1.898737	10.834409	5.031182	0.012131	-0.008458	0.001105
O	4.351879	2.967192	1.335608	0.012075	-0.008433	0.001084
O	-0.212316	4.798696	5.055280	0.061017	-0.024244	-0.015455
O	2.665458	9.002905	1.311510	0.061159	-0.024279	-0.015486
O	0.511030	11.699496	4.494905	0.061175	0.024300	-0.015494
O	1.942113	2.102105	1.871885	0.061006	0.024227	-0.015450
O	0.525580	2.169271	5.472081	0.001569	0.007424	0.003090
O	1.927562	11.632329	0.894709	0.001575	0.007483	0.003073
O	-0.226867	9.070071	4.078104	0.001573	-0.007473	0.003076
O	2.680009	4.731529	2.288686	0.001572	-0.007436	0.003082
O	0.058846	0.698526	2.444964	-0.007114	-0.017909	-0.005032
O	2.394296	13.103075	3.921826	-0.007106	-0.017926	-0.005038
O	4.548725	7.599326	0.738431	-0.007117	0.017944	-0.005041
O	-2.095583	6.202275	5.628359	-0.007104	0.017887	-0.005033
O	-2.459230	13.184059	5.445139	0.007638	-0.003070	0.009443
O	4.912372	0.617542	0.921651	0.007647	-0.003087	0.009439
O	2.757943	6.283259	4.105046	0.007642	0.003091	0.009440
O	-0.304801	7.518342	2.261744	0.007647	0.003072	0.009446
O	-0.175430	2.374756	0.744070	0.011449	0.004543	-0.006209
O	2.628573	11.426844	5.622720	0.011483	0.004557	-0.006208
O	4.783002	9.275557	2.439325	0.011477	-0.004556	-0.006211
O	-2.329859	4.526044	3.927465	0.011445	-0.004543	-0.006209
O	-1.223866	12.517207	2.155216	0.003887	0.012761	-0.003661
O	3.677009	1.284394	4.211574	0.003889	0.012782	-0.003656
O	5.831438	5.616407	1.028179	0.003891	-0.012788	-0.003658
O	-3.378295	8.185194	5.338611	0.003881	-0.012758	-0.003660
H	-0.637445	12.195109	2.878812	-0.021749	0.046328	0.028242
H	3.090587	1.606491	3.487978	-0.021640	0.046253	0.028128
H	5.245016	5.294309	0.304583	-0.021668	-0.046283	0.028163
H	-2.791874	8.507292	6.062207	-0.021710	-0.046290	0.028190

51 f = 26.555702 THz 166.854396 2PiTHz 885.802843 cm-1 109.825595 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.009618	-0.001957	-0.009554
Li	-1.316675	4.156264	2.365404	0.009612	0.001959	0.009553
Li	-3.471104	2.744536	5.548798	0.009606	-0.001958	0.009548
Li	5.924247	11.057064	0.817991	-0.009623	0.001958	-0.009560
Na	2.049025	6.784862	1.629696	-0.001606	0.001936	0.001582
Na	0.404117	7.016739	4.737094	0.001604	-0.001937	-0.001582
Na	2.558546	13.685662	1.553699	0.001606	0.001938	-0.001581
Na	-0.105403	0.115939	4.813091	-0.001605	-0.001936	0.001583
B	4.155007	8.978944	1.168663	-0.051203	0.057050	0.035677
B	-1.701865	4.822656	5.198127	0.051140	-0.056894	-0.035649
B	0.452564	2.078144	2.014732	0.051203	0.056986	-0.035668
B	2.000578	11.723457	4.352058	-0.051161	-0.057000	0.035655
B	-2.733891	11.746082	5.839177	0.020232	0.075155	-0.030642
B	5.187034	2.055518	0.527613	-0.020221	-0.075179	0.030656
B	3.032605	4.845282	3.711007	-0.020229	0.075068	0.030638
B	-0.579463	8.956318	2.655782	0.020227	-0.075239	-0.030656
B	-0.983708	0.054306	1.827988	-0.000632	-0.002114	-0.000856
B	3.436850	13.747295	4.538802	0.000635	0.002110	0.000857
B	5.591279	6.955106	1.355407	0.000635	-0.002114	0.000860
B	-3.138137	6.846495	5.011383	-0.000630	0.002111	-0.000851
Si	0.631772	3.486686	4.508512	-0.007722	0.019384	-0.004473
Si	1.821370	10.314915	1.858278	0.007737	-0.019386	0.004482
Si	-0.333059	10.387486	5.041673	0.007730	0.019390	0.004486
Si	2.786201	3.414115	1.325117	-0.007727	-0.019381	-0.004467
O	0.061445	3.072947	3.041906	-0.001858	-0.006775	-0.000582
O	2.391697	10.728653	3.324884	0.001844	0.006781	0.000586
O	4.546126	9.973747	0.141489	0.001850	-0.006783	0.000585
O	-2.092984	3.827853	6.225301	-0.001851	0.006766	-0.000579
O	2.197450	3.933608	4.519003	-0.005287	-0.014622	0.002724
O	0.255692	9.867992	1.847787	0.005302	0.014646	-0.002734
O	-1.898737	10.834409	5.031182	0.005298	-0.014631	-0.002728
O	4.351879	2.967192	1.335608	-0.005298	0.014644	0.002732
O	-0.212316	4.798696	5.055280	-0.009919	-0.007614	0.002030
O	2.665458	9.002905	1.311510	0.009950	0.007594	-0.002039
O	0.511030	11.699496	4.494905	0.009931	-0.007608	-0.002036
O	1.942113	2.102105	1.871885	-0.009946	0.007595	0.002034

O	0.525580	2.169271	5.472081	0.001282	-0.006350	-0.002412
O	1.927562	11.632329	0.894709	-0.001300	0.006354	0.002385
O	-0.226867	9.070071	4.078104	-0.001293	-0.006349	0.002391
O	2.680009	4.731529	2.288686	0.001292	0.006357	-0.002404
O	0.058846	0.698526	2.444964	-0.015218	-0.032668	0.008461
O	2.394296	13.103075	3.921826	0.015211	0.032658	-0.008456
O	4.548725	7.599326	0.738431	0.015220	-0.032689	-0.008467
O	-2.095583	6.202275	5.628359	-0.015205	0.032621	0.008446
O	-2.459230	13.184059	5.445139	0.003092	-0.038907	0.019699
O	4.912372	0.617542	0.921651	-0.003095	0.038912	-0.019703
O	2.757943	6.283259	4.105046	-0.003084	-0.038862	-0.019676
O	-0.304801	7.518342	2.261744	0.003100	0.038942	0.019714
O	-0.175430	2.374756	0.744070	0.013538	0.003707	0.009826
O	2.628573	11.426844	5.622720	-0.013537	-0.003694	-0.009831
O	4.783002	9.275557	2.439325	-0.013553	0.003706	-0.009832
O	-2.329859	4.526044	3.927465	0.013524	-0.003696	0.009824
O	-1.223866	12.517207	2.155216	0.014172	-0.005476	0.007149
O	3.677009	1.284394	4.211574	-0.014164	0.005481	-0.007149
O	5.831438	5.616407	1.028179	-0.014170	-0.005485	-0.007155
O	-3.378295	8.185194	5.338611	0.014160	0.005465	0.007141
H	-0.637445	12.195109	2.878812	-0.059701	0.045579	0.085768
H	3.090587	1.606491	3.487978	0.059635	-0.045573	-0.085704
H	5.245016	5.294309	0.304583	0.059645	0.045608	-0.085745
H	-2.791874	8.507292	6.062207	-0.059683	-0.045507	0.085694

52 f = 26.341569 THz 165.508959 2PiTHz 878.660133 cm-1 108.940011 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004720	-0.001552	-0.008060
Li	-1.316675	4.156264	2.365404	-0.004707	-0.001553	-0.008050
Li	-3.471104	2.744536	5.548798	0.004719	-0.001554	0.008060
Li	5.924247	11.057064	0.817991	0.004706	-0.001549	0.008049
Na	2.049025	6.784862	1.629696	0.001665	0.000280	0.000987
Na	0.404117	7.016739	4.737094	0.001669	0.000279	0.000986
Na	2.558546	13.685662	1.553699	-0.001667	0.000280	-0.000988
Na	-0.105403	0.115939	4.813091	-0.001668	0.000278	-0.000986

B	4.155007	8.978944	1.168663	0.038218	-0.075623	-0.012548
B	-1.701865	4.822656	5.198127	0.038236	-0.075685	-0.012566
B	0.452564	2.078144	2.014732	-0.038221	-0.075625	0.012548
B	2.000578	11.723457	4.352058	-0.038272	-0.075707	0.012586
B	-2.733891	11.746082	5.839177	0.002883	0.088657	-0.016668
B	5.187034	2.055518	0.527613	0.002871	0.088530	-0.016610
B	3.032605	4.845282	3.711007	-0.002884	0.088607	0.016639
B	-0.579463	8.956318	2.655782	-0.002862	0.088546	0.016630
B	-0.983708	0.054306	1.827988	-0.000322	0.002020	0.001491
B	3.436850	13.747295	4.538802	-0.000315	0.002018	0.001492
B	5.591279	6.955106	1.355407	0.000317	0.002016	-0.001491
B	-3.138137	6.846495	5.011383	0.000325	0.002023	-0.001488
Si	0.631772	3.486686	4.508512	-0.005952	0.001148	0.009775
Si	1.821370	10.314915	1.858278	-0.005939	0.001115	0.009782
Si	-0.333059	10.387486	5.041673	0.005956	0.001143	-0.009780
Si	2.786201	3.414115	1.325117	0.005937	0.001133	-0.009775
O	0.061445	3.072947	3.041906	0.002928	0.007610	-0.002373
O	2.391697	10.728653	3.324884	0.002936	0.007623	-0.002353
O	4.546126	9.973747	0.141489	-0.002935	0.007607	0.002363
O	-2.092984	3.827853	6.225301	-0.002927	0.007626	0.002358
O	2.197450	3.933608	4.519003	-0.004640	-0.013007	0.002163
O	0.255692	9.867992	1.847787	-0.004642	-0.013006	0.002157
O	-1.898737	10.834409	5.031182	0.004646	-0.013025	-0.002166
O	4.351879	2.967192	1.335608	0.004645	-0.012999	-0.002161
O	-0.212316	4.798696	5.055280	-0.012650	0.010393	-0.002238
O	2.665458	9.002905	1.311510	-0.012661	0.010412	-0.002235
O	0.511030	11.699496	4.494905	0.012661	0.010396	0.002236
O	1.942113	2.102105	1.871885	0.012655	0.010403	0.002237
O	0.525580	2.169271	5.472081	0.007370	-0.009331	0.007515
O	1.927562	11.632329	0.894709	0.007376	-0.009312	0.007515
O	-0.226867	9.070071	4.078104	-0.007376	-0.009320	-0.007510
O	2.680009	4.731529	2.288686	-0.007370	-0.009331	-0.007519
O	0.058846	0.698526	2.444964	0.008285	0.029283	-0.008644
O	2.394296	13.103075	3.921826	0.008316	0.029326	-0.008643
O	4.548725	7.599326	0.738431	-0.008293	0.029284	0.008633
O	-2.095583	6.202275	5.628359	-0.008297	0.029310	0.008648

O	-2.459230	13.184059	5.445139	0.008711	-0.043225	0.021271
O	4.912372	0.617542	0.921651	0.008713	-0.043182	0.021247
O	2.757943	6.283259	4.105046	-0.008718	-0.043218	-0.021262
O	-0.304801	7.518342	2.261744	-0.008708	-0.043174	-0.021245
O	-0.175430	2.374756	0.744070	-0.012917	-0.001737	-0.009958
O	2.628573	11.426844	5.622720	-0.012944	-0.001743	-0.009978
O	4.783002	9.275557	2.439325	0.012926	-0.001739	0.009963
O	-2.329859	4.526044	3.927465	0.012933	-0.001741	0.009968
O	-1.223866	12.517207	2.155216	-0.008376	0.010495	-0.008091
O	3.677009	1.284394	4.211574	-0.008393	0.010492	-0.008098
O	5.831438	5.616407	1.028179	0.008376	0.010486	0.008089
O	-3.378295	8.185194	5.338611	0.008389	0.010499	0.008098
H	-0.637445	12.195109	2.878812	0.010321	-0.036976	-0.047931
H	3.090587	1.606491	3.487978	0.010378	-0.037053	-0.048029
H	5.245016	5.294309	0.304583	-0.010333	-0.036992	0.047941
H	-2.791874	8.507292	6.062207	-0.010379	-0.036995	0.048001

53 f = 26.223260 THz 164.765601 2PiTHz 874.713765 cm-1 108.450724 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002542	-0.001123	0.000054
Li	-1.316675	4.156264	2.365404	-0.002564	0.001116	-0.000065
Li	-3.471104	2.744536	5.548798	0.002549	0.001120	0.000058
Li	5.924247	11.057064	0.817991	-0.002563	-0.001118	-0.000066
Na	2.049025	6.784862	1.629696	-0.001539	0.001210	0.001384
Na	0.404117	7.016739	4.737094	0.001537	-0.001211	-0.001384
Na	2.558546	13.685662	1.553699	-0.001541	-0.001212	0.001381
Na	-0.105403	0.115939	4.813091	0.001534	0.001209	-0.001387
B	4.155007	8.978944	1.168663	-0.033957	0.086530	0.009754
B	-1.701865	4.822656	5.198127	0.033779	-0.086391	-0.009640
B	0.452564	2.078144	2.014732	-0.033953	-0.086536	0.009757
B	2.000578	11.723457	4.352058	0.033774	0.086355	-0.009626
B	-2.733891	11.746082	5.839177	-0.005169	-0.082248	0.016860
B	5.187034	2.055518	0.527613	0.005249	0.082506	-0.016932
B	3.032605	4.845282	3.711007	-0.005206	0.082291	0.016862
B	-0.579463	8.956318	2.655782	0.005218	-0.082504	-0.016942

B	-0.983708	0.054306	1.827988	0.000687	-0.000505	0.001646
B	3.436850	13.747295	4.538802	-0.000680	0.000510	-0.001631
B	5.591279	6.955106	1.355407	0.000687	0.000502	0.001643
B	-3.138137	6.846495	5.011383	-0.000676	-0.000513	-0.001633
Si	0.631772	3.486686	4.508512	-0.007690	0.001713	0.010627
Si	1.821370	10.314915	1.858278	0.007716	-0.001769	-0.010617
Si	-0.333059	10.387486	5.041673	-0.007679	-0.001706	0.010624
Si	2.786201	3.414115	1.325117	0.007718	0.001772	-0.010619
O	0.061445	3.072947	3.041906	0.002168	0.011652	0.004512
O	2.391697	10.728653	3.324884	-0.002141	-0.011647	-0.004521
O	4.546126	9.973747	0.141489	0.002156	-0.011659	0.004517
O	-2.092984	3.827853	6.225301	-0.002153	0.011646	-0.004523
O	2.197450	3.933608	4.519003	-0.002684	-0.009505	0.000233
O	0.255692	9.867992	1.847787	0.002695	0.009552	-0.000251
O	-1.898737	10.834409	5.031182	-0.002688	0.009510	0.000235
O	4.351879	2.967192	1.335608	0.002695	-0.009547	-0.000250
O	-0.212316	4.798696	5.055280	-0.007880	0.004255	-0.003648
O	2.665458	9.002905	1.311510	0.007910	-0.004220	0.003647
O	0.511030	11.699496	4.494905	-0.007897	-0.004253	-0.003644
O	1.942113	2.102105	1.871885	0.007891	0.004225	0.003651
O	0.525580	2.169271	5.472081	0.004573	-0.005472	0.000893
O	1.927562	11.632329	0.894709	-0.004571	0.005484	-0.000881
O	-0.226867	9.070071	4.078104	0.004569	0.005468	0.000890
O	2.680009	4.731529	2.288686	-0.004574	-0.005491	-0.000883
O	0.058846	0.698526	2.444964	0.008002	0.032367	-0.009726
O	2.394296	13.103075	3.921826	-0.007956	-0.032266	0.009676
O	4.548725	7.599326	0.738431	0.008005	-0.032361	-0.009716
O	-2.095583	6.202275	5.628359	-0.007955	0.032284	0.009691
O	-2.459230	13.184059	5.445139	-0.005733	0.041666	-0.019596
O	4.912372	0.617542	0.921651	0.005741	-0.041787	0.019651
O	2.757943	6.283259	4.105046	-0.005747	-0.041687	-0.019608
O	-0.304801	7.518342	2.261744	0.005732	0.041788	0.019645
O	-0.175430	2.374756	0.744070	-0.010377	-0.000852	-0.007936
O	2.628573	11.426844	5.622720	0.010333	0.000832	0.007907
O	4.783002	9.275557	2.439325	-0.010366	0.000847	-0.007937
O	-2.329859	4.526044	3.927465	0.010352	-0.000841	0.007911

O	-1.223866	12.517207	2.155216	-0.006308	0.013738	-0.007200
O	3.677009	1.284394	4.211574	0.006303	-0.013711	0.007186
O	5.831438	5.616407	1.028179	-0.006305	-0.013737	-0.007202
O	-3.378295	8.185194	5.338611	0.006310	0.013716	0.007188
H	-0.637445	12.195109	2.878812	0.001174	-0.064405	-0.047643
H	3.090587	1.606491	3.487978	-0.001305	0.064220	0.047615
H	5.245016	5.294309	0.304583	0.001155	0.064425	-0.047636
H	-2.791874	8.507292	6.062207	-0.001346	-0.064209	0.047653

54 f = 26.066333 THz 163.779599 2PiTHz 869.479242 cm-1 107.801726 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.007200	0.001175	0.003446
Li	-1.316675	4.156264	2.365404	0.007199	0.001183	0.003450
Li	-3.471104	2.744536	5.548798	0.007207	-0.001179	0.003453
Li	5.924247	11.057064	0.817991	0.007194	-0.001181	0.003447
Na	2.049025	6.784862	1.629696	0.001517	0.000282	0.000991
Na	0.404117	7.016739	4.737094	0.001525	0.000275	0.000988
Na	2.558546	13.685662	1.553699	0.001520	-0.000279	0.000991
Na	-0.105403	0.115939	4.813091	0.001521	-0.000278	0.000988
B	4.155007	8.978944	1.168663	0.050778	-0.061471	-0.032875
B	-1.701865	4.822656	5.198127	0.050939	-0.061714	-0.032955
B	0.452564	2.078144	2.014732	0.050836	0.061467	-0.032918
B	2.000578	11.723457	4.352058	0.050867	0.061692	-0.032899
B	-2.733891	11.746082	5.839177	-0.014802	-0.085730	0.023146
B	5.187034	2.055518	0.527613	-0.014827	-0.085505	0.023120
B	3.032605	4.845282	3.711007	-0.014831	0.085803	0.023189
B	-0.579463	8.956318	2.655782	-0.014801	0.085484	0.023084
B	-0.983708	0.054306	1.827988	-0.003160	-0.000792	-0.003151
B	3.436850	13.747295	4.538802	-0.003160	-0.000788	-0.003154
B	5.591279	6.955106	1.355407	-0.003159	0.000790	-0.003152
B	-3.138137	6.846495	5.011383	-0.003159	0.000790	-0.003152
Si	0.631772	3.486686	4.508512	-0.013368	0.019208	-0.002399
Si	1.821370	10.314915	1.858278	-0.013345	0.019189	-0.002440
Si	-0.333059	10.387486	5.041673	-0.013360	-0.019176	-0.002408
Si	2.786201	3.414115	1.325117	-0.013345	-0.019220	-0.002436

O	0.061445	3.072947	3.041906	-0.002344	-0.007871	-0.001887
O	2.391697	10.728653	3.324884	-0.002339	-0.007903	-0.001904
O	4.546126	9.973747	0.141489	-0.002335	0.007871	-0.001885
O	-2.092984	3.827853	6.225301	-0.002350	0.007906	-0.001904
O	2.197450	3.933608	4.519003	-0.001171	-0.013228	0.005208
O	0.255692	9.867992	1.847787	-0.001158	-0.013180	0.005206
O	-1.898737	10.834409	5.031182	-0.001169	0.013215	0.005207
O	4.351879	2.967192	1.335608	-0.001162	0.013191	0.005207
O	-0.212316	4.798696	5.055280	-0.001493	-0.010982	-0.001071
O	2.665458	9.002905	1.311510	-0.001452	-0.010987	-0.001061
O	0.511030	11.699496	4.494905	-0.001491	0.010962	-0.001065
O	1.942113	2.102105	1.871885	-0.001450	0.011008	-0.001064
O	0.525580	2.169271	5.472081	0.000804	-0.002774	-0.002025
O	1.927562	11.632329	0.894709	0.000786	-0.002760	-0.002011
O	-0.226867	9.070071	4.078104	0.000802	0.002762	-0.002019
O	2.680009	4.731529	2.288686	0.000785	0.002767	-0.002019
O	0.058846	0.698526	2.444964	-0.013918	-0.028449	0.010819
O	2.394296	13.103075	3.921826	-0.013935	-0.028518	0.010828
O	4.548725	7.599326	0.738431	-0.013905	0.028436	0.010816
O	-2.095583	6.202275	5.628359	-0.013951	0.028541	0.010835
O	-2.459230	13.184059	5.445139	-0.000082	0.038077	-0.016494
O	4.912372	0.617542	0.921651	-0.000075	0.037982	-0.016456
O	2.757943	6.283259	4.105046	-0.000083	-0.038116	-0.016510
O	-0.304801	7.518342	2.261744	-0.000077	-0.037970	-0.016446
O	-0.175430	2.374756	0.744070	0.010229	0.003403	0.010749
O	2.628573	11.426844	5.622720	0.010255	0.003405	0.010761
O	4.783002	9.275557	2.439325	0.010225	-0.003402	0.010737
O	-2.329859	4.526044	3.927465	0.010268	-0.003407	0.010780
O	-1.223866	12.517207	2.155216	0.000394	-0.009481	0.004466
O	3.677009	1.284394	4.211574	0.000400	-0.009505	0.004484
O	5.831438	5.616407	1.028179	0.000380	0.009482	0.004465
O	-3.378295	8.185194	5.338611	0.000418	0.009509	0.004488
H	-0.637445	12.195109	2.878812	0.054211	0.071692	0.003908
H	3.090587	1.606491	3.487978	0.054300	0.071858	0.003951
H	5.245016	5.294309	0.304583	0.054292	-0.071672	0.003829
H	-2.791874	8.507292	6.062207	0.054216	-0.071895	0.004050

55 f = 24.907514 THz 156.498526 2PiTHz 830.825211 cm-1 103.009235
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001433	0.000103	-0.001936
Li	-1.316675	4.156264	2.365404	-0.001436	-0.000096	0.001928
Li	-3.471104	2.744536	5.548798	0.001435	-0.000103	-0.001941
Li	5.924247	11.057064	0.817991	-0.001436	0.000095	0.001921
Na	2.049025	6.784862	1.629696	-0.000174	-0.000294	-0.000356
Na	0.404117	7.016739	4.737094	0.000176	0.000293	0.000359
Na	2.558546	13.685662	1.553699	-0.000177	0.000291	-0.000358
Na	-0.105403	0.115939	4.813091	0.000173	-0.000296	0.000357
B	4.155007	8.978944	1.168663	-0.015270	0.051364	-0.009658
B	-1.701865	4.822656	5.198127	0.015271	-0.051433	0.009675
B	0.452564	2.078144	2.014732	-0.015262	-0.051418	-0.009688
B	2.000578	11.723457	4.352058	0.015285	0.051386	0.009644
B	-2.733891	11.746082	5.839177	-0.012116	0.070156	-0.024297
B	5.187034	2.055518	0.527613	0.012138	-0.070298	0.024303
B	3.032605	4.845282	3.711007	-0.012124	-0.070242	-0.024300
B	-0.579463	8.956318	2.655782	0.012129	0.070201	0.024297
B	-0.983708	0.054306	1.827988	-0.003242	-0.005762	0.003070
B	3.436850	13.747295	4.538802	0.003235	0.005760	-0.003073
B	5.591279	6.955106	1.355407	-0.003243	0.005750	0.003072
B	-3.138137	6.846495	5.011383	0.003234	-0.005772	-0.003067
Si	0.631772	3.486686	4.508512	0.002706	0.033723	-0.000102
Si	1.821370	10.314915	1.858278	-0.002702	-0.033694	0.000107
Si	-0.333059	10.387486	5.041673	0.002706	-0.033685	-0.000114
Si	2.786201	3.414115	1.325117	-0.002705	0.033729	0.000093
O	0.061445	3.072947	3.041906	-0.005822	0.010101	-0.006274
O	2.391697	10.728653	3.324884	0.005809	-0.010091	0.006276
O	4.546126	9.973747	0.141489	-0.005808	-0.010085	-0.006274
O	-2.092984	3.827853	6.225301	0.005825	0.010107	0.006274
O	2.197450	3.933608	4.519003	-0.002560	0.014038	-0.003187
O	0.255692	9.867992	1.847787	0.002546	-0.014029	0.003185
O	-1.898737	10.834409	5.031182	-0.002551	-0.014024	-0.003179
O	4.351879	2.967192	1.335608	0.002559	0.014046	0.003193

O	-0.212316	4.798696	5.055280	0.013780	-0.011741	-0.006969
O	2.665458	9.002905	1.311510	-0.013758	0.011731	0.006967
O	0.511030	11.699496	4.494905	0.013745	0.011714	-0.006960
O	1.942113	2.102105	1.871885	-0.013794	-0.011756	0.006977
O	0.525580	2.169271	5.472081	-0.004755	-0.016540	0.013153
O	1.927562	11.632329	0.894709	0.004747	0.016545	-0.013152
O	-0.226867	9.070071	4.078104	-0.004751	0.016545	0.013151
O	2.680009	4.731529	2.288686	0.004749	-0.016537	-0.013150
O	0.058846	0.698526	2.444964	-0.032736	-0.020527	-0.019563
O	2.394296	13.103075	3.921826	0.032700	0.020495	0.019540
O	4.548725	7.599326	0.738431	-0.032709	0.020486	-0.019557
O	-2.095583	6.202275	5.628359	0.032725	-0.020536	0.019543
O	-2.459230	13.184059	5.445139	-0.026410	0.012043	-0.025032
O	4.912372	0.617542	0.921651	0.026441	-0.012007	0.025048
O	2.757943	6.283259	4.105046	-0.026418	-0.012051	-0.025055
O	-0.304801	7.518342	2.261744	0.026432	0.011994	0.025022
O	-0.175430	2.374756	0.744070	0.009571	0.019598	-0.005459
O	2.628573	11.426844	5.622720	-0.009580	-0.019588	0.005469
O	4.783002	9.275557	2.439325	0.009564	-0.019571	-0.005452
O	-2.329859	4.526044	3.927465	-0.009585	0.019613	0.005479
O	-1.223866	12.517207	2.155216	0.007438	0.048011	-0.013045
O	3.677009	1.284394	4.211574	-0.007402	-0.047990	0.013045
O	5.831438	5.616407	1.028179	0.007409	-0.047959	-0.013030
O	-3.378295	8.185194	5.338611	-0.007425	0.048039	0.013055
H	-0.637445	12.195109	2.878812	0.001854	0.044994	-0.008627
H	3.090587	1.606491	3.487978	-0.001985	-0.044830	0.008815
H	5.245016	5.294309	0.304583	0.001954	-0.044895	-0.008729
H	-2.791874	8.507292	6.062207	-0.001929	0.044908	0.008756

56 f = 24.639755 THz 154.816143 2PiTHz 821.893717 cm-1 101.901870 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000296	-0.005191	-0.002909
Li	-1.316675	4.156264	2.365404	0.000299	-0.005179	-0.002907
Li	-3.471104	2.744536	5.548798	-0.000297	-0.005181	0.002910
Li	5.924247	11.057064	0.817991	-0.000298	-0.005188	0.002910

Na	2.049025	6.784862	1.629696	-0.000251	0.000496	0.000232
Na	0.404117	7.016739	4.737094	-0.000250	0.000495	0.000236
Na	2.558546	13.685662	1.553699	0.000250	0.000495	-0.000236
Na	-0.105403	0.115939	4.813091	0.000251	0.000496	-0.000231
B	4.155007	8.978944	1.168663	-0.012757	0.068950	-0.008870
B	-1.701865	4.822656	5.198127	-0.012705	0.068888	-0.008896
B	0.452564	2.078144	2.014732	0.012720	0.068899	0.008897
B	2.000578	11.723457	4.352058	0.012741	0.068939	0.008868
B	-2.733891	11.746082	5.839177	-0.010422	0.070385	-0.013875
B	5.187034	2.055518	0.527613	-0.010403	0.070290	-0.013876
B	3.032605	4.845282	3.711007	0.010402	0.070293	0.013871
B	-0.579463	8.956318	2.655782	0.010423	0.070373	0.013875
B	-0.983708	0.054306	1.827988	-0.000822	0.008259	0.001226
B	3.436850	13.747295	4.538802	-0.000829	0.008272	0.001228
B	5.591279	6.955106	1.355407	0.000834	0.008276	-0.001232
B	-3.138137	6.846495	5.011383	0.000817	0.008257	-0.001223
Si	0.631772	3.486686	4.508512	-0.004705	-0.030566	-0.004559
Si	1.821370	10.314915	1.858278	-0.004706	-0.030604	-0.004551
Si	-0.333059	10.387486	5.041673	0.004712	-0.030598	0.004554
Si	2.786201	3.414115	1.325117	0.004699	-0.030570	0.004558
O	0.061445	3.072947	3.041906	0.008774	-0.013981	0.000547
O	2.391697	10.728653	3.324884	0.008755	-0.013991	0.000517
O	4.546126	9.973747	0.141489	-0.008755	-0.013991	-0.000520
O	-2.092984	3.827853	6.225301	-0.008775	-0.013982	-0.000543
O	2.197450	3.933608	4.519003	0.001294	-0.012176	0.008596
O	0.255692	9.867992	1.847787	0.001316	-0.012178	0.008599
O	-1.898737	10.834409	5.031182	-0.001315	-0.012184	-0.008605
O	4.351879	2.967192	1.335608	-0.001296	-0.012173	-0.008592
O	-0.212316	4.798696	5.055280	-0.006396	0.011594	0.006908
O	2.665458	9.002905	1.311510	-0.006408	0.011624	0.006914
O	0.511030	11.699496	4.494905	0.006408	0.011617	-0.006910
O	1.942113	2.102105	1.871885	0.006397	0.011600	-0.006910
O	0.525580	2.169271	5.472081	0.004518	0.010233	-0.004699
O	1.927562	11.632329	0.894709	0.004531	0.010244	-0.004693
O	-0.226867	9.070071	4.078104	-0.004529	0.010241	0.004696
O	2.680009	4.731529	2.288686	-0.004517	0.010232	0.004695

O	0.058846	0.698526	2.444964	0.031655	0.017322	0.017936
O	2.394296	13.103075	3.921826	0.031682	0.017335	0.017951
O	4.548725	7.599326	0.738431	-0.031686	0.017344	-0.017949
O	-2.095583	6.202275	5.628359	-0.031649	0.017312	-0.017937
O	-2.459230	13.184059	5.445139	-0.022515	0.009479	-0.026165
O	4.912372	0.617542	0.921651	-0.022507	0.009467	-0.026135
O	2.757943	6.283259	4.105046	0.022500	0.009459	0.026124
O	-0.304801	7.518342	2.261744	0.022523	0.009488	0.026176
O	-0.175430	2.374756	0.744070	-0.009051	-0.020071	0.008099
O	2.628573	11.426844	5.622720	-0.009076	-0.020102	0.008107
O	4.783002	9.275557	2.439325	0.009072	-0.020102	-0.008112
O	-2.329859	4.526044	3.927465	0.009057	-0.020071	-0.008096
O	-1.223866	12.517207	2.155216	-0.012980	-0.044526	0.009772
O	3.677009	1.284394	4.211574	-0.012976	-0.044582	0.009781
O	5.831438	5.616407	1.028179	0.012971	-0.044590	-0.009781
O	-3.378295	8.185194	5.338611	0.012978	-0.044519	-0.009768
H	-0.637445	12.195109	2.878812	0.054426	-0.036783	-0.036562
H	3.090587	1.606491	3.487978	0.054324	-0.036845	-0.036472
H	5.245016	5.294309	0.304583	-0.054298	-0.036851	0.036448
H	-2.791874	8.507292	6.062207	-0.054410	-0.036744	0.036536

57 f = 23.785333 THz 149.447657 2PiTHz 793.393295 cm-1 98.368267 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.010633	-0.000354	-0.015560
Li	-1.316675	4.156264	2.365404	0.010648	0.000352	0.015598
Li	-3.471104	2.744536	5.548798	-0.010609	0.000367	-0.015544
Li	5.924247	11.057064	0.817991	0.010672	-0.000339	0.015621
Na	2.049025	6.784862	1.629696	-0.001142	0.001022	-0.000618
Na	0.404117	7.016739	4.737094	0.001144	-0.001019	0.000632
Na	2.558546	13.685662	1.553699	-0.001140	-0.001018	-0.000627
Na	-0.105403	0.115939	4.813091	0.001146	0.001024	0.000623
B	4.155007	8.978944	1.168663	-0.023362	-0.026283	0.031164
B	-1.701865	4.822656	5.198127	0.023120	0.026271	-0.031083
B	0.452564	2.078144	2.014732	-0.023224	0.026188	0.031064
B	2.000578	11.723457	4.352058	0.023244	-0.026386	-0.031184

B	-2.733891	11.746082	5.839177	-0.014387	0.024288	0.026803
B	5.187034	2.055518	0.527613	0.014428	-0.024500	-0.026606
B	3.032605	4.845282	3.711007	-0.014356	-0.024330	0.026645
B	-0.579463	8.956318	2.655782	0.014468	0.024464	-0.026772
B	-0.983708	0.054306	1.827988	0.010593	-0.000349	0.006159
B	3.436850	13.747295	4.538802	-0.010612	0.000351	-0.006136
B	5.591279	6.955106	1.355407	0.010627	0.000336	0.006168
B	-3.138137	6.846495	5.011383	-0.010576	-0.000359	-0.006128
Si	0.631772	3.486686	4.508512	-0.000215	0.007356	-0.005200
Si	1.821370	10.314915	1.858278	0.000232	-0.007334	0.005124
Si	-0.333059	10.387486	5.041673	-0.000242	-0.007357	-0.005171
Si	2.786201	3.414115	1.325117	0.000201	0.007329	0.005156
O	0.061445	3.072947	3.041906	0.014485	0.004477	0.034590
O	2.391697	10.728653	3.324884	-0.014542	-0.004515	-0.034773
O	4.546126	9.973747	0.141489	0.014568	-0.004496	0.034702
O	-2.092984	3.827853	6.225301	-0.014462	0.004496	-0.034655
O	2.197450	3.933608	4.519003	-0.024042	-0.002533	-0.005778
O	0.255692	9.867992	1.847787	0.024220	0.002521	0.005788
O	-1.898737	10.834409	5.031182	-0.024142	0.002568	-0.005804
O	4.351879	2.967192	1.335608	0.024115	-0.002488	0.005764
O	-0.212316	4.798696	5.055280	0.019427	-0.044290	-0.004537
O	2.665458	9.002905	1.311510	-0.019595	0.044499	0.004646
O	0.511030	11.699496	4.494905	0.019488	0.044444	-0.004574
O	1.942113	2.102105	1.871885	-0.019521	-0.044338	0.004600
O	0.525580	2.169271	5.472081	-0.005983	0.030525	-0.022645
O	1.927562	11.632329	0.894709	0.005966	-0.030709	0.022794
O	-0.226867	9.070071	4.078104	-0.005969	-0.030652	-0.022709
O	2.680009	4.731529	2.288686	0.005981	0.030580	0.022720
O	0.058846	0.698526	2.444964	0.010701	0.011906	-0.009443
O	2.394296	13.103075	3.921826	-0.010839	-0.011891	0.009371
O	4.548725	7.599326	0.738431	0.010773	-0.011889	-0.009440
O	-2.095583	6.202275	5.628359	-0.010769	0.011900	0.009372
O	-2.459230	13.184059	5.445139	-0.000762	0.008719	-0.014274
O	4.912372	0.617542	0.921651	0.000905	-0.008811	0.014343
O	2.757943	6.283259	4.105046	-0.000808	-0.008729	-0.014255
O	-0.304801	7.518342	2.261744	0.000853	0.008808	0.014364

O	-0.175430	2.374756	0.744070	0.006133	-0.003563	0.002297
O	2.628573	11.426844	5.622720	-0.006094	0.003612	-0.002228
O	4.783002	9.275557	2.439325	0.006103	0.003571	0.002250
O	-2.329859	4.526044	3.927465	-0.006125	-0.003594	-0.002268
O	-1.223866	12.517207	2.155216	-0.025119	-0.002028	-0.000642
O	3.677009	1.284394	4.211574	0.024998	0.002191	0.000603
O	5.831438	5.616407	1.028179	-0.025066	0.002058	-0.000645
O	-3.378295	8.185194	5.338611	0.025035	-0.002150	0.000610
H	-0.637445	12.195109	2.878812	0.209754	-0.047294	-0.205012
H	3.090587	1.606491	3.487978	-0.208313	0.047161	0.203602
H	5.245016	5.294309	0.304583	0.209138	0.047244	-0.204457
H	-2.791874	8.507292	6.062207	-0.208841	-0.047177	0.204072

58 f = 23.667052 THz 148.704472 2PiTHz 789.447847 cm-1 97.879094 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.007338	0.002008	-0.012767
Li	-1.316675	4.156264	2.365404	-0.007298	0.001999	-0.012696
Li	-3.471104	2.744536	5.548798	-0.007336	-0.001998	-0.012763
Li	5.924247	11.057064	0.817991	-0.007299	-0.002010	-0.012697
Na	2.049025	6.784862	1.629696	-0.000599	-0.000020	-0.001070
Na	0.404117	7.016739	4.737094	-0.000593	-0.000026	-0.001059
Na	2.558546	13.685662	1.553699	-0.000598	0.000020	-0.001062
Na	-0.105403	0.115939	4.813091	-0.000594	0.000026	-0.001067
B	4.155007	8.978944	1.168663	0.029935	-0.028559	0.007146
B	-1.701865	4.822656	5.198127	0.030005	-0.028480	0.007030
B	0.452564	2.078144	2.014732	0.029933	0.028583	0.007165
B	2.000578	11.723457	4.352058	0.030006	0.028457	0.007008
B	-2.733891	11.746082	5.839177	-0.024075	0.046509	-0.012028
B	5.187034	2.055518	0.527613	-0.024038	0.046470	-0.012128
B	3.032605	4.845282	3.711007	-0.024099	-0.046551	-0.012046
B	-0.579463	8.956318	2.655782	-0.024015	-0.046420	-0.012105
B	-0.983708	0.054306	1.827988	-0.002787	-0.004776	-0.007674
B	3.436850	13.747295	4.538802	-0.002819	-0.004788	-0.007709
B	5.591279	6.955106	1.355407	-0.002780	0.004782	-0.007684
B	-3.138137	6.846495	5.011383	-0.002822	0.004788	-0.007700

Si	0.631772	3.486686	4.508512	0.001208	-0.003571	0.011653
Si	1.821370	10.314915	1.858278	0.001212	-0.003587	0.011672
Si	-0.333059	10.387486	5.041673	0.001211	0.003561	0.011640
Si	2.786201	3.414115	1.325117	0.001212	0.003595	0.011682
O	0.061445	3.072947	3.041906	-0.006641	0.005095	0.020132
O	2.391697	10.728653	3.324884	-0.006693	0.005080	0.019987
O	4.546126	9.973747	0.141489	-0.006635	-0.005094	0.020118
O	-2.092984	3.827853	6.225301	-0.006700	-0.005081	0.020003
O	2.197450	3.933608	4.519003	-0.021069	0.009020	0.006675
O	0.255692	9.867992	1.847787	-0.020979	0.009022	0.006694
O	-1.898737	10.834409	5.031182	-0.021062	-0.009026	0.006660
O	4.351879	2.967192	1.335608	-0.020989	-0.009020	0.006707
O	-0.212316	4.798696	5.055280	0.031748	-0.015882	-0.017934
O	2.665458	9.002905	1.311510	0.031649	-0.015722	-0.017919
O	0.511030	11.699496	4.494905	0.031720	0.015873	-0.017924
O	1.942113	2.102105	1.871885	0.031674	0.015728	-0.017926
O	0.525580	2.169271	5.472081	0.000813	0.014735	-0.025186
O	1.927562	11.632329	0.894709	0.000844	0.014638	-0.025058
O	-0.226867	9.070071	4.078104	0.000806	-0.014729	-0.025157
O	2.680009	4.731529	2.288686	0.000846	-0.014642	-0.025091
O	0.058846	0.698526	2.444964	0.018006	-0.000592	0.019625
O	2.394296	13.103075	3.921826	0.017949	-0.000664	0.019668
O	4.548725	7.599326	0.738431	0.017985	0.000593	0.019612
O	-2.095583	6.202275	5.628359	0.017967	0.000663	0.019682
O	-2.459230	13.184059	5.445139	-0.024999	0.018433	-0.022976
O	4.912372	0.617542	0.921651	-0.024998	0.018411	-0.022937
O	2.757943	6.283259	4.105046	-0.025015	-0.018435	-0.022990
O	-0.304801	7.518342	2.261744	-0.024988	-0.018403	-0.022922
O	-0.175430	2.374756	0.744070	-0.000828	-0.010658	-0.005924
O	2.628573	11.426844	5.622720	-0.000845	-0.010622	-0.005936
O	4.783002	9.275557	2.439325	-0.000813	0.010648	-0.005906
O	-2.329859	4.526044	3.927465	-0.000854	0.010629	-0.005953
O	-1.223866	12.517207	2.155216	0.014840	-0.034381	0.008454
O	3.677009	1.284394	4.211574	0.014928	-0.034337	0.008447
O	5.831438	5.616407	1.028179	0.014827	0.034354	0.008456
O	-3.378295	8.185194	5.338611	0.014942	0.034364	0.008449

H	-0.637445	12.195109	2.878812	-0.193357	0.010635	0.196459
H	3.090587	1.606491	3.487978	-0.194113	0.010803	0.197165
H	5.245016	5.294309	0.304583	-0.193211	-0.010610	0.196307
H	-2.791874	8.507292	6.062207	-0.194288	-0.010826	0.197343

59 f = 23.459788 THz 147.402196 2PiTHz 782.534278 cm-1 97.021920 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.005623	0.000888	-0.005235
Li	-1.316675	4.156264	2.365404	-0.005666	0.000884	-0.005312
Li	-3.471104	2.744536	5.548798	0.005666	0.000890	0.005302
Li	5.924247	11.057064	0.817991	0.005631	0.000892	0.005260
Na	2.049025	6.784862	1.629696	-0.000461	0.001300	-0.000715
Na	0.404117	7.016739	4.737094	-0.000468	0.001305	-0.000712
Na	2.558546	13.685662	1.553699	0.000467	0.001305	0.000712
Na	-0.105403	0.115939	4.813091	0.000462	0.001303	0.000716
B	4.155007	8.978944	1.168663	-0.049574	-0.019468	0.033584
B	-1.701865	4.822656	5.198127	-0.049537	-0.019695	0.033716
B	0.452564	2.078144	2.014732	0.049645	-0.019548	-0.033693
B	2.000578	11.723457	4.352058	0.049481	-0.019584	-0.033593
B	-2.733891	11.746082	5.839177	-0.013287	0.007209	0.050699
B	5.187034	2.055518	0.527613	-0.013417	0.007406	0.050739
B	3.032605	4.845282	3.711007	0.013337	0.007266	-0.050777
B	-0.579463	8.956318	2.655782	0.013354	0.007324	-0.050681
B	-0.983708	0.054306	1.827988	-0.009283	-0.001023	-0.003712
B	3.436850	13.747295	4.538802	-0.009259	-0.001027	-0.003687
B	5.591279	6.955106	1.355407	0.009255	-0.001022	0.003700
B	-3.138137	6.846495	5.011383	0.009287	-0.001022	0.003710
Si	0.631772	3.486686	4.508512	0.009114	-0.003775	-0.008743
Si	1.821370	10.314915	1.858278	0.009135	-0.003765	-0.008796
Si	-0.333059	10.387486	5.041673	-0.009126	-0.003758	0.008774
Si	2.786201	3.414115	1.325117	-0.009135	-0.003788	0.008766
O	0.061445	3.072947	3.041906	-0.021335	-0.008167	-0.034995
O	2.391697	10.728653	3.324884	-0.021283	-0.008169	-0.034944
O	4.546126	9.973747	0.141489	0.021302	-0.008162	0.034893
O	-2.092984	3.827853	6.225301	0.021322	-0.008170	0.035064

O	2.197450	3.933608	4.519003	0.032302	0.010785	0.005536
O	0.255692	9.867992	1.847787	0.032285	0.010771	0.005493
O	-1.898737	10.834409	5.031182	-0.032237	0.010780	-0.005513
O	4.351879	2.967192	1.335608	-0.032360	0.010786	-0.005504
O	-0.212316	4.798696	5.055280	-0.018484	0.052253	0.013844
O	2.665458	9.002905	1.311510	-0.018512	0.052170	0.013893
O	0.511030	11.699496	4.494905	0.018433	0.052130	-0.013847
O	1.942113	2.102105	1.871885	0.018577	0.052312	-0.013897
O	0.525580	2.169271	5.472081	-0.005332	-0.044654	0.017554
O	1.927562	11.632329	0.894709	-0.005374	-0.044603	0.017552
O	-0.226867	9.070071	4.078104	0.005367	-0.044573	-0.017484
O	2.680009	4.731529	2.288686	0.005338	-0.044690	-0.017646
O	0.058846	0.698526	2.444964	-0.012830	0.001481	0.010356
O	2.394296	13.103075	3.921826	-0.012857	0.001543	0.010240
O	4.548725	7.599326	0.738431	0.012808	0.001554	-0.010296
O	-2.095583	6.202275	5.628359	0.012900	0.001459	-0.010288
O	-2.459230	13.184059	5.445139	0.005308	-0.005374	-0.012300
O	4.912372	0.617542	0.921651	0.005252	-0.005340	-0.012392
O	2.757943	6.283259	4.105046	-0.005312	-0.005338	0.012336
O	-0.304801	7.518342	2.261744	-0.005262	-0.005357	0.012345
O	-0.175430	2.374756	0.744070	0.013231	0.004107	0.010789
O	2.628573	11.426844	5.622720	0.013254	0.004109	0.010839
O	4.783002	9.275557	2.439325	-0.013260	0.004080	-0.010830
O	-2.329859	4.526044	3.927465	-0.013212	0.004138	-0.010801
O	-1.223866	12.517207	2.155216	-0.009840	0.002403	-0.001523
O	3.677009	1.284394	4.211574	-0.009873	0.002487	-0.001542
O	5.831438	5.616407	1.028179	0.009907	0.002395	0.001515
O	-3.378295	8.185194	5.338611	0.009777	0.002519	0.001556
H	-0.637445	12.195109	2.878812	0.107736	0.006719	-0.088525
H	3.090587	1.606491	3.487978	0.108147	0.006668	-0.088947
H	5.245016	5.294309	0.304583	-0.108378	0.006607	0.089119
H	-2.791874	8.507292	6.062207	-0.107307	0.006864	0.088155

60 f = 23.434661 THz 147.244320 2PiTHz 781.696138 cm-1 96.918004
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.001841	0.000753	-0.009342
Li	-1.316675	4.156264	2.365404	0.001809	-0.000737	0.009304
Li	-3.471104	2.744536	5.548798	0.001829	0.000742	0.009328
Li	5.924247	11.057064	0.817991	-0.001822	-0.000747	-0.009318
Na	2.049025	6.784862	1.629696	-0.000425	0.001066	-0.000570
Na	0.404117	7.016739	4.737094	0.000422	-0.001062	0.000567
Na	2.558546	13.685662	1.553699	0.000424	0.001066	0.000570
Na	-0.105403	0.115939	4.813091	-0.000423	-0.001063	-0.000568
B	4.155007	8.978944	1.168663	0.038547	-0.052724	0.007616
B	-1.701865	4.822656	5.198127	-0.038651	0.052723	-0.007553
B	0.452564	2.078144	2.014732	-0.038558	-0.052752	-0.007630
B	2.000578	11.723457	4.352058	0.038679	0.052674	0.007512
B	-2.733891	11.746082	5.839177	-0.026431	0.044225	-0.008277
B	5.187034	2.055518	0.527613	0.026415	-0.044240	0.008395
B	3.032605	4.845282	3.711007	0.026438	0.044240	0.008304
B	-0.579463	8.956318	2.655782	-0.026395	-0.044211	-0.008413
B	-0.983708	0.054306	1.827988	-0.000500	-0.000358	0.002477
B	3.436850	13.747295	4.538802	0.000477	0.000353	-0.002502
B	5.591279	6.955106	1.355407	0.000507	-0.000359	-0.002496
B	-3.138137	6.846495	5.011383	-0.000475	0.000357	0.002476
Si	0.631772	3.486686	4.508512	0.006493	-0.005112	-0.006758
Si	1.821370	10.314915	1.858278	-0.006459	0.005093	0.006737
Si	-0.333059	10.387486	5.041673	-0.006484	-0.005103	0.006757
Si	2.786201	3.414115	1.325117	0.006470	0.005095	-0.006738
O	0.061445	3.072947	3.041906	0.004310	0.000146	-0.023563
O	2.391697	10.728653	3.324884	-0.004379	-0.000152	0.023463
O	4.546126	9.973747	0.141489	-0.004316	0.000132	0.023561
O	-2.092984	3.827853	6.225301	0.004354	-0.000165	-0.023487
O	2.197450	3.933608	4.519003	0.020657	-0.001982	-0.010732
O	0.255692	9.867992	1.847787	-0.020573	0.002016	0.010753
O	-1.898737	10.834409	5.031182	-0.020661	-0.001986	0.010738
O	4.351879	2.967192	1.335608	0.020597	0.002004	-0.010746
O	-0.212316	4.798696	5.055280	-0.034044	0.018255	0.018431
O	2.665458	9.002905	1.311510	0.033981	-0.018101	-0.018400
O	0.511030	11.699496	4.494905	0.034038	0.018246	-0.018433
O	1.942113	2.102105	1.871885	-0.033998	-0.018138	0.018405

O	0.525580	2.169271	5.472081	-0.000758	-0.009788	0.031067
O	1.927562	11.632329	0.894709	0.000749	0.009671	-0.031000
O	-0.226867	9.070071	4.078104	0.000760	-0.009792	-0.031053
O	2.680009	4.731529	2.288686	-0.000752	0.009704	0.031023
O	0.058846	0.698526	2.444964	-0.019641	-0.009461	-0.019256
O	2.394296	13.103075	3.921826	0.019600	0.009445	0.019292
O	4.548725	7.599326	0.738431	0.019636	-0.009444	0.019263
O	-2.095583	6.202275	5.628359	-0.019620	0.009467	-0.019280
O	-2.459230	13.184059	5.445139	-0.016101	0.006323	-0.018466
O	4.912372	0.617542	0.921651	0.016108	-0.006324	0.018437
O	2.757943	6.283259	4.105046	0.016091	0.006320	0.018468
O	-0.304801	7.518342	2.261744	-0.016125	-0.006329	-0.018428
O	-0.175430	2.374756	0.744070	-0.003816	0.014725	0.000748
O	2.628573	11.426844	5.622720	0.003844	-0.014694	-0.000728
O	4.783002	9.275557	2.439325	0.003816	0.014705	-0.000753
O	-2.329859	4.526044	3.927465	-0.003831	-0.014720	0.000727
O	-1.223866	12.517207	2.155216	0.020194	0.040803	-0.012834
O	3.677009	1.284394	4.211574	-0.020202	-0.040782	0.012827
O	5.831438	5.616407	1.028179	-0.020156	0.040786	0.012822
O	-3.378295	8.185194	5.338611	0.020231	-0.040808	-0.012832
H	-0.637445	12.195109	2.878812	-0.153722	0.047462	0.129015
H	3.090587	1.606491	3.487978	0.153832	-0.047384	-0.129078
H	5.245016	5.294309	0.304583	0.153344	0.047351	-0.128654
H	-2.791874	8.507292	6.062207	-0.154140	-0.047474	0.129368

61 f = 23.195893 THz 145.744094 2PiTHz 773.731680 cm-1 95.930537
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.011443	0.011755	-0.017425
Li	-1.316675	4.156264	2.365404	-0.011434	0.011738	-0.017409
Li	-3.471104	2.744536	5.548798	-0.011447	-0.011752	-0.017415
Li	5.924247	11.057064	0.817991	-0.011446	-0.011754	-0.017440
Na	2.049025	6.784862	1.629696	-0.000754	0.002511	-0.001213
Na	0.404117	7.016739	4.737094	-0.000748	0.002510	-0.001214
Na	2.558546	13.685662	1.553699	-0.000748	-0.002509	-0.001215
Na	-0.105403	0.115939	4.813091	-0.000755	-0.002513	-0.001215

B	4.155007	8.978944	1.168663	-0.012173	0.035005	-0.017174
B	-1.701865	4.822656	5.198127	-0.012071	0.034977	-0.017178
B	0.452564	2.078144	2.014732	-0.012087	-0.034947	-0.017176
B	2.000578	11.723457	4.352058	-0.012075	-0.035065	-0.017207
B	-2.733891	11.746082	5.839177	0.016542	-0.032733	0.018785
B	5.187034	2.055518	0.527613	0.016500	-0.032600	0.018671
B	3.032605	4.845282	3.711007	0.016514	0.032655	0.018689
B	-0.579463	8.956318	2.655782	0.016556	0.032761	0.018682
B	-0.983708	0.054306	1.827988	0.001736	0.001345	-0.014795
B	3.436850	13.747295	4.538802	0.001733	0.001338	-0.014800
B	5.591279	6.955106	1.355407	0.001747	-0.001334	-0.014789
B	-3.138137	6.846495	5.011383	0.001730	-0.001342	-0.014786
Si	0.631772	3.486686	4.508512	0.014956	-0.007811	-0.003405
Si	1.821370	10.314915	1.858278	0.014989	-0.007801	-0.003442
Si	-0.333059	10.387486	5.041673	0.014973	0.007803	-0.003422
Si	2.786201	3.414115	1.325117	0.014969	0.007801	-0.003411
O	0.061445	3.072947	3.041906	-0.003704	0.002961	-0.017386
O	2.391697	10.728653	3.324884	-0.003726	0.002949	-0.017445
O	4.546126	9.973747	0.141489	-0.003688	-0.002950	-0.017408
O	-2.092984	3.827853	6.225301	-0.003712	-0.002964	-0.017389
O	2.197450	3.933608	4.519003	0.009812	0.009814	-0.008438
O	0.255692	9.867992	1.847787	0.009878	0.009834	-0.008456
O	-1.898737	10.834409	5.031182	0.009818	-0.009806	-0.008448
O	4.351879	2.967192	1.335608	0.009818	-0.009833	-0.008461
O	-0.212316	4.798696	5.055280	-0.019914	0.018975	0.009427
O	2.665458	9.002905	1.311510	-0.019987	0.019065	0.009468
O	0.511030	11.699496	4.494905	-0.019958	-0.018984	0.009435
O	1.942113	2.102105	1.871885	-0.019930	-0.019004	0.009433
O	0.525580	2.169271	5.472081	-0.004568	-0.009840	0.024988
O	1.927562	11.632329	0.894709	-0.004609	-0.009944	0.025020
O	-0.226867	9.070071	4.078104	-0.004580	0.009854	0.025020
O	2.680009	4.731529	2.288686	-0.004582	0.009867	0.024977
O	0.058846	0.698526	2.444964	-0.019680	-0.019414	-0.006922
O	2.394296	13.103075	3.921826	-0.019758	-0.019396	-0.006980
O	4.548725	7.599326	0.738431	-0.019740	0.019406	-0.006988
O	-2.095583	6.202275	5.628359	-0.019701	0.019410	-0.006936

O	-2.459230	13.184059	5.445139	0.007430	0.013424	0.010671
O	4.912372	0.617542	0.921651	0.007367	0.013413	0.010635
O	2.757943	6.283259	4.105046	0.007383	-0.013413	0.010642
O	-0.304801	7.518342	2.261744	0.007440	-0.013439	0.010691
O	-0.175430	2.374756	0.744070	-0.008165	0.010920	0.000781
O	2.628573	11.426844	5.622720	-0.008153	0.010934	0.000848
O	4.783002	9.275557	2.439325	-0.008195	-0.010924	0.000820
O	-2.329859	4.526044	3.927465	-0.008161	-0.010931	0.000795
O	-1.223866	12.517207	2.155216	0.029259	0.024382	-0.003363
O	3.677009	1.284394	4.211574	0.029250	0.024456	-0.003375
O	5.831438	5.616407	1.028179	0.029227	-0.024458	-0.003367
O	-3.378295	8.185194	5.338611	0.029243	-0.024396	-0.003361
H	-0.637445	12.195109	2.878812	-0.235957	0.092394	0.234194
H	3.090587	1.606491	3.487978	-0.235685	0.092387	0.233914
H	5.245016	5.294309	0.304583	-0.235530	-0.092307	0.233750
H	-2.791874	8.507292	6.062207	-0.235708	-0.092355	0.233953

62 f = 23.004465 THz 144.541318 2PiTHz 767.346339 cm-1 95.138855
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.012219	0.007144	-0.017574
Li	-1.316675	4.156264	2.365404	-0.012175	0.007138	-0.017480
Li	-3.471104	2.744536	5.548798	0.012169	0.007132	0.017468
Li	5.924247	11.057064	0.817991	0.012204	0.007128	0.017559
Na	2.049025	6.784862	1.629696	-0.001721	0.001217	-0.001898
Na	0.404117	7.016739	4.737094	-0.001713	0.001202	-0.001892
Na	2.558546	13.685662	1.553699	0.001713	0.001202	0.001892
Na	-0.105403	0.115939	4.813091	0.001719	0.001213	0.001896
B	4.155007	8.978944	1.168663	0.022878	0.009778	-0.001170
B	-1.701865	4.822656	5.198127	0.022504	0.009678	-0.001044
B	0.452564	2.078144	2.014732	-0.022496	0.009683	0.001039
B	2.000578	11.723457	4.352058	-0.022911	0.009706	0.001139
B	-2.733891	11.746082	5.839177	0.010310	-0.039957	-0.026714
B	5.187034	2.055518	0.527613	0.010234	-0.039808	-0.026338
B	3.032605	4.845282	3.711007	-0.010242	-0.039815	0.026338
B	-0.579463	8.956318	2.655782	-0.010279	-0.039882	0.026751

B	-0.983708	0.054306	1.827988	-0.001746	-0.000115	0.012436
B	3.436850	13.747295	4.538802	-0.001706	-0.000109	0.012453
B	5.591279	6.955106	1.355407	0.001709	-0.000101	-0.012469
B	-3.138137	6.846495	5.011383	0.001750	-0.000111	-0.012449
Si	0.631772	3.486686	4.508512	0.002019	-0.001047	0.000429
Si	1.821370	10.314915	1.858278	0.001956	-0.001057	0.000538
Si	-0.333059	10.387486	5.041673	-0.001939	-0.001051	-0.000546
Si	2.786201	3.414115	1.325117	-0.002013	-0.001040	-0.000424
O	0.061445	3.072947	3.041906	0.008891	-0.003630	0.002523
O	2.391697	10.728653	3.324884	0.009034	-0.003597	0.002620
O	4.546126	9.973747	0.141489	-0.009033	-0.003597	-0.002656
O	-2.092984	3.827853	6.225301	-0.008898	-0.003636	-0.002520
O	2.197450	3.933608	4.519003	-0.015278	0.000217	-0.002695
O	0.255692	9.867992	1.847787	-0.015470	0.000150	-0.002726
O	-1.898737	10.834409	5.031182	0.015497	0.000142	0.002709
O	4.351879	2.967192	1.335608	0.015273	0.000213	0.002698
O	-0.212316	4.798696	5.055280	-0.000315	-0.001806	-0.006959
O	2.665458	9.002905	1.311510	-0.000273	-0.002023	-0.007077
O	0.511030	11.699496	4.494905	0.000230	-0.002049	0.007099
O	1.942113	2.102105	1.871885	0.000325	-0.001812	0.006955
O	0.525580	2.169271	5.472081	0.006574	0.014765	0.003987
O	1.927562	11.632329	0.894709	0.006684	0.015037	0.004010
O	-0.226867	9.070071	4.078104	-0.006690	0.015055	-0.003963
O	2.680009	4.731529	2.288686	-0.006570	0.014761	-0.003990
O	0.058846	0.698526	2.444964	-0.003600	0.000337	-0.005351
O	2.394296	13.103075	3.921826	-0.003544	0.000218	-0.005344
O	4.548725	7.599326	0.738431	0.003508	0.000250	0.005330
O	-2.095583	6.202275	5.628359	0.003601	0.000352	0.005361
O	-2.459230	13.184059	5.445139	0.016218	0.003584	0.008082
O	4.912372	0.617542	0.921651	0.016234	0.003512	0.008019
O	2.757943	6.283259	4.105046	-0.016245	0.003503	-0.008025
O	-0.304801	7.518342	2.261744	-0.016200	0.003585	-0.008059
O	-0.175430	2.374756	0.744070	-0.015964	0.001161	-0.002952
O	2.628573	11.426844	5.622720	-0.016151	0.001211	-0.003112
O	4.783002	9.275557	2.439325	0.016146	0.001185	0.003113
O	-2.329859	4.526044	3.927465	0.015962	0.001160	0.002943

O	-1.223866	12.517207	2.155216	-0.025251	0.006678	0.001096
O	3.677009	1.284394	4.211574	-0.025127	0.006746	0.001071
O	5.831438	5.616407	1.028179	0.025149	0.006692	-0.001076
O	-3.378295	8.185194	5.338611	0.025271	0.006688	-0.001092
H	-0.637445	12.195109	2.878812	0.303682	-0.061155	-0.290342
H	3.090587	1.606491	3.487978	0.302561	-0.060858	-0.289244
H	5.245016	5.294309	0.304583	-0.302697	-0.060937	0.289374
H	-2.791874	8.507292	6.062207	-0.303938	-0.061219	0.290594

63 f = 22.936628 THz 144.115081 2PiTHz 765.083519 cm-1 94.858301 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.007321	0.000445	-0.015200
Li	-1.316675	4.156264	2.365404	0.007397	-0.000486	0.015337
Li	-3.471104	2.744536	5.548798	-0.007407	-0.000498	-0.015338
Li	5.924247	11.057064	0.817991	0.007314	0.000440	0.015205
Na	2.049025	6.784862	1.629696	-0.001637	0.001906	-0.000664
Na	0.404117	7.016739	4.737094	0.001650	-0.001911	0.000656
Na	2.558546	13.685662	1.553699	-0.001650	-0.001913	-0.000657
Na	-0.105403	0.115939	4.813091	0.001639	0.001905	0.000664
B	4.155007	8.978944	1.168663	0.053867	0.004682	-0.009620
B	-1.701865	4.822656	5.198127	-0.054083	-0.004699	0.009578
B	0.452564	2.078144	2.014732	0.054053	-0.004767	-0.009613
B	2.000578	11.723457	4.352058	-0.053885	0.004651	0.009591
B	-2.733891	11.746082	5.839177	0.002970	-0.014127	-0.050573
B	5.187034	2.055518	0.527613	-0.003008	0.014340	0.050808
B	3.032605	4.845282	3.711007	0.003041	0.014434	-0.050776
B	-0.579463	8.956318	2.655782	-0.002971	-0.014098	0.050581
B	-0.983708	0.054306	1.827988	-0.004048	0.000938	-0.000758
B	3.436850	13.747295	4.538802	0.004065	-0.000929	0.000654
B	5.591279	6.955106	1.355407	-0.004056	-0.000934	-0.000673
B	-3.138137	6.846495	5.011383	0.004064	0.000940	0.000737
Si	0.631772	3.486686	4.508512	0.011115	0.001783	-0.018782
Si	1.821370	10.314915	1.858278	-0.011104	-0.001789	0.018757
Si	-0.333059	10.387486	5.041673	0.011115	-0.001783	-0.018747
Si	2.786201	3.414115	1.325117	-0.011100	0.001787	0.018774

O	0.061445	3.072947	3.041906	-0.017016	-0.005533	-0.012913
O	2.391697	10.728653	3.324884	0.016945	0.005561	0.012862
O	4.546126	9.973747	0.141489	-0.016959	0.005547	-0.012880
O	-2.092984	3.827853	6.225301	0.017007	-0.005540	0.012874
O	2.197450	3.933608	4.519003	0.025195	0.008680	0.003027
O	0.255692	9.867992	1.847787	-0.025046	-0.008679	-0.003023
O	-1.898737	10.834409	5.031182	0.025065	-0.008678	0.003016
O	4.351879	2.967192	1.335608	-0.025160	0.008682	-0.003037
O	-0.212316	4.798696	5.055280	-0.005029	0.027562	0.018723
O	2.665458	9.002905	1.311510	0.005001	-0.027483	-0.018646
O	0.511030	11.699496	4.494905	-0.005011	-0.027503	0.018652
O	1.942113	2.102105	1.871885	0.004982	0.027527	-0.018701
O	0.525580	2.169271	5.472081	-0.017697	-0.036718	-0.002191
O	1.927562	11.632329	0.894709	0.017633	0.036565	0.002185
O	-0.226867	9.070071	4.078104	-0.017624	0.036568	-0.002158
O	2.680009	4.731529	2.288686	0.017693	-0.036693	0.002242
O	0.058846	0.698526	2.444964	-0.007889	0.019640	-0.004990
O	2.394296	13.103075	3.921826	0.007897	-0.019672	0.005036
O	4.548725	7.599326	0.738431	-0.007898	-0.019623	-0.005002
O	-2.095583	6.202275	5.628359	0.007862	0.019688	0.005002
O	-2.459230	13.184059	5.445139	-0.002980	0.014594	0.004304
O	4.912372	0.617542	0.921651	0.002866	-0.014626	-0.004351
O	2.757943	6.283259	4.105046	-0.002866	-0.014602	0.004377
O	-0.304801	7.518342	2.261744	0.002958	0.014612	-0.004300
O	-0.175430	2.374756	0.744070	0.028620	-0.005838	0.025786
O	2.628573	11.426844	5.622720	-0.028482	0.005868	-0.025761
O	4.783002	9.275557	2.439325	0.028484	0.005824	0.025725
O	-2.329859	4.526044	3.927465	-0.028615	-0.005897	-0.025803
O	-1.223866	12.517207	2.155216	-0.018868	-0.004776	0.001963
O	3.677009	1.284394	4.211574	0.019063	0.004775	-0.001982
O	5.831438	5.616407	1.028179	-0.019043	0.004743	0.001971
O	-3.378295	8.185194	5.338611	0.018878	-0.004848	-0.001976
H	-0.637445	12.195109	2.878812	0.179122	-0.043226	-0.176057
H	3.090587	1.606491	3.487978	-0.181316	0.043741	0.178159
H	5.245016	5.294309	0.304583	0.181179	0.043639	-0.178018
H	-2.791874	8.507292	6.062207	-0.179160	-0.043310	0.176083

64 f = 22.721266 THz 142.761924 2PiTHz 757.899829 cm-1 93.967636

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.006308	0.011506	-0.017236
Li	-1.316675	4.156264	2.365404	0.006342	-0.011523	0.017279
Li	-3.471104	2.744536	5.548798	0.006333	0.011523	0.017254
Li	5.924247	11.057064	0.817991	-0.006309	-0.011506	-0.017240
Na	2.049025	6.784862	1.629696	-0.001887	0.001976	-0.002044
Na	0.404117	7.016739	4.737094	0.001890	-0.001975	0.002043
Na	2.558546	13.685662	1.553699	0.001888	0.001975	0.002042
Na	-0.105403	0.115939	4.813091	-0.001887	-0.001974	-0.002044
B	4.155007	8.978944	1.168663	0.008423	0.008210	-0.008854
B	-1.701865	4.822656	5.198127	-0.008435	-0.008265	0.008865
B	0.452564	2.078144	2.014732	-0.008420	0.008258	0.008884
B	2.000578	11.723457	4.352058	0.008403	-0.008218	-0.008835
B	-2.733891	11.746082	5.839177	0.017337	-0.045387	0.028357
B	5.187034	2.055518	0.527613	-0.017342	0.045435	-0.028368
B	3.032605	4.845282	3.711007	-0.017335	-0.045411	-0.028384
B	-0.579463	8.956318	2.655782	0.017346	0.045399	0.028374
B	-0.983708	0.054306	1.827988	-0.004622	0.003106	0.003964
B	3.436850	13.747295	4.538802	0.004612	-0.003101	-0.003929
B	5.591279	6.955106	1.355407	0.004608	0.003096	-0.003923
B	-3.138137	6.846495	5.011383	-0.004620	-0.003103	0.003968
Si	0.631772	3.486686	4.508512	-0.000837	-0.005602	0.013729
Si	1.821370	10.314915	1.858278	0.000811	0.005618	-0.013738
Si	-0.333059	10.387486	5.041673	0.000820	-0.005616	-0.013748
Si	2.786201	3.414115	1.325117	-0.000833	0.005604	0.013736
O	0.061445	3.072947	3.041906	-0.002079	0.007189	0.010773
O	2.391697	10.728653	3.324884	0.002105	-0.007202	-0.010752
O	4.546126	9.973747	0.141489	0.002097	0.007208	-0.010760
O	-2.092984	3.827853	6.225301	-0.002079	-0.007188	0.010771
O	2.197450	3.933608	4.519003	-0.007037	-0.002645	0.001164
O	0.255692	9.867992	1.847787	0.007029	0.002626	-0.001160
O	-1.898737	10.834409	5.031182	0.007038	-0.002630	-0.001159
O	4.351879	2.967192	1.335608	-0.007044	0.002641	0.001160

O	-0.212316	4.798696	5.055280	0.016588	-0.006305	-0.003593
O	2.665458	9.002905	1.311510	-0.016587	0.006269	0.003592
O	0.511030	11.699496	4.494905	-0.016591	-0.006288	0.003599
O	1.942113	2.102105	1.871885	0.016582	0.006302	-0.003601
O	0.525580	2.169271	5.472081	0.009046	0.014737	-0.011385
O	1.927562	11.632329	0.894709	-0.009046	-0.014730	0.011358
O	-0.226867	9.070071	4.078104	-0.009051	0.014744	0.011364
O	2.680009	4.731529	2.288686	0.009054	-0.014742	-0.011378
O	0.058846	0.698526	2.444964	0.018232	-0.008430	0.013688
O	2.394296	13.103075	3.921826	-0.018226	0.008481	-0.013727
O	4.548725	7.599326	0.738431	-0.018228	-0.008489	-0.013726
O	-2.095583	6.202275	5.628359	0.018233	0.008445	0.013699
O	-2.459230	13.184059	5.445139	0.018265	0.001164	0.013585
O	4.912372	0.617542	0.921651	-0.018232	-0.001173	-0.013572
O	2.757943	6.283259	4.105046	-0.018229	0.001175	-0.013575
O	-0.304801	7.518342	2.261744	0.018273	-0.001157	0.013583
O	-0.175430	2.374756	0.744070	-0.002410	-0.001216	-0.019167
O	2.628573	11.426844	5.622720	0.002411	0.001175	0.019197
O	4.783002	9.275557	2.439325	0.002423	-0.001177	0.019199
O	-2.329859	4.526044	3.927465	-0.002417	0.001201	-0.019192
O	-1.223866	12.517207	2.155216	0.023951	-0.017065	-0.000255
O	3.677009	1.284394	4.211574	-0.023993	0.017039	0.000255
O	5.831438	5.616407	1.028179	-0.024017	-0.017037	0.000250
O	-3.378295	8.185194	5.338611	0.023940	0.017060	-0.000257
H	-0.637445	12.195109	2.878812	-0.275951	0.047155	0.266709
H	3.090587	1.606491	3.487978	0.276266	-0.047278	-0.267033
H	5.245016	5.294309	0.304583	0.276526	0.047315	-0.267279
H	-2.791874	8.507292	6.062207	-0.275878	-0.047155	0.266640

65 f = 22.037936 THz 138.468434 2PiTHz 735.106389 cm-1 91.141609
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002117	-0.007543	-0.014736
Li	-1.316675	4.156264	2.365404	0.002834	-0.007981	-0.015619
Li	-3.471104	2.744536	5.548798	-0.002834	-0.007974	0.015616
Li	5.924247	11.057064	0.817991	-0.002117	-0.007549	0.014740

Na	2.049025	6.784862	1.629696	-0.000148	-0.000048	0.001046
Na	0.404117	7.016739	4.737094	-0.000084	-0.000056	0.001064
Na	2.558546	13.685662	1.553699	0.000084	-0.000059	-0.001064
Na	-0.105403	0.115939	4.813091	0.000148	-0.000046	-0.001045
B	4.155007	8.978944	1.168663	0.012496	-0.001751	0.037399
B	-1.701865	4.822656	5.198127	0.012093	-0.001881	0.038641
B	0.452564	2.078144	2.014732	-0.012113	-0.001880	-0.038641
B	2.000578	11.723457	4.352058	-0.012479	-0.001754	-0.037406
B	-2.733891	11.746082	5.839177	-0.034251	0.008049	-0.005511
B	5.187034	2.055518	0.527613	-0.035599	0.008541	-0.005390
B	3.032605	4.845282	3.711007	0.035585	0.008522	0.005389
B	-0.579463	8.956318	2.655782	0.034262	0.008067	0.005512
B	-0.983708	0.054306	1.827988	0.000760	-0.001902	-0.016255
B	3.436850	13.747295	4.538802	-0.000146	-0.001526	-0.014767
B	5.591279	6.955106	1.355407	0.000143	-0.001535	0.014775
B	-3.138137	6.846495	5.011383	-0.000756	-0.001891	0.016245
Si	0.631772	3.486686	4.508512	-0.010283	-0.002221	0.031487
Si	1.821370	10.314915	1.858278	-0.010356	-0.002330	0.030410
Si	-0.333059	10.387486	5.041673	0.010349	-0.002335	-0.030414
Si	2.786201	3.414115	1.325117	0.010293	-0.002215	-0.031483
O	0.061445	3.072947	3.041906	-0.010172	0.010376	-0.011951
O	2.391697	10.728653	3.324884	-0.009482	0.009841	-0.011583
O	4.546126	9.973747	0.141489	0.009478	0.009840	0.011578
O	-2.092984	3.827853	6.225301	0.010176	0.010378	0.011955
O	2.197450	3.933608	4.519003	0.005018	-0.001606	0.003842
O	0.255692	9.867992	1.847787	0.004801	-0.001753	0.003890
O	-1.898737	10.834409	5.031182	-0.004796	-0.001743	-0.003886
O	4.351879	2.967192	1.335608	-0.005023	-0.001615	-0.003847
O	-0.212316	4.798696	5.055280	-0.015973	-0.006376	-0.017794
O	2.665458	9.002905	1.311510	-0.015574	-0.006115	-0.017367
O	0.511030	11.699496	4.494905	0.015561	-0.006113	0.017366
O	1.942113	2.102105	1.871885	0.015985	-0.006380	0.017796
O	0.525580	2.169271	5.472081	0.024866	0.009566	0.020930
O	1.927562	11.632329	0.894709	0.024263	0.009541	0.020323
O	-0.226867	9.070071	4.078104	-0.024260	0.009542	-0.020314
O	2.680009	4.731529	2.288686	-0.024866	0.009562	-0.020932

O	0.058846	0.698526	2.444964	0.008733	-0.048664	0.048204
O	2.394296	13.103075	3.921826	0.008067	-0.046598	0.045351
O	4.548725	7.599326	0.738431	-0.008057	-0.046604	-0.045349
O	-2.095583	6.202275	5.628359	-0.008745	-0.048659	-0.048207
O	-2.459230	13.184059	5.445139	-0.012776	0.006403	-0.013382
O	4.912372	0.617542	0.921651	-0.014371	0.005598	-0.013855
O	2.757943	6.283259	4.105046	0.014384	0.005588	0.013866
O	-0.304801	7.518342	2.261744	0.012763	0.006415	0.013372
O	-0.175430	2.374756	0.744070	-0.020204	0.026506	-0.057232
O	2.628573	11.426844	5.622720	-0.020650	0.024707	-0.054491
O	4.783002	9.275557	2.439325	0.020658	0.024690	0.054495
O	-2.329859	4.526044	3.927465	0.020192	0.026524	0.057222
O	-1.223866	12.517207	2.155216	0.004875	0.006045	0.005412
O	3.677009	1.284394	4.211574	0.005417	0.005444	0.004999
O	5.831438	5.616407	1.028179	-0.005416	0.005429	-0.005003
O	-3.378295	8.185194	5.338611	-0.004878	0.006058	-0.005407
H	-0.637445	12.195109	2.878812	0.026659	0.044519	0.004060
H	3.090587	1.606491	3.487978	0.020218	0.044189	0.009335
H	5.245016	5.294309	0.304583	-0.020217	0.044212	-0.009356
H	-2.791874	8.507292	6.062207	-0.026658	0.044502	-0.004045

66 f = 22.031121 THz 138.425616 2PiTHz 734.879074 cm-1 91.113426 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.013859	0.008130	0.018239
Li	-1.316675	4.156264	2.365404	0.013676	-0.007724	-0.017363
Li	-3.471104	2.744536	5.548798	-0.013684	-0.007705	0.017412
Li	5.924247	11.057064	0.817991	0.013803	0.008129	-0.018145
Na	2.049025	6.784862	1.629696	-0.001226	0.000221	-0.000587
Na	0.404117	7.016739	4.737094	0.001237	-0.000231	0.000541
Na	2.558546	13.685662	1.553699	-0.001231	-0.000221	-0.000545
Na	-0.105403	0.115939	4.813091	0.001227	0.000230	0.000584
B	4.155007	8.978944	1.168663	0.006963	0.002785	-0.023315
B	-1.701865	4.822656	5.198127	-0.007601	-0.002685	0.021278
B	0.452564	2.078144	2.014732	0.007575	-0.002700	-0.021339
B	2.000578	11.723457	4.352058	-0.006975	0.002754	0.023187

B	-2.733891	11.746082	5.839177	0.025164	-0.008513	-0.001285
B	5.187034	2.055518	0.527613	-0.023402	0.008127	0.001505
B	3.032605	4.845282	3.711007	0.023367	0.008091	-0.001548
B	-0.579463	8.956318	2.655782	-0.025214	-0.008541	0.001231
B	-0.983708	0.054306	1.827988	0.017893	-0.007265	-0.028882
B	3.436850	13.747295	4.538802	-0.017886	0.007337	0.029617
B	5.591279	6.955106	1.355407	0.017948	0.007361	-0.029734
B	-3.138137	6.846495	5.011383	-0.017895	-0.007259	0.028858
Si	0.631772	3.486686	4.508512	0.002260	0.002237	0.019396
Si	1.821370	10.314915	1.858278	-0.001729	-0.002143	-0.020910
Si	-0.333059	10.387486	5.041673	0.001758	-0.002101	0.020999
Si	2.786201	3.414115	1.325117	-0.002245	0.002260	-0.019347
O	0.061445	3.072947	3.041906	-0.012474	0.009884	-0.006292
O	2.391697	10.728653	3.324884	0.012959	-0.010361	0.006902
O	4.546126	9.973747	0.141489	-0.013016	-0.010414	-0.006934
O	-2.092984	3.827853	6.225301	0.012448	0.009849	0.006284
O	2.197450	3.933608	4.519003	0.003432	0.002703	-0.001572
O	0.255692	9.867992	1.847787	-0.003659	-0.002611	0.001334
O	-1.898737	10.834409	5.031182	0.003688	-0.002628	-0.001363
O	4.351879	2.967192	1.335608	-0.003421	0.002701	0.001555
O	-0.212316	4.798696	5.055280	-0.006884	-0.004370	-0.007503
O	2.665458	9.002905	1.311510	0.007687	0.004711	0.008416
O	0.511030	11.699496	4.494905	-0.007682	0.004674	-0.008394
O	1.942113	2.102105	1.871885	0.006900	-0.004387	0.007516
O	0.525580	2.169271	5.472081	0.010451	0.000114	0.010650
O	1.927562	11.632329	0.894709	-0.011664	-0.000565	-0.011679
O	-0.226867	9.070071	4.078104	0.011715	-0.000611	0.011749
O	2.680009	4.731529	2.288686	-0.010416	0.000079	-0.010618
O	0.058846	0.698526	2.444964	0.013186	-0.038883	0.054373
O	2.394296	13.103075	3.921826	-0.013581	0.041183	-0.056613
O	4.548725	7.599326	0.738431	0.013678	0.041416	0.056914
O	-2.095583	6.202275	5.628359	-0.013134	-0.038772	-0.054247
O	-2.459230	13.184059	5.445139	0.032853	0.016530	0.009421
O	4.912372	0.617542	0.921651	-0.032254	-0.016869	-0.008750
O	2.757943	6.283259	4.105046	0.032164	-0.016820	0.008709
O	-0.304801	7.518342	2.261744	-0.033063	0.016648	-0.009477

O	-0.175430	2.374756	0.744070	0.011096	0.035539	-0.051518
O	2.628573	11.426844	5.622720	-0.010066	-0.036763	0.054239
O	4.783002	9.275557	2.439325	0.010117	-0.036977	-0.054497
O	-2.329859	4.526044	3.927465	-0.011089	0.035460	0.051402
O	-1.223866	12.517207	2.155216	-0.009881	0.012250	0.007761
O	3.677009	1.284394	4.211574	0.009628	-0.012506	-0.008022
O	5.831438	5.616407	1.028179	-0.009643	-0.012597	0.008028
O	-3.378295	8.185194	5.338611	0.009890	0.012213	-0.007766
H	-0.637445	12.195109	2.878812	0.116791	0.006604	-0.095902
H	3.090587	1.606491	3.487978	-0.117998	-0.008815	0.095594
H	5.245016	5.294309	0.304583	0.118297	-0.008883	-0.095841
H	-2.791874	8.507292	6.062207	-0.116783	0.006595	0.095895

67 f = 21.939382 THz 137.849203 2PiTHz 731.818990 cm-1 90.734023 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.014566	0.005659	0.015329
Li	-1.316675	4.156264	2.365404	0.014633	-0.005683	-0.015443
Li	-3.471104	2.744536	5.548798	0.014636	0.005686	-0.015451
Li	5.924247	11.057064	0.817991	-0.014601	-0.005682	0.015368
Na	2.049025	6.784862	1.629696	-0.001339	-0.000130	-0.000112
Na	0.404117	7.016739	4.737094	0.001339	0.000134	0.000128
Na	2.558546	13.685662	1.553699	0.001340	-0.000133	0.000130
Na	-0.105403	0.115939	4.813091	-0.001342	0.000130	-0.000114
B	4.155007	8.978944	1.168663	-0.000623	0.009392	-0.024951
B	-1.701865	4.822656	5.198127	0.000628	-0.009391	0.025093
B	0.452564	2.078144	2.014732	0.000646	0.009398	0.025137
B	2.000578	11.723457	4.352058	-0.000592	-0.009392	-0.024978
B	-2.733891	11.746082	5.839177	-0.009952	-0.003029	-0.003106
B	5.187034	2.055518	0.527613	0.010052	0.002988	0.003178
B	3.032605	4.845282	3.711007	0.009970	-0.003003	0.003179
B	-0.579463	8.956318	2.655782	-0.009951	0.003034	-0.003114
B	-0.983708	0.054306	1.827988	-0.021613	0.008694	0.033914
B	3.436850	13.747295	4.538802	0.021592	-0.008694	-0.033827
B	5.591279	6.955106	1.355407	0.021545	0.008681	-0.033774
B	-3.138137	6.846495	5.011383	-0.021602	-0.008675	0.033871

Si	0.631772	3.486686	4.508512	-0.009147	0.008680	-0.013938
Si	1.821370	10.314915	1.858278	0.009138	-0.008619	0.013822
Si	-0.333059	10.387486	5.041673	0.009110	0.008631	0.013805
Si	2.786201	3.414115	1.325117	-0.009177	-0.008677	-0.013892
O	0.061445	3.072947	3.041906	0.011510	-0.008308	0.008931
O	2.391697	10.728653	3.324884	-0.011457	0.008248	-0.008897
O	4.546126	9.973747	0.141489	-0.011433	-0.008233	-0.008891
O	-2.092984	3.827853	6.225301	0.011498	0.008291	0.008916
O	2.197450	3.933608	4.519003	-0.005594	-0.006034	0.006592
O	0.255692	9.867992	1.847787	0.005554	0.006035	-0.006566
O	-1.898737	10.834409	5.031182	0.005558	-0.006016	-0.006554
O	4.351879	2.967192	1.335608	-0.005578	0.006044	0.006602
O	-0.212316	4.798696	5.055280	0.002205	-0.009461	-0.005147
O	2.665458	9.002905	1.311510	-0.002188	0.009418	0.005125
O	0.511030	11.699496	4.494905	-0.002194	-0.009423	0.005127
O	1.942113	2.102105	1.871885	0.002174	0.009474	-0.005173
O	0.525580	2.169271	5.472081	-0.007031	-0.006276	-0.016616
O	1.927562	11.632329	0.894709	0.006949	0.006208	0.016523
O	-0.226867	9.070071	4.078104	0.006951	-0.006220	0.016513
O	2.680009	4.731529	2.288686	-0.006991	0.006260	-0.016589
O	0.058846	0.698526	2.444964	-0.011400	0.043797	-0.056852
O	2.394296	13.103075	3.921826	0.011318	-0.043534	0.056563
O	4.548725	7.599326	0.738431	0.011280	0.043465	0.056447
O	-2.095583	6.202275	5.628359	-0.011408	-0.043745	-0.056806
O	-2.459230	13.184059	5.445139	-0.035215	-0.017068	-0.003629
O	4.912372	0.617542	0.921651	0.035360	0.017115	0.003696
O	2.757943	6.283259	4.105046	0.035370	-0.017159	0.003687
O	-0.304801	7.518342	2.261744	-0.035123	0.016989	-0.003616
O	-0.175430	2.374756	0.744070	-0.008653	-0.042996	0.048681
O	2.628573	11.426844	5.622720	0.008684	0.042811	-0.048393
O	4.783002	9.275557	2.439325	0.008613	-0.042715	-0.048292
O	-2.329859	4.526044	3.927465	-0.008708	0.042991	0.048625
O	-1.223866	12.517207	2.155216	0.006576	-0.019272	-0.005809
O	3.677009	1.284394	4.211574	-0.006571	0.019211	0.005782
O	5.831438	5.616407	1.028179	-0.006542	-0.019182	0.005776
O	-3.378295	8.185194	5.338611	0.006567	0.019267	-0.005786

H	-0.637445	12.195109	2.878812	-0.082816	-0.027901	0.062205
H	3.090587	1.606491	3.487978	0.082403	0.027800	-0.061914
H	5.245016	5.294309	0.304583	0.082202	-0.027812	-0.061719
H	-2.791874	8.507292	6.062207	-0.082610	0.027871	0.062067

68 f = 21.857900 THz 137.337239 2PiTHz 729.101058 cm-1 90.397043
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.009519	-0.000631	-0.017771
Li	-1.316675	4.156264	2.365404	0.009501	-0.000639	-0.017720
Li	-3.471104	2.744536	5.548798	0.009426	0.000586	-0.017651
Li	5.924247	11.057064	0.817991	0.009577	0.000671	-0.017809
Na	2.049025	6.784862	1.629696	-0.000516	0.001183	0.000744
Na	0.404117	7.016739	4.737094	-0.000519	0.001183	0.000728
Na	2.558546	13.685662	1.553699	-0.000524	-0.001183	0.000726
Na	-0.105403	0.115939	4.813091	-0.000511	-0.001180	0.000745
B	4.155007	8.978944	1.168663	0.007761	-0.006992	0.027738
B	-1.701865	4.822656	5.198127	0.007713	-0.006897	0.027758
B	0.452564	2.078144	2.014732	0.007783	0.006940	0.027667
B	2.000578	11.723457	4.352058	0.007712	0.006965	0.027865
B	-2.733891	11.746082	5.839177	0.014016	-0.002427	0.011913
B	5.187034	2.055518	0.527613	0.013940	-0.002404	0.011953
B	3.032605	4.845282	3.711007	0.014011	0.002478	0.011911
B	-0.579463	8.956318	2.655782	0.013893	0.002342	0.011976
B	-0.983708	0.054306	1.827988	-0.006698	0.001207	0.016824
B	3.436850	13.747295	4.538802	-0.006918	0.001293	0.017153
B	5.591279	6.955106	1.355407	-0.006859	-0.001260	0.017043
B	-3.138137	6.846495	5.011383	-0.006776	-0.001232	0.016931
Si	0.631772	3.486686	4.508512	-0.008367	0.009834	-0.019020
Si	1.821370	10.314915	1.858278	-0.008386	0.009866	-0.019138
Si	-0.333059	10.387486	5.041673	-0.008401	-0.009865	-0.019066
Si	2.786201	3.414115	1.325117	-0.008386	-0.009838	-0.019068
O	0.061445	3.072947	3.041906	0.011781	-0.011062	0.006450
O	2.391697	10.728653	3.324884	0.011889	-0.011117	0.006548
O	4.546126	9.973747	0.141489	0.011833	0.011097	0.006501
O	-2.092984	3.827853	6.225301	0.011831	0.011079	0.006494

O	2.197450	3.933608	4.519003	-0.005869	-0.002308	0.006702
O	0.255692	9.867992	1.847787	-0.005950	-0.002341	0.006705
O	-1.898737	10.834409	5.031182	-0.005904	0.002345	0.006739
O	4.351879	2.967192	1.335608	-0.005887	0.002318	0.006679
O	-0.212316	4.798696	5.055280	-0.001056	-0.009582	-0.006433
O	2.665458	9.002905	1.311510	-0.001010	-0.009609	-0.006427
O	0.511030	11.699496	4.494905	-0.001045	0.009621	-0.006456
O	1.942113	2.102105	1.871885	-0.001066	0.009581	-0.006420
O	0.525580	2.169271	5.472081	-0.011947	-0.011169	-0.016114
O	1.927562	11.632329	0.894709	-0.012000	-0.011180	-0.016279
O	-0.226867	9.070071	4.078104	-0.011948	0.011183	-0.016209
O	2.680009	4.731529	2.288686	-0.011976	0.011163	-0.016180
O	0.058846	0.698526	2.444964	-0.017093	0.047150	-0.054864
O	2.394296	13.103075	3.921826	-0.017214	0.047502	-0.055387
O	4.548725	7.599326	0.738431	-0.017176	-0.047381	-0.055200
O	-2.095583	6.202275	5.628359	-0.017168	-0.047278	-0.055091
O	-2.459230	13.184059	5.445139	0.033029	0.016969	0.011502
O	4.912372	0.617542	0.921651	0.032671	0.016759	0.011455
O	2.757943	6.283259	4.105046	0.032822	-0.016861	0.011503
O	-0.304801	7.518342	2.261744	0.032949	-0.016952	0.011458
O	-0.175430	2.374756	0.744070	-0.003975	-0.040559	0.054196
O	2.628573	11.426844	5.622720	-0.004152	-0.040948	0.054603
O	4.783002	9.275557	2.439325	-0.004150	0.040856	0.054436
O	-2.329859	4.526044	3.927465	-0.004057	0.040705	0.054379
O	-1.223866	12.517207	2.155216	0.000804	-0.015232	-0.002570
O	3.677009	1.284394	4.211574	0.000906	-0.015398	-0.002636
O	5.831438	5.616407	1.028179	0.000858	0.015378	-0.002597
O	-3.378295	8.185194	5.338611	0.000868	0.015274	-0.002595
H	-0.637445	12.195109	2.878812	-0.065822	-0.016296	0.049913
H	3.090587	1.606491	3.487978	-0.066919	-0.016393	0.050842
H	5.245016	5.294309	0.304583	-0.066389	0.016406	0.050405
H	-2.791874	8.507292	6.062207	-0.066442	0.016237	0.050477

69 f = 21.571011 THz 135.534661 2PiTHz 719.531463 cm-1 89.210564
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.013439	-0.009793	-0.017221
Li	-1.316675	4.156264	2.365404	0.013364	-0.009805	-0.017081
Li	-3.471104	2.744536	5.548798	-0.013365	-0.009785	0.017075
Li	5.924247	11.057064	0.817991	-0.013438	-0.009794	0.017232
Na	2.049025	6.784862	1.629696	-0.000233	0.001393	0.000503
Na	0.404117	7.016739	4.737094	-0.000234	0.001389	0.000513
Na	2.558546	13.685662	1.553699	0.000237	0.001392	-0.000513
Na	-0.105403	0.115939	4.813091	0.000232	0.001387	-0.000502
B	4.155007	8.978944	1.168663	-0.012485	0.007514	-0.019727
B	-1.701865	4.822656	5.198127	-0.012380	0.007514	-0.019414
B	0.452564	2.078144	2.014732	0.012251	0.007478	0.019219
B	2.000578	11.723457	4.352058	0.012540	0.007530	0.019804
B	-2.733891	11.746082	5.839177	0.029405	-0.004074	-0.013071
B	5.187034	2.055518	0.527613	0.028696	-0.003999	-0.012832
B	3.032605	4.845282	3.711007	-0.028907	-0.004037	0.012846
B	-0.579463	8.956318	2.655782	-0.029336	-0.004071	0.013039
B	-0.983708	0.054306	1.827988	0.015502	0.001555	-0.006115
B	3.436850	13.747295	4.538802	0.015739	0.001597	-0.006190
B	5.591279	6.955106	1.355407	-0.015730	0.001586	0.006205
B	-3.138137	6.846495	5.011383	-0.015539	0.001577	0.006083
Si	0.631772	3.486686	4.508512	0.021537	-0.000679	-0.012216
Si	1.821370	10.314915	1.858278	0.021705	-0.000658	-0.012588
Si	-0.333059	10.387486	5.041673	-0.021781	-0.000694	0.012564
Si	2.786201	3.414115	1.325117	-0.021366	-0.000586	0.012311
O	0.061445	3.072947	3.041906	0.004309	-0.001047	0.001519
O	2.391697	10.728653	3.324884	0.004513	-0.001180	0.001586
O	4.546126	9.973747	0.141489	-0.004478	-0.001151	-0.001576
O	-2.092984	3.827853	6.225301	-0.004394	-0.001131	-0.001523
O	2.197450	3.933608	4.519003	-0.017320	0.009510	-0.005907
O	0.255692	9.867992	1.847787	-0.017545	0.009552	-0.005924
O	-1.898737	10.834409	5.031182	0.017566	0.009594	0.005966
O	4.351879	2.967192	1.335608	0.017278	0.009430	0.005806
O	-0.212316	4.798696	5.055280	0.027392	0.004416	0.008717
O	2.665458	9.002905	1.311510	0.027701	0.004503	0.008868
O	0.511030	11.699496	4.494905	-0.027739	0.004548	-0.008890
O	1.942113	2.102105	1.871885	-0.027282	0.004317	-0.008663

O	0.525580	2.169271	5.472081	-0.011994	-0.000051	-0.000479
O	1.927562	11.632329	0.894709	-0.012310	-0.000156	-0.000667
O	-0.226867	9.070071	4.078104	0.012288	-0.000123	0.000622
O	2.680009	4.731529	2.288686	0.012073	-0.000149	0.000574
O	0.058846	0.698526	2.444964	0.023278	-0.009338	0.030364
O	2.394296	13.103075	3.921826	0.023497	-0.009119	0.030413
O	4.548725	7.599326	0.738431	-0.023471	-0.009175	-0.030427
O	-2.095583	6.202275	5.628359	-0.023316	-0.009180	-0.030292
O	-2.459230	13.184059	5.445139	-0.049271	-0.054672	-0.001334
O	4.912372	0.617542	0.921651	-0.048634	-0.053930	-0.001413
O	2.757943	6.283259	4.105046	0.048761	-0.054129	0.001394
O	-0.304801	7.518342	2.261744	0.049213	-0.054598	0.001332
O	-0.175430	2.374756	0.744070	0.049806	0.036597	-0.016981
O	2.628573	11.426844	5.622720	0.050629	0.036923	-0.016721
O	4.783002	9.275557	2.439325	-0.050539	0.036900	0.016766
O	-2.329859	4.526044	3.927465	-0.050043	0.036630	0.016827
O	-1.223866	12.517207	2.155216	-0.008082	0.015080	-0.007138
O	3.677009	1.284394	4.211574	-0.007998	0.015239	-0.007238
O	5.831438	5.616407	1.028179	0.007997	0.015222	0.007235
O	-3.378295	8.185194	5.338611	0.008084	0.015111	0.007177
H	-0.637445	12.195109	2.878812	0.016294	-0.016476	-0.039522
H	3.090587	1.606491	3.487978	0.014086	-0.016401	-0.037902
H	5.245016	5.294309	0.304583	-0.014147	-0.016262	0.037861
H	-2.791874	8.507292	6.062207	-0.015869	-0.016617	0.039313

70 f = 21.480656 THz 134.966942 2PiTHz 716.517537 cm-1 88.836884 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.006021	0.007818	0.006921
Li	-1.316675	4.156264	2.365404	-0.006025	0.007822	0.006859
Li	-3.471104	2.744536	5.548798	-0.006014	-0.007819	0.006855
Li	5.924247	11.057064	0.817991	-0.006072	-0.007851	0.006973
Na	2.049025	6.784862	1.629696	-0.000550	-0.001465	-0.000773
Na	0.404117	7.016739	4.737094	-0.000545	-0.001477	-0.000770
Na	2.558546	13.685662	1.553699	-0.000542	0.001480	-0.000774
Na	-0.105403	0.115939	4.813091	-0.000552	0.001466	-0.000771

B	4.155007	8.978944	1.168663	0.021864	-0.003404	0.024848
B	-1.701865	4.822656	5.198127	0.021721	-0.003411	0.024622
B	0.452564	2.078144	2.014732	0.021693	0.003399	0.024595
B	2.000578	11.723457	4.352058	0.021924	0.003440	0.024932
B	-2.733891	11.746082	5.839177	0.037205	-0.008393	-0.000886
B	5.187034	2.055518	0.527613	0.036764	-0.008383	-0.000816
B	3.032605	4.845282	3.711007	0.036817	0.008344	-0.000823
B	-0.579463	8.956318	2.655782	0.037074	0.008427	-0.000839
B	-0.983708	0.054306	1.827988	0.016542	0.002197	-0.004307
B	3.436850	13.747295	4.538802	0.016778	0.002162	-0.004477
B	5.591279	6.955106	1.355407	0.016691	-0.002173	-0.004410
B	-3.138137	6.846495	5.011383	0.016579	-0.002182	-0.004356
Si	0.631772	3.486686	4.508512	-0.028686	0.013673	-0.014499
Si	1.821370	10.314915	1.858278	-0.028899	0.013785	-0.014667
Si	-0.333059	10.387486	5.041673	-0.028974	-0.013800	-0.014601
Si	2.786201	3.414115	1.325117	-0.028674	-0.013663	-0.014530
O	0.061445	3.072947	3.041906	0.011990	-0.014272	-0.003579
O	2.391697	10.728653	3.324884	0.012124	-0.014387	-0.003594
O	4.546126	9.973747	0.141489	0.012095	0.014369	-0.003594
O	-2.092984	3.827853	6.225301	0.012005	0.014288	-0.003585
O	2.197450	3.933608	4.519003	0.010614	-0.013104	0.016301
O	0.255692	9.867992	1.847787	0.010663	-0.013200	0.016413
O	-1.898737	10.834409	5.031182	0.010729	0.013221	0.016424
O	4.351879	2.967192	1.335608	0.010602	0.013109	0.016304
O	-0.212316	4.798696	5.055280	-0.022711	-0.014595	-0.007419
O	2.665458	9.002905	1.311510	-0.022833	-0.014730	-0.007469
O	0.511030	11.699496	4.494905	-0.022953	0.014764	-0.007511
O	1.942113	2.102105	1.871885	-0.022671	0.014568	-0.007400
O	0.525580	2.169271	5.472081	-0.011705	-0.016336	-0.010076
O	1.927562	11.632329	0.894709	-0.011865	-0.016480	-0.010185
O	-0.226867	9.070071	4.078104	-0.011812	0.016477	-0.010181
O	2.680009	4.731529	2.288686	-0.011726	0.016342	-0.010079
O	0.058846	0.698526	2.444964	0.014956	0.011356	0.011669
O	2.394296	13.103075	3.921826	0.015059	0.011491	0.011769
O	4.548725	7.599326	0.738431	0.014990	-0.011495	0.011674
O	-2.095583	6.202275	5.628359	0.014952	-0.011382	0.011670

O	-2.459230	13.184059	5.445139	-0.041920	-0.052688	0.003211
O	4.912372	0.617542	0.921651	-0.041471	-0.052192	0.003146
O	2.757943	6.283259	4.105046	-0.041511	0.052216	0.003157
O	-0.304801	7.518342	2.261744	-0.041740	0.052514	0.003200
O	-0.175430	2.374756	0.744070	0.049919	0.025154	0.007875
O	2.628573	11.426844	5.622720	0.050482	0.025385	0.008003
O	4.783002	9.275557	2.439325	0.050300	-0.025275	0.008020
O	-2.329859	4.526044	3.927465	0.049962	-0.025157	0.007907
O	-1.223866	12.517207	2.155216	-0.002559	0.011281	-0.011336
O	3.677009	1.284394	4.211574	-0.002593	0.011398	-0.011364
O	5.831438	5.616407	1.028179	-0.002574	-0.011356	-0.011346
O	-3.378295	8.185194	5.338611	-0.002556	-0.011284	-0.011329
H	-0.637445	12.195109	2.878812	-0.094423	0.005694	0.060840
H	3.090587	1.606491	3.487978	-0.095068	0.005520	0.061126
H	5.245016	5.294309	0.304583	-0.094856	-0.005540	0.061022
H	-2.791874	8.507292	6.062207	-0.094643	-0.005717	0.061025

71 f = 21.457529 THz 134.821629 2PiTHz 715.746094 cm-1 88.741238 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.007264	-0.001414	-0.011418
Li	-1.316675	4.156264	2.365404	-0.007439	0.001554	0.011659
Li	-3.471104	2.744536	5.548798	0.007448	0.001556	-0.011668
Li	5.924247	11.057064	0.817991	-0.007252	-0.001413	0.011397
Na	2.049025	6.784862	1.629696	0.000493	-0.000124	-0.001312
Na	0.404117	7.016739	4.737094	-0.000490	0.000111	0.001313
Na	2.558546	13.685662	1.553699	0.000490	0.000103	-0.001312
Na	-0.105403	0.115939	4.813091	-0.000493	-0.000131	0.001313
B	4.155007	8.978944	1.168663	-0.014236	0.003103	-0.031206
B	-1.701865	4.822656	5.198127	0.014326	-0.003175	0.031344
B	0.452564	2.078144	2.014732	-0.014352	-0.003179	-0.031369
B	2.000578	11.723457	4.352058	0.014175	0.003092	0.031115
B	-2.733891	11.746082	5.839177	0.041025	-0.002334	-0.015950
B	5.187034	2.055518	0.527613	-0.041432	0.002441	0.016143
B	3.032605	4.845282	3.711007	0.041388	0.002422	-0.016145
B	-0.579463	8.956318	2.655782	-0.041150	-0.002369	0.015953

B	-0.983708	0.054306	1.827988	-0.019212	-0.000463	0.011226
B	3.436850	13.747295	4.538802	0.018959	0.000446	-0.011103
B	5.591279	6.955106	1.355407	-0.019006	0.000449	0.011115
B	-3.138137	6.846495	5.011383	0.019186	-0.000463	-0.011215
Si	0.631772	3.486686	4.508512	-0.020690	0.003354	0.022167
Si	1.821370	10.314915	1.858278	0.020478	-0.003382	-0.022016
Si	-0.333059	10.387486	5.041673	-0.020388	-0.003336	0.022069
Si	2.786201	3.414115	1.325117	0.020724	0.003368	-0.022146
O	0.061445	3.072947	3.041906	-0.011142	0.006471	-0.003310
O	2.391697	10.728653	3.324884	0.011107	-0.006462	0.003307
O	4.546126	9.973747	0.141489	-0.011139	-0.006502	-0.003301
O	-2.092984	3.827853	6.225301	0.011137	0.006458	0.003311
O	2.197450	3.933608	4.519003	0.018873	-0.007408	0.005235
O	0.255692	9.867992	1.847787	-0.018677	0.007313	-0.005210
O	-1.898737	10.834409	5.031182	0.018642	0.007265	0.005146
O	4.351879	2.967192	1.335608	-0.018888	-0.007424	-0.005265
O	-0.212316	4.798696	5.055280	-0.031053	-0.011634	-0.013455
O	2.665458	9.002905	1.311510	0.030764	0.011623	0.013390
O	0.511030	11.699496	4.494905	-0.030699	0.011581	-0.013360
O	1.942113	2.102105	1.871885	0.031072	-0.011642	0.013469
O	0.525580	2.169271	5.472081	0.018576	0.001808	0.006992
O	1.927562	11.632329	0.894709	-0.018422	-0.001784	-0.006985
O	-0.226867	9.070071	4.078104	0.018464	-0.001846	0.007029
O	2.680009	4.731529	2.288686	-0.018563	0.001778	-0.006971
O	0.058846	0.698526	2.444964	-0.014284	-0.005928	-0.011385
O	2.394296	13.103075	3.921826	0.013918	0.006105	0.010860
O	4.548725	7.599326	0.738431	-0.013955	0.006162	-0.010869
O	-2.095583	6.202275	5.628359	0.014258	-0.005911	0.011360
O	-2.459230	13.184059	5.445139	-0.043005	-0.045486	0.005508
O	4.912372	0.617542	0.921651	0.043786	0.046319	-0.005473
O	2.757943	6.283259	4.105046	-0.043719	0.046258	0.005472
O	-0.304801	7.518342	2.261744	0.043129	-0.045638	-0.005513
O	-0.175430	2.374756	0.744070	-0.048204	-0.024424	-0.007141
O	2.628573	11.426844	5.622720	0.047458	0.023829	0.007427
O	4.783002	9.275557	2.439325	-0.047608	0.023888	-0.007479
O	-2.329859	4.526044	3.927465	0.048143	-0.024388	0.007124

O	-1.223866	12.517207	2.155216	-0.004104	-0.010745	0.005687
O	3.677009	1.284394	4.211574	0.004215	0.010492	-0.005579
O	5.831438	5.616407	1.028179	-0.004216	0.010531	0.005610
O	-3.378295	8.185194	5.338611	0.004101	-0.010726	-0.005665
H	-0.637445	12.195109	2.878812	0.131346	-0.013309	-0.099386
H	3.090587	1.606491	3.487978	-0.131478	0.013473	0.099854
H	5.245016	5.294309	0.304583	0.131794	0.013454	-0.100054
H	-2.791874	8.507292	6.062207	-0.131151	-0.013282	0.099234

72 f = 21.358965 THz 134.202333 2PiTHz 712.458350 cm-1 88.333609 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.003723	-0.000824	-0.008756
Li	-1.316675	4.156264	2.365404	-0.003743	0.000858	0.008762
Li	-3.471104	2.744536	5.548798	-0.003795	-0.000897	0.008834
Li	5.924247	11.057064	0.817991	0.003686	0.000792	-0.008711
Na	2.049025	6.784862	1.629696	0.001013	-0.001382	-0.000149
Na	0.404117	7.016739	4.737094	-0.001020	0.001373	0.000154
Na	2.558546	13.685662	1.553699	-0.001020	-0.001369	0.000153
Na	-0.105403	0.115939	4.813091	0.001015	0.001386	-0.000152
B	4.155007	8.978944	1.168663	-0.021947	0.004910	-0.033118
B	-1.701865	4.822656	5.198127	0.022077	-0.004923	0.033247
B	0.452564	2.078144	2.014732	0.022123	0.004946	0.033336
B	2.000578	11.723457	4.352058	-0.021923	-0.004895	-0.033080
B	-2.733891	11.746082	5.839177	-0.037977	0.003504	0.005796
B	5.187034	2.055518	0.527613	0.038336	-0.003589	-0.005863
B	3.032605	4.845282	3.711007	0.038222	0.003565	-0.005802
B	-0.579463	8.956318	2.655782	-0.038031	-0.003527	0.005823
B	-0.983708	0.054306	1.827988	0.020503	-0.001460	-0.009472
B	3.436850	13.747295	4.538802	-0.020280	0.001481	0.009366
B	5.591279	6.955106	1.355407	-0.020309	-0.001473	0.009379
B	-3.138137	6.846495	5.011383	0.020422	0.001462	-0.009423
Si	0.631772	3.486686	4.508512	-0.031842	0.016436	-0.014424
Si	1.821370	10.314915	1.858278	0.031676	-0.016330	0.014286
Si	-0.333059	10.387486	5.041673	0.031627	0.016333	0.014305
Si	2.786201	3.414115	1.325117	-0.031926	-0.016443	-0.014373

O	0.061445	3.072947	3.041906	0.014021	-0.013976	-0.000890
O	2.391697	10.728653	3.324884	-0.013910	0.013861	0.000866
O	4.546126	9.973747	0.141489	-0.013918	-0.013857	0.000866
O	-2.092984	3.827853	6.225301	0.013994	0.013973	-0.000897
O	2.197450	3.933608	4.519003	0.010684	-0.015449	0.016980
O	0.255692	9.867992	1.847787	-0.010648	0.015365	-0.016866
O	-1.898737	10.834409	5.031182	-0.010608	-0.015338	-0.016854
O	4.351879	2.967192	1.335608	0.010762	0.015486	0.017002
O	-0.212316	4.798696	5.055280	-0.022161	-0.018730	-0.008891
O	2.665458	9.002905	1.311510	0.022080	0.018635	0.008861
O	0.511030	11.699496	4.494905	0.022010	-0.018626	0.008843
O	1.942113	2.102105	1.871885	-0.022283	0.018753	-0.008926
O	0.525580	2.169271	5.472081	-0.013194	-0.016794	-0.014749
O	1.927562	11.632329	0.894709	0.013074	0.016676	0.014676
O	-0.226867	9.070071	4.078104	0.013096	-0.016673	0.014668
O	2.680009	4.731529	2.288686	-0.013146	0.016798	-0.014748
O	0.058846	0.698526	2.444964	0.010647	0.016907	0.005850
O	2.394296	13.103075	3.921826	-0.010418	-0.016917	-0.005561
O	4.548725	7.599326	0.738431	-0.010480	0.016871	-0.005651
O	-2.095583	6.202275	5.628359	0.010551	-0.016957	0.005714
O	-2.459230	13.184059	5.445139	0.039455	0.048953	-0.005061
O	4.912372	0.617542	0.921651	-0.040026	-0.049603	0.005067
O	2.757943	6.283259	4.105046	-0.039808	0.049381	0.005068
O	-0.304801	7.518342	2.261744	0.039587	-0.049099	-0.005045
O	-0.175430	2.374756	0.744070	0.050928	0.019495	0.012596
O	2.628573	11.426844	5.622720	-0.050351	-0.019105	-0.012663
O	4.783002	9.275557	2.439325	-0.050470	0.019210	-0.012601
O	-2.329859	4.526044	3.927465	0.050727	-0.019334	0.012663
O	-1.223866	12.517207	2.155216	-0.003094	0.009745	-0.003581
O	3.677009	1.284394	4.211574	0.003047	-0.009568	0.003478
O	5.831438	5.616407	1.028179	0.003068	0.009620	0.003496
O	-3.378295	8.185194	5.338611	-0.003075	-0.009674	-0.003558
H	-0.637445	12.195109	2.878812	-0.055804	-0.023670	0.019243
H	3.090587	1.606491	3.487978	0.055186	0.023721	-0.018934
H	5.245016	5.294309	0.304583	0.055042	-0.023764	-0.018750
H	-2.791874	8.507292	6.062207	-0.055749	0.023650	0.019278

73 f = 20.333926 THz 127.761825 2PiTHz 678.266743 cm-1 84.094389
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.006396	0.002692	0.000986
Li	-1.316675	4.156264	2.365404	0.006401	-0.002703	-0.000992
Li	-3.471104	2.744536	5.548798	-0.006394	-0.002687	0.000996
Li	5.924247	11.057064	0.817991	0.006408	0.002707	-0.000984
Na	2.049025	6.784862	1.629696	0.002905	-0.000135	0.001796
Na	0.404117	7.016739	4.737094	-0.002908	0.000131	-0.001802
Na	2.558546	13.685662	1.553699	0.002909	0.000134	0.001802
Na	-0.105403	0.115939	4.813091	-0.002904	-0.000132	-0.001796
B	4.155007	8.978944	1.168663	0.004173	-0.006099	-0.007420
B	-1.701865	4.822656	5.198127	-0.004185	0.006119	0.007402
B	0.452564	2.078144	2.014732	0.004184	0.006116	-0.007411
B	2.000578	11.723457	4.352058	-0.004180	-0.006101	0.007418
B	-2.733891	11.746082	5.839177	-0.001483	-0.000740	0.005054
B	5.187034	2.055518	0.527613	0.001495	0.000740	-0.005074
B	3.032605	4.845282	3.711007	-0.001502	0.000741	0.005074
B	-0.579463	8.956318	2.655782	0.001473	-0.000738	-0.005051
B	-0.983708	0.054306	1.827988	-0.072989	0.040540	0.092419
B	3.436850	13.747295	4.538802	0.072986	-0.040534	-0.092410
B	5.591279	6.955106	1.355407	-0.072988	-0.040530	0.092409
B	-3.138137	6.846495	5.011383	0.072957	0.040525	-0.092382
Si	0.631772	3.486686	4.508512	0.012221	-0.001167	0.006715
Si	1.821370	10.314915	1.858278	-0.012207	0.001161	-0.006722
Si	-0.333059	10.387486	5.041673	0.012218	0.001168	0.006720
Si	2.786201	3.414115	1.325117	-0.012218	-0.001161	-0.006712
O	0.061445	3.072947	3.041906	-0.009761	0.010039	-0.000083
O	2.391697	10.728653	3.324884	0.009761	-0.010041	0.000093
O	4.546126	9.973747	0.141489	-0.009773	-0.010050	-0.000092
O	-2.092984	3.827853	6.225301	0.009748	0.010029	0.000081
O	2.197450	3.933608	4.519003	-0.004821	0.011932	-0.006839
O	0.255692	9.867992	1.847787	0.004812	-0.011931	0.006830
O	-1.898737	10.834409	5.031182	-0.004816	-0.011935	-0.006833
O	4.351879	2.967192	1.335608	0.004824	0.011936	0.006842

O	-0.212316	4.798696	5.055280	-0.000304	-0.004938	-0.001414
O	2.665458	9.002905	1.311510	0.000327	0.004957	0.001417
O	0.511030	11.699496	4.494905	-0.000312	0.004945	-0.001417
O	1.942113	2.102105	1.871885	0.000317	-0.004950	0.001414
O	0.525580	2.169271	5.472081	0.000315	-0.000372	0.002552
O	1.927562	11.632329	0.894709	-0.000317	0.000372	-0.002559
O	-0.226867	9.070071	4.078104	0.000319	0.000373	0.002558
O	2.680009	4.731529	2.288686	-0.000309	-0.000371	-0.002551
O	0.058846	0.698526	2.444964	0.030204	-0.020493	-0.008730
O	2.394296	13.103075	3.921826	-0.030196	0.020494	0.008735
O	4.548725	7.599326	0.738431	0.030191	0.020490	-0.008746
O	-2.095583	6.202275	5.628359	-0.030191	-0.020483	0.008727
O	-2.459230	13.184059	5.445139	-0.004982	0.027792	0.030365
O	4.912372	0.617542	0.921651	0.004972	-0.027802	-0.030372
O	2.757943	6.283259	4.105046	-0.004968	-0.027796	0.030355
O	-0.304801	7.518342	2.261744	0.004993	0.027776	-0.030366
O	-0.175430	2.374756	0.744070	0.008180	0.007330	-0.013665
O	2.628573	11.426844	5.622720	-0.008184	-0.007337	0.013674
O	4.783002	9.275557	2.439325	0.008162	-0.007318	-0.013660
O	-2.329859	4.526044	3.927465	-0.008192	0.007334	0.013667
O	-1.223866	12.517207	2.155216	0.014259	-0.005887	-0.022333
O	3.677009	1.284394	4.211574	-0.014257	0.005880	0.022330
O	5.831438	5.616407	1.028179	0.014259	0.005884	-0.022330
O	-3.378295	8.185194	5.338611	-0.014253	-0.005887	0.022322
H	-0.637445	12.195109	2.878812	0.005713	-0.020278	-0.022304
H	3.090587	1.606491	3.487978	-0.005701	0.020260	0.022293
H	5.245016	5.294309	0.304583	0.005672	0.020266	-0.022266
H	-2.791874	8.507292	6.062207	-0.005707	-0.020260	0.022287

74 f = 20.238523 THz 127.162391 2PiTHz 675.084444 cm-1 83.699834
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004164	-0.004927	-0.002852
Li	-1.316675	4.156264	2.365404	0.004159	0.004922	0.002863
Li	-3.471104	2.744536	5.548798	0.004159	-0.004920	0.002861
Li	5.924247	11.057064	0.817991	-0.004163	0.004928	-0.002849

Na	2.049025	6.784862	1.629696	0.002674	0.000158	0.001649
Na	0.404117	7.016739	4.737094	-0.002677	-0.000162	-0.001657
Na	2.558546	13.685662	1.553699	-0.002676	0.000161	-0.001656
Na	-0.105403	0.115939	4.813091	0.002673	-0.000159	0.001649
B	4.155007	8.978944	1.168663	0.006766	-0.000412	-0.014882
B	-1.701865	4.822656	5.198127	-0.006765	0.000433	0.014887
B	0.452564	2.078144	2.014732	-0.006762	-0.000426	0.014882
B	2.000578	11.723457	4.352058	0.006771	0.000419	-0.014883
B	-2.733891	11.746082	5.839177	0.007396	-0.008204	-0.004779
B	5.187034	2.055518	0.527613	-0.007384	0.008204	0.004787
B	3.032605	4.845282	3.711007	-0.007388	-0.008195	0.004783
B	-0.579463	8.956318	2.655782	0.007394	0.008217	-0.004785
B	-0.983708	0.054306	1.827988	0.072383	-0.040216	-0.091906
B	3.436850	13.747295	4.538802	-0.072391	0.040213	0.091915
B	5.591279	6.955106	1.355407	-0.072405	-0.040223	0.091931
B	-3.138137	6.846495	5.011383	0.072412	0.040226	-0.091942
Si	0.631772	3.486686	4.508512	0.007045	0.000187	-0.006913
Si	1.821370	10.314915	1.858278	-0.007045	-0.000183	0.006913
Si	-0.333059	10.387486	5.041673	-0.007048	0.000188	0.006914
Si	2.786201	3.414115	1.325117	0.007042	-0.000184	-0.006916
O	0.061445	3.072947	3.041906	0.005458	-0.005498	0.004732
O	2.391697	10.728653	3.324884	-0.005459	0.005498	-0.004732
O	4.546126	9.973747	0.141489	-0.005455	-0.005502	-0.004739
O	-2.092984	3.827853	6.225301	0.005466	0.005498	0.004727
O	2.197450	3.933608	4.519003	-0.007924	0.008862	-0.005098
O	0.255692	9.867992	1.847787	0.007928	-0.008860	0.005082
O	-1.898737	10.834409	5.031182	0.007925	0.008862	0.005093
O	4.351879	2.967192	1.335608	-0.007929	-0.008861	-0.005089
O	-0.212316	4.798696	5.055280	0.005189	-0.000882	0.000440
O	2.665458	9.002905	1.311510	-0.005210	0.000868	-0.000439
O	0.511030	11.699496	4.494905	-0.005198	-0.000872	-0.000440
O	1.942113	2.102105	1.871885	0.005201	0.000878	0.000439
O	0.525580	2.169271	5.472081	-0.005126	-0.001378	-0.007268
O	1.927562	11.632329	0.894709	0.005119	0.001373	0.007265
O	-0.226867	9.070071	4.078104	0.005124	-0.001385	0.007278
O	2.680009	4.731529	2.288686	-0.005120	0.001367	-0.007259

O	0.058846	0.698526	2.444964	-0.028614	0.021947	0.005153
O	2.394296	13.103075	3.921826	0.028612	-0.021939	-0.005163
O	4.548725	7.599326	0.738431	0.028624	0.021956	-0.005151
O	-2.095583	6.202275	5.628359	-0.028610	-0.021938	0.005177
O	-2.459230	13.184059	5.445139	0.003649	-0.029333	-0.028857
O	4.912372	0.617542	0.921651	-0.003648	0.029340	0.028854
O	2.757943	6.283259	4.105046	-0.003672	-0.029329	0.028860
O	-0.304801	7.518342	2.261744	0.003635	0.029350	-0.028864
O	-0.175430	2.374756	0.744070	-0.007042	-0.012635	0.012511
O	2.628573	11.426844	5.622720	0.007053	0.012633	-0.012511
O	4.783002	9.275557	2.439325	0.007053	-0.012644	-0.012513
O	-2.329859	4.526044	3.927465	-0.007040	0.012620	0.012508
O	-1.223866	12.517207	2.155216	-0.012133	0.001191	0.023036
O	3.677009	1.284394	4.211574	0.012138	-0.001196	-0.023041
O	5.831438	5.616407	1.028179	0.012144	0.001183	-0.023047
O	-3.378295	8.185194	5.338611	-0.012139	-0.001208	0.023039
H	-0.637445	12.195109	2.878812	-0.041208	0.025600	0.058039
H	3.090587	1.606491	3.487978	0.041153	-0.025599	-0.057988
H	5.245016	5.294309	0.304583	0.041153	0.025594	-0.057994
H	-2.791874	8.507292	6.062207	-0.041196	-0.025610	0.058024

75 f = 19.873605 THz 124.869545 2PiTHz 662.912097 cm-1 82.190654 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.011724	-0.018352	-0.007998
Li	-1.316675	4.156264	2.365404	0.011729	-0.018373	-0.007989
Li	-3.471104	2.744536	5.548798	-0.011733	-0.018374	0.007995
Li	5.924247	11.057064	0.817991	-0.011726	-0.018357	0.008003
Na	2.049025	6.784862	1.629696	-0.000789	0.001599	0.000304
Na	0.404117	7.016739	4.737094	-0.000791	0.001598	0.000315
Na	2.558546	13.685662	1.553699	0.000792	0.001600	-0.000315
Na	-0.105403	0.115939	4.813091	0.000790	0.001599	-0.000304
B	4.155007	8.978944	1.168663	0.000924	0.003814	0.001546
B	-1.701865	4.822656	5.198127	0.000929	0.003820	0.001561
B	0.452564	2.078144	2.014732	-0.000928	0.003822	-0.001568
B	2.000578	11.723457	4.352058	-0.000923	0.003808	-0.001549

B	-2.733891	11.746082	5.839177	-0.001800	-0.000906	0.003939
B	5.187034	2.055518	0.527613	-0.001794	-0.000904	0.003936
B	3.032605	4.845282	3.711007	0.001800	-0.000906	-0.003941
B	-0.579463	8.956318	2.655782	0.001797	-0.000901	-0.003937
B	-0.983708	0.054306	1.827988	-0.077494	0.035632	0.094825
B	3.436850	13.747295	4.538802	-0.077489	0.035618	0.094805
B	5.591279	6.955106	1.355407	0.077440	0.035592	-0.094748
B	-3.138137	6.846495	5.011383	0.077438	0.035605	-0.094755
Si	0.631772	3.486686	4.508512	0.008865	-0.001691	0.005944
Si	1.821370	10.314915	1.858278	0.008874	-0.001680	0.005948
Si	-0.333059	10.387486	5.041673	-0.008875	-0.001679	-0.005944
Si	2.786201	3.414115	1.325117	-0.008870	-0.001692	-0.005939
O	0.061445	3.072947	3.041906	-0.012019	0.013997	-0.002052
O	2.391697	10.728653	3.324884	-0.012034	0.014007	-0.002036
O	4.546126	9.973747	0.141489	0.012032	0.014003	0.002034
O	-2.092984	3.827853	6.225301	0.012017	0.013995	0.002051
O	2.197450	3.933608	4.519003	-0.004532	0.010980	-0.003757
O	0.255692	9.867992	1.847787	-0.004525	0.010975	-0.003773
O	-1.898737	10.834409	5.031182	0.004528	0.010981	0.003773
O	4.351879	2.967192	1.335608	0.004536	0.010984	0.003757
O	-0.212316	4.798696	5.055280	0.000694	-0.006611	-0.001455
O	2.665458	9.002905	1.311510	0.000667	-0.006624	-0.001448
O	0.511030	11.699496	4.494905	-0.000668	-0.006624	0.001447
O	1.942113	2.102105	1.871885	-0.000697	-0.006612	0.001454
O	0.525580	2.169271	5.472081	-0.000747	-0.000680	0.006393
O	1.927562	11.632329	0.894709	-0.000759	-0.000693	0.006371
O	-0.226867	9.070071	4.078104	0.000760	-0.000696	-0.006367
O	2.680009	4.731529	2.288686	0.000749	-0.000680	-0.006389
O	0.058846	0.698526	2.444964	0.026535	-0.014336	-0.021532
O	2.394296	13.103075	3.921826	0.026525	-0.014333	-0.021540
O	4.548725	7.599326	0.738431	-0.026509	-0.014324	0.021530
O	-2.095583	6.202275	5.628359	-0.026512	-0.014321	0.021524
O	-2.459230	13.184059	5.445139	0.013907	-0.016474	-0.030273
O	4.912372	0.617542	0.921651	0.013901	-0.016498	-0.030272
O	2.757943	6.283259	4.105046	-0.013897	-0.016479	0.030252
O	-0.304801	7.518342	2.261744	-0.013899	-0.016467	0.030251

O	-0.175430	2.374756	0.744070	0.004829	0.001225	-0.007862
O	2.628573	11.426844	5.622720	0.004835	0.001218	-0.007850
O	4.783002	9.275557	2.439325	-0.004837	0.001212	0.007850
O	-2.329859	4.526044	3.927465	-0.004822	0.001220	0.007851
O	-1.223866	12.517207	2.155216	0.016760	-0.004721	-0.020577
O	3.677009	1.284394	4.211574	0.016760	-0.004723	-0.020565
O	5.831438	5.616407	1.028179	-0.016748	-0.004727	0.020553
O	-3.378295	8.185194	5.338611	-0.016748	-0.004716	0.020559
H	-0.637445	12.195109	2.878812	-0.013339	-0.011006	0.000001
H	3.090587	1.606491	3.487978	-0.013365	-0.010973	0.000050
H	5.245016	5.294309	0.304583	0.013363	-0.010970	-0.000054
H	-2.791874	8.507292	6.062207	0.013327	-0.011000	-0.000002

76 f = 19.757382 THz 124.139295 2PiTHz 659.035320 cm-1 81.709995
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.005136	0.007215	0.006014
Li	-1.316675	4.156264	2.365404	-0.005146	0.007205	0.006008
Li	-3.471104	2.744536	5.548798	-0.005142	-0.007204	0.006001
Li	5.924247	11.057064	0.817991	-0.005124	-0.007191	0.006013
Na	2.049025	6.784862	1.629696	0.000792	-0.001115	-0.000566
Na	0.404117	7.016739	4.737094	0.000793	-0.001113	-0.000576
Na	2.558546	13.685662	1.553699	0.000792	0.001113	-0.000576
Na	-0.105403	0.115939	4.813091	0.000792	0.001113	-0.000566
B	4.155007	8.978944	1.168663	0.004090	0.002741	-0.006196
B	-1.701865	4.822656	5.198127	0.004093	0.002751	-0.006204
B	0.452564	2.078144	2.014732	0.004087	-0.002743	-0.006200
B	2.000578	11.723457	4.352058	0.004096	-0.002755	-0.006199
B	-2.733891	11.746082	5.839177	0.004179	-0.005701	-0.000687
B	5.187034	2.055518	0.527613	0.004177	-0.005705	-0.000680
B	3.032605	4.845282	3.711007	0.004172	0.005706	-0.000685
B	-0.579463	8.956318	2.655782	0.004178	0.005703	-0.000674
B	-0.983708	0.054306	1.827988	-0.080318	0.038139	0.096573
B	3.436850	13.747295	4.538802	-0.080346	0.038142	0.096580
B	5.591279	6.955106	1.355407	-0.080380	-0.038160	0.096627
B	-3.138137	6.846495	5.011383	-0.080388	-0.038164	0.096653

Si	0.631772	3.486686	4.508512	-0.003026	-0.001143	0.005914
Si	1.821370	10.314915	1.858278	-0.003009	-0.001147	0.005924
Si	-0.333059	10.387486	5.041673	-0.003009	0.001153	0.005923
Si	2.786201	3.414115	1.325117	-0.003014	0.001136	0.005924
O	0.061445	3.072947	3.041906	-0.002838	0.005819	-0.002311
O	2.391697	10.728653	3.324884	-0.002857	0.005836	-0.002303
O	4.546126	9.973747	0.141489	-0.002863	-0.005847	-0.002311
O	-2.092984	3.827853	6.225301	-0.002853	-0.005830	-0.002304
O	2.197450	3.933608	4.519003	0.002646	-0.003693	-0.001681
O	0.255692	9.867992	1.847787	0.002642	-0.003677	-0.001712
O	-1.898737	10.834409	5.031182	0.002636	0.003671	-0.001702
O	4.351879	2.967192	1.335608	0.002648	0.003684	-0.001698
O	-0.212316	4.798696	5.055280	-0.003128	-0.001184	-0.001712
O	2.665458	9.002905	1.311510	-0.003134	-0.001180	-0.001718
O	0.511030	11.699496	4.494905	-0.003126	0.001188	-0.001721
O	1.942113	2.102105	1.871885	-0.003143	0.001189	-0.001711
O	0.525580	2.169271	5.472081	0.000754	0.003093	0.006841
O	1.927562	11.632329	0.894709	0.000746	0.003098	0.006842
O	-0.226867	9.070071	4.078104	0.000749	-0.003104	0.006860
O	2.680009	4.731529	2.288686	0.000748	-0.003085	0.006830
O	0.058846	0.698526	2.444964	0.026395	-0.017416	-0.017383
O	2.394296	13.103075	3.921826	0.026391	-0.017430	-0.017388
O	4.548725	7.599326	0.738431	0.026407	0.017436	-0.017403
O	-2.095583	6.202275	5.628359	0.026411	0.017427	-0.017401
O	-2.459230	13.184059	5.445139	0.009565	-0.017503	-0.030388
O	4.912372	0.617542	0.921651	0.009561	-0.017517	-0.030377
O	2.757943	6.283259	4.105046	0.009576	0.017526	-0.030403
O	-0.304801	7.518342	2.261744	0.009572	0.017513	-0.030400
O	-0.175430	2.374756	0.744070	0.003891	0.006309	-0.005013
O	2.628573	11.426844	5.622720	0.003897	0.006306	-0.005005
O	4.783002	9.275557	2.439325	0.003896	-0.006302	-0.005005
O	-2.329859	4.526044	3.927465	0.003896	-0.006311	-0.005021
O	-1.223866	12.517207	2.155216	0.019440	-0.002092	-0.021927
O	3.677009	1.284394	4.211574	0.019445	-0.002100	-0.021925
O	5.831438	5.616407	1.028179	0.019453	0.002099	-0.021933
O	-3.378295	8.185194	5.338611	0.019455	0.002102	-0.021941

H	-0.637445	12.195109	2.878812	-0.025403	-0.004174	0.012687
H	3.090587	1.606491	3.487978	-0.025411	-0.004157	0.012712
H	5.245016	5.294309	0.304583	-0.025406	0.004166	0.012699
H	-2.791874	8.507292	6.062207	-0.025437	0.004184	0.012711

77 f = 19.270613 THz 121.080832 2PiTHz 642.798436 cm-1 79.696877
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.009912	0.013621	-0.019508
Li	-1.316675	4.156264	2.365404	0.009949	-0.013576	0.019491
Li	-3.471104	2.744536	5.548798	-0.009998	-0.013623	-0.019492
Li	5.924247	11.057064	0.817991	0.009872	0.013585	0.019513
Na	2.049025	6.784862	1.629696	0.001674	-0.002389	0.001373
Na	0.404117	7.016739	4.737094	-0.001678	0.002416	-0.001386
Na	2.558546	13.685662	1.553699	0.001675	0.002410	0.001384
Na	-0.105403	0.115939	4.813091	-0.001678	-0.002396	-0.001374
B	4.155007	8.978944	1.168663	-0.010522	0.000675	-0.022056
B	-1.701865	4.822656	5.198127	0.010465	-0.000587	0.021961
B	0.452564	2.078144	2.014732	-0.010473	-0.000557	-0.021992
B	2.000578	11.723457	4.352058	0.010512	0.000700	0.022040
B	-2.733891	11.746082	5.839177	-0.016628	0.006985	-0.015524
B	5.187034	2.055518	0.527613	0.016510	-0.006898	0.015485
B	3.032605	4.845282	3.711007	-0.016523	-0.006918	-0.015499
B	-0.579463	8.956318	2.655782	0.016623	0.006960	0.015509
B	-0.983708	0.054306	1.827988	-0.003102	0.008927	0.007286
B	3.436850	13.747295	4.538802	0.003227	-0.008991	-0.007385
B	5.591279	6.955106	1.355407	-0.003200	-0.008981	0.007361
B	-3.138137	6.846495	5.011383	0.003134	0.008935	-0.007298
Si	0.631772	3.486686	4.508512	-0.021845	-0.026647	-0.013763
Si	1.821370	10.314915	1.858278	0.021932	0.026772	0.013831
Si	-0.333059	10.387486	5.041673	-0.021945	0.026770	-0.013814
Si	2.786201	3.414115	1.325117	0.021829	-0.026654	0.013775
O	0.061445	3.072947	3.041906	0.018444	-0.005689	-0.024458
O	2.391697	10.728653	3.324884	-0.018637	0.005729	0.024559
O	4.546126	9.973747	0.141489	0.018675	0.005761	-0.024553
O	-2.092984	3.827853	6.225301	-0.018387	-0.005637	0.024468

O	2.197450	3.933608	4.519003	-0.001773	-0.009941	0.053388
O	0.255692	9.867992	1.847787	0.001821	0.009955	-0.053519
O	-1.898737	10.834409	5.031182	-0.001823	0.009953	0.053511
O	4.351879	2.967192	1.335608	0.001768	-0.009936	-0.053398
O	-0.212316	4.798696	5.055280	0.041880	0.021709	0.002067
O	2.665458	9.002905	1.311510	-0.042169	-0.021977	-0.002041
O	0.511030	11.699496	4.494905	0.042143	-0.021956	0.002047
O	1.942113	2.102105	1.871885	-0.041910	0.021740	-0.002047
O	0.525580	2.169271	5.472081	0.017965	0.041708	0.053440
O	1.927562	11.632329	0.894709	-0.018042	-0.041817	-0.053601
O	-0.226867	9.070071	4.078104	0.018053	-0.041829	0.053608
O	2.680009	4.731529	2.288686	-0.017944	0.041682	-0.053428
O	0.058846	0.698526	2.444964	0.002519	-0.001898	0.001545
O	2.394296	13.103075	3.921826	-0.002539	0.001994	-0.001549
O	4.548725	7.599326	0.738431	0.002546	0.001997	0.001583
O	-2.095583	6.202275	5.628359	-0.002511	-0.001906	-0.001513
O	-2.459230	13.184059	5.445139	0.000844	0.009971	-0.001252
O	4.912372	0.617542	0.921651	-0.000837	-0.009968	0.001294
O	2.757943	6.283259	4.105046	0.000833	-0.009961	-0.001291
O	-0.304801	7.518342	2.261744	-0.000854	0.009970	0.001253
O	-0.175430	2.374756	0.744070	-0.008161	0.008078	0.010385
O	2.628573	11.426844	5.622720	0.008222	-0.008125	-0.010481
O	4.783002	9.275557	2.439325	-0.008204	-0.008140	0.010427
O	-2.329859	4.526044	3.927465	0.008173	0.008065	-0.010451
O	-1.223866	12.517207	2.155216	-0.003233	0.012256	-0.007812
O	3.677009	1.284394	4.211574	0.003160	-0.012351	0.007850
O	5.831438	5.616407	1.028179	-0.003171	-0.012342	-0.007831
O	-3.378295	8.185194	5.338611	0.003220	0.012269	0.007828
H	-0.637445	12.195109	2.878812	0.044694	-0.004647	-0.055460
H	3.090587	1.606491	3.487978	-0.044464	0.004484	0.055215
H	5.245016	5.294309	0.304583	0.044502	0.004468	-0.055225
H	-2.791874	8.507292	6.062207	-0.044640	-0.004642	0.055424

78 f = 19.079860 THz 119.882297 2PiTHz 636.435609 cm-1 78.907987 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.001824	-0.001464	-0.022762
Li	-1.316675	4.156264	2.365404	0.001794	-0.001450	-0.022848
Li	-3.471104	2.744536	5.548798	-0.001790	-0.001435	0.022855
Li	5.924247	11.057064	0.817991	-0.001812	-0.001462	0.022754
Na	2.049025	6.784862	1.629696	-0.000587	0.004113	-0.002150
Na	0.404117	7.016739	4.737094	-0.000576	0.004098	-0.002135
Na	2.558546	13.685662	1.553699	0.000578	0.004103	0.002136
Na	-0.105403	0.115939	4.813091	0.000588	0.004111	0.002150
B	4.155007	8.978944	1.168663	-0.010169	0.021084	-0.014284
B	-1.701865	4.822656	5.198127	-0.010202	0.021087	-0.014400
B	0.452564	2.078144	2.014732	0.010207	0.021086	0.014404
B	2.000578	11.723457	4.352058	0.010168	0.021078	0.014306
B	-2.733891	11.746082	5.839177	-0.022837	0.015081	-0.007695
B	5.187034	2.055518	0.527613	-0.022922	0.015120	-0.007767
B	3.032605	4.845282	3.711007	0.022933	0.015121	0.007764
B	-0.579463	8.956318	2.655782	0.022847	0.015078	0.007698
B	-0.983708	0.054306	1.827988	0.010632	-0.009621	-0.006939
B	3.436850	13.747295	4.538802	0.010615	-0.009582	-0.006914
B	5.591279	6.955106	1.355407	-0.010616	-0.009581	0.006895
B	-3.138137	6.846495	5.011383	-0.010648	-0.009622	0.006952
Si	0.631772	3.486686	4.508512	0.024028	0.025977	0.014940
Si	1.821370	10.314915	1.858278	0.023934	0.025853	0.014868
Si	-0.333059	10.387486	5.041673	-0.023927	0.025860	-0.014868
Si	2.786201	3.414115	1.325117	-0.024029	0.025980	-0.014933
O	0.061445	3.072947	3.041906	-0.027951	0.009905	0.019976
O	2.391697	10.728653	3.324884	-0.027847	0.009857	0.019883
O	4.546126	9.973747	0.141489	0.027832	0.009838	-0.019885
O	-2.092984	3.827853	6.225301	0.027933	0.009888	-0.019981
O	2.197450	3.933608	4.519003	0.000103	0.016344	-0.048359
O	0.255692	9.867992	1.847787	0.000111	0.016283	-0.048097
O	-1.898737	10.834409	5.031182	-0.000111	0.016276	0.048100
O	4.351879	2.967192	1.335608	-0.000097	0.016340	0.048358
O	-0.212316	4.798696	5.055280	-0.042633	-0.030722	-0.004354
O	2.665458	9.002905	1.311510	-0.042464	-0.030618	-0.004342
O	0.511030	11.699496	4.494905	0.042464	-0.030619	0.004323
O	1.942113	2.102105	1.871885	0.042639	-0.030736	0.004346

O	0.525580	2.169271	5.472081	-0.015288	-0.040794	-0.043460
O	1.927562	11.632329	0.894709	-0.015214	-0.040598	-0.043221
O	-0.226867	9.070071	4.078104	0.015203	-0.040587	0.043216
O	2.680009	4.731529	2.288686	0.015280	-0.040784	0.043460
O	0.058846	0.698526	2.444964	-0.002062	0.005879	-0.000120
O	2.394296	13.103075	3.921826	-0.002054	0.005866	-0.000100
O	4.548725	7.599326	0.738431	0.002047	0.005868	0.000090
O	-2.095583	6.202275	5.628359	0.002070	0.005896	0.000124
O	-2.459230	13.184059	5.445139	0.005583	-0.000949	0.001977
O	4.912372	0.617542	0.921651	0.005590	-0.000919	0.001974
O	2.757943	6.283259	4.105046	-0.005604	-0.000900	-0.001980
O	-0.304801	7.518342	2.261744	-0.005578	-0.000976	-0.001979
O	-0.175430	2.374756	0.744070	0.008006	-0.007731	-0.018768
O	2.628573	11.426844	5.622720	0.007976	-0.007695	-0.018706
O	4.783002	9.275557	2.439325	-0.007976	-0.007688	0.018731
O	-2.329859	4.526044	3.927465	-0.007990	-0.007742	0.018762
O	-1.223866	12.517207	2.155216	-0.009839	-0.019618	0.004507
O	3.677009	1.284394	4.211574	-0.009849	-0.019560	0.004480
O	5.831438	5.616407	1.028179	0.009854	-0.019567	-0.004470
O	-3.378295	8.185194	5.338611	0.009840	-0.019614	-0.004510
H	-0.637445	12.195109	2.878812	0.025069	-0.020453	-0.024877
H	3.090587	1.606491	3.487978	0.025253	-0.020467	-0.025100
H	5.245016	5.294309	0.304583	-0.025246	-0.020485	0.025115
H	-2.791874	8.507292	6.062207	-0.025057	-0.020448	0.024863

79 f = 18.855045 THz 118.469741 2PiTHz 628.936579 cm-1 77.978226 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.026853	-0.013142	0.021704
Li	-1.316675	4.156264	2.365404	-0.026835	0.013115	-0.021699
Li	-3.471104	2.744536	5.548798	-0.026870	-0.013123	-0.021717
Li	5.924247	11.057064	0.817991	0.026775	0.013123	0.021648
Na	2.049025	6.784862	1.629696	-0.000466	0.002306	0.000604
Na	0.404117	7.016739	4.737094	0.000457	-0.002310	-0.000629
Na	2.558546	13.685662	1.553699	0.000456	0.002309	-0.000630
Na	-0.105403	0.115939	4.813091	-0.000466	-0.002303	0.000606

B	4.155007	8.978944	1.168663	0.014058	0.003579	0.038631
B	-1.701865	4.822656	5.198127	-0.014118	-0.003585	-0.038799
B	0.452564	2.078144	2.014732	-0.014111	0.003590	-0.038795
B	2.000578	11.723457	4.352058	0.014068	-0.003579	0.038639
B	-2.733891	11.746082	5.839177	0.043839	0.006042	0.001541
B	5.187034	2.055518	0.527613	-0.043989	-0.006058	-0.001532
B	3.032605	4.845282	3.711007	-0.043988	0.006059	-0.001537
B	-0.579463	8.956318	2.655782	0.043827	-0.006045	0.001535
B	-0.983708	0.054306	1.827988	0.027121	-0.000336	0.013166
B	3.436850	13.747295	4.538802	-0.027024	0.000326	-0.013136
B	5.591279	6.955106	1.355407	-0.027027	-0.000327	-0.013125
B	-3.138137	6.846495	5.011383	0.027112	0.000331	0.013176
Si	0.631772	3.486686	4.508512	-0.009251	0.018052	-0.006167
Si	1.821370	10.314915	1.858278	0.009236	-0.018012	0.006142
Si	-0.333059	10.387486	5.041673	0.009238	0.018008	0.006145
Si	2.786201	3.414115	1.325117	-0.009256	-0.018050	-0.006169
O	0.061445	3.072947	3.041906	0.040328	-0.046130	0.006687
O	2.391697	10.728653	3.324884	-0.040361	0.046044	-0.006676
O	4.546126	9.973747	0.141489	-0.040280	-0.045997	-0.006666
O	-2.092984	3.827853	6.225301	0.040371	0.046154	0.006687
O	2.197450	3.933608	4.519003	0.011163	-0.032466	0.016840
O	0.255692	9.867992	1.847787	-0.011094	0.032319	-0.016675
O	-1.898737	10.834409	5.031182	-0.011123	-0.032357	-0.016744
O	4.351879	2.967192	1.335608	0.011150	0.032453	0.016816
O	-0.212316	4.798696	5.055280	0.001078	-0.007793	0.034616
O	2.665458	9.002905	1.311510	-0.001034	0.007816	-0.034498
O	0.511030	11.699496	4.494905	-0.001010	-0.007870	-0.034521
O	1.942113	2.102105	1.871885	0.001097	0.007769	0.034611
O	0.525580	2.169271	5.472081	0.028626	0.011478	-0.003857
O	1.927562	11.632329	0.894709	-0.028531	-0.011454	0.003835
O	-0.226867	9.070071	4.078104	-0.028522	0.011503	0.003800
O	2.680009	4.731529	2.288686	0.028633	-0.011460	-0.003870
O	0.058846	0.698526	2.444964	0.005699	0.024346	0.010761
O	2.394296	13.103075	3.921826	-0.005696	-0.024225	-0.010771
O	4.548725	7.599326	0.738431	-0.005699	0.024231	-0.010760
O	-2.095583	6.202275	5.628359	0.005698	-0.024337	0.010771

O	-2.459230	13.184059	5.445139	-0.011383	0.022773	-0.007268
O	4.912372	0.617542	0.921651	0.011447	-0.022818	0.007305
O	2.757943	6.283259	4.105046	0.011452	0.022820	0.007300
O	-0.304801	7.518342	2.261744	-0.011366	-0.022781	-0.007276
O	-0.175430	2.374756	0.744070	-0.036090	-0.000071	-0.024619
O	2.628573	11.426844	5.622720	0.035965	0.000048	0.024562
O	4.783002	9.275557	2.439325	0.035944	-0.000049	0.024541
O	-2.329859	4.526044	3.927465	-0.036105	0.000063	-0.024621
O	-1.223866	12.517207	2.155216	-0.009212	0.001746	-0.008538
O	3.677009	1.284394	4.211574	0.009180	-0.001753	0.008519
O	5.831438	5.616407	1.028179	0.009183	0.001760	0.008517
O	-3.378295	8.185194	5.338611	-0.009204	-0.001745	-0.008544
H	-0.637445	12.195109	2.878812	-0.031225	-0.039174	-0.009535
H	3.090587	1.606491	3.487978	0.031013	0.039034	0.009597
H	5.245016	5.294309	0.304583	0.030980	-0.039043	0.009631
H	-2.791874	8.507292	6.062207	-0.031279	0.039145	-0.009477

80 f = 18.843770 THz 118.398898 2PiTHz 628.560485 cm-1 77.931596 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.022822	0.018160	-0.015282
Li	-1.316675	4.156264	2.365404	-0.022679	0.018105	-0.015197
Li	-3.471104	2.744536	5.548798	-0.022740	-0.018129	-0.015197
Li	5.924247	11.057064	0.817991	-0.022748	-0.018133	-0.015254
Na	2.049025	6.784862	1.629696	-0.002416	0.001909	-0.001313
Na	0.404117	7.016739	4.737094	-0.002415	0.001918	-0.001310
Na	2.558546	13.685662	1.553699	-0.002416	-0.001915	-0.001308
Na	-0.105403	0.115939	4.813091	-0.002415	-0.001913	-0.001313
B	4.155007	8.978944	1.168663	-0.012178	-0.003810	-0.042194
B	-1.701865	4.822656	5.198127	-0.012151	-0.003785	-0.042102
B	0.452564	2.078144	2.014732	-0.012135	0.003806	-0.042088
B	2.000578	11.723457	4.352058	-0.012190	0.003806	-0.042211
B	-2.733891	11.746082	5.839177	-0.047411	-0.003829	0.002004
B	5.187034	2.055518	0.527613	-0.047280	-0.003802	0.002007
B	3.032605	4.845282	3.711007	-0.047266	0.003819	0.002007
B	-0.579463	8.956318	2.655782	-0.047405	0.003824	0.002005

B	-0.983708	0.054306	1.827988	0.021342	0.004604	0.017381
B	3.436850	13.747295	4.538802	0.021411	0.004614	0.017433
B	5.591279	6.955106	1.355407	0.021414	-0.004604	0.017424
B	-3.138137	6.846495	5.011383	0.021327	-0.004621	0.017394
Si	0.631772	3.486686	4.508512	-0.007344	0.014657	-0.008049
Si	1.821370	10.314915	1.858278	-0.007398	0.014698	-0.008084
Si	-0.333059	10.387486	5.041673	-0.007383	-0.014708	-0.008078
Si	2.786201	3.414115	1.325117	-0.007375	-0.014632	-0.008063
O	0.061445	3.072947	3.041906	0.038515	-0.046584	0.005024
O	2.391697	10.728653	3.324884	0.038724	-0.046761	0.005030
O	4.546126	9.973747	0.141489	0.038637	0.046712	0.005029
O	-2.092984	3.827853	6.225301	0.038601	0.046626	0.005010
O	2.197450	3.933608	4.519003	0.007445	-0.029172	0.015697
O	0.255692	9.867992	1.847787	0.007467	-0.029264	0.015750
O	-1.898737	10.834409	5.031182	0.007487	0.029284	0.015783
O	4.351879	2.967192	1.335608	0.007428	0.029169	0.015703
O	-0.212316	4.798696	5.055280	0.003421	-0.005873	0.035204
O	2.665458	9.002905	1.311510	0.003466	-0.005837	0.035298
O	0.511030	11.699496	4.494905	0.003430	0.005899	0.035316
O	1.942113	2.102105	1.871885	0.003477	0.005807	0.035198
O	0.525580	2.169271	5.472081	0.029830	0.013112	-0.002449
O	1.927562	11.632329	0.894709	0.029935	0.013124	-0.002470
O	-0.226867	9.070071	4.078104	0.029915	-0.013147	-0.002459
O	2.680009	4.731529	2.288686	0.029855	-0.013118	-0.002433
O	0.058846	0.698526	2.444964	0.007147	0.024676	0.009627
O	2.394296	13.103075	3.921826	0.007165	0.024734	0.009679
O	4.548725	7.599326	0.738431	0.007170	-0.024738	0.009668
O	-2.095583	6.202275	5.628359	0.007147	-0.024658	0.009647
O	-2.459230	13.184059	5.445139	0.012201	-0.022179	0.004457
O	4.912372	0.617542	0.921651	0.012159	-0.022110	0.004443
O	2.757943	6.283259	4.105046	0.012162	0.022112	0.004436
O	-0.304801	7.518342	2.261744	0.012183	0.022185	0.004458
O	-0.175430	2.374756	0.744070	-0.038017	-0.000685	-0.022504
O	2.628573	11.426844	5.622720	-0.038158	-0.000675	-0.022567
O	4.783002	9.275557	2.439325	-0.038129	0.000675	-0.022559
O	-2.329859	4.526044	3.927465	-0.038048	0.000670	-0.022491

O	-1.223866	12.517207	2.155216	-0.003519	0.001928	-0.009358
O	3.677009	1.284394	4.211574	-0.003552	0.001947	-0.009390
O	5.831438	5.616407	1.028179	-0.003542	-0.001943	-0.009385
O	-3.378295	8.185194	5.338611	-0.003521	-0.001952	-0.009361
H	-0.637445	12.195109	2.878812	-0.077559	-0.023081	0.037234
H	3.090587	1.606491	3.487978	-0.077561	-0.023207	0.037108
H	5.245016	5.294309	0.304583	-0.077646	0.023190	0.037200
H	-2.791874	8.507292	6.062207	-0.077447	0.023089	0.037122

81 f = 18.683366 THz 117.391052 2PiTHz 623.209994 cm-1 77.268219 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.060819	-0.022934	0.033072
Li	-1.316675	4.156264	2.365404	-0.060634	0.022907	-0.032955
Li	-3.471104	2.744536	5.548798	0.060605	0.022865	0.032943
Li	5.924247	11.057064	0.817991	-0.060854	-0.022973	-0.033101
Na	2.049025	6.784862	1.629696	0.000084	0.005549	-0.002081
Na	0.404117	7.016739	4.737094	-0.000081	-0.005535	0.002078
Na	2.558546	13.685662	1.553699	0.000078	-0.005547	-0.002080
Na	-0.105403	0.115939	4.813091	-0.000087	0.005540	0.002079
B	4.155007	8.978944	1.168663	-0.004418	0.004741	-0.010219
B	-1.701865	4.822656	5.198127	0.004394	-0.004741	0.010161
B	0.452564	2.078144	2.014732	-0.004413	-0.004747	-0.010193
B	2.000578	11.723457	4.352058	0.004390	0.004742	0.010158
B	-2.733891	11.746082	5.839177	0.002963	0.005307	0.005448
B	5.187034	2.055518	0.527613	-0.002995	-0.005320	-0.005409
B	3.032605	4.845282	3.711007	0.002973	-0.005308	0.005411
B	-0.579463	8.956318	2.655782	-0.003021	0.005331	-0.005441
B	-0.983708	0.054306	1.827988	-0.003577	0.005698	0.009520
B	3.436850	13.747295	4.538802	0.003639	-0.005719	-0.009557
B	5.591279	6.955106	1.355407	-0.003606	-0.005726	0.009585
B	-3.138137	6.846495	5.011383	0.003583	0.005692	-0.009502
Si	0.631772	3.486686	4.508512	-0.005609	-0.003152	-0.001719
Si	1.821370	10.314915	1.858278	0.005609	0.003167	0.001721
Si	-0.333059	10.387486	5.041673	-0.005618	0.003145	-0.001732
Si	2.786201	3.414115	1.325117	0.005605	-0.003159	0.001714

O	0.061445	3.072947	3.041906	0.065536	-0.039383	0.003632
O	2.391697	10.728653	3.324884	-0.065703	0.039453	-0.003642
O	4.546126	9.973747	0.141489	0.065781	0.039528	0.003649
O	-2.092984	3.827853	6.225301	-0.065470	-0.039333	-0.003627
O	2.197450	3.933608	4.519003	-0.018104	0.016958	-0.034643
O	0.255692	9.867992	1.847787	0.018172	-0.017036	0.034773
O	-1.898737	10.834409	5.031182	-0.018169	-0.017002	-0.034779
O	4.351879	2.967192	1.335608	0.018096	0.016962	0.034618
O	-0.212316	4.798696	5.055280	0.023713	0.046597	-0.014406
O	2.665458	9.002905	1.311510	-0.023813	-0.046807	0.014500
O	0.511030	11.699496	4.494905	0.023801	-0.046776	-0.014452
O	1.942113	2.102105	1.871885	-0.023736	0.046639	0.014440
O	0.525580	2.169271	5.472081	0.010540	-0.025955	-0.016184
O	1.927562	11.632329	0.894709	-0.010534	0.026111	0.016278
O	-0.226867	9.070071	4.078104	0.010580	0.026064	-0.016260
O	2.680009	4.731529	2.288686	-0.010524	-0.025994	0.016206
O	0.058846	0.698526	2.444964	-0.001476	-0.006090	0.012896
O	2.394296	13.103075	3.921826	0.001489	0.006147	-0.012923
O	4.548725	7.599326	0.738431	-0.001481	0.006105	0.012933
O	-2.095583	6.202275	5.628359	0.001475	-0.006107	-0.012899
O	-2.459230	13.184059	5.445139	-0.007865	-0.003549	0.006452
O	4.912372	0.617542	0.921651	0.007859	0.003526	-0.006413
O	2.757943	6.283259	4.105046	-0.007841	0.003531	0.006422
O	-0.304801	7.518342	2.261744	0.007885	-0.003518	-0.006437
O	-0.175430	2.374756	0.744070	-0.018202	0.003313	-0.008403
O	2.628573	11.426844	5.622720	0.018213	-0.003327	0.008415
O	4.783002	9.275557	2.439325	-0.018266	-0.003324	-0.008442
O	-2.329859	4.526044	3.927465	0.018181	0.003319	0.008387
O	-1.223866	12.517207	2.155216	-0.000986	0.006399	0.001860
O	3.677009	1.284394	4.211574	0.000948	-0.006382	-0.001857
O	5.831438	5.616407	1.028179	-0.000958	-0.006387	0.001838
O	-3.378295	8.185194	5.338611	0.000987	0.006397	-0.001867
H	-0.637445	12.195109	2.878812	0.062146	-0.011339	-0.057264
H	3.090587	1.606491	3.487978	-0.062115	0.011236	0.057149
H	5.245016	5.294309	0.304583	0.062010	0.011274	-0.057116
H	-2.791874	8.507292	6.062207	-0.062221	-0.011337	0.057312

82 f = 18.649504 THz 117.178287 2PiTHz 622.080462 cm-1 77.128175

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.059882	-0.016602	0.035125
Li	-1.316675	4.156264	2.365404	0.060155	-0.016752	0.035210
Li	-3.471104	2.744536	5.548798	-0.060123	-0.016735	-0.035185
Li	5.924247	11.057064	0.817991	-0.059902	-0.016611	-0.035141
Na	2.049025	6.784862	1.629696	0.001041	0.000293	-0.000188
Na	0.404117	7.016739	4.737094	0.001044	0.000306	-0.000193
Na	2.558546	13.685662	1.553699	-0.001046	0.000304	0.000193
Na	-0.105403	0.115939	4.813091	-0.001041	0.000296	0.000188
B	4.155007	8.978944	1.168663	-0.005866	0.003339	-0.005916
B	-1.701865	4.822656	5.198127	-0.005875	0.003348	-0.005948
B	0.452564	2.078144	2.014732	0.005892	0.003353	0.005979
B	2.000578	11.723457	4.352058	0.005850	0.003338	0.005865
B	-2.733891	11.746082	5.839177	0.004003	0.001117	0.007639
B	5.187034	2.055518	0.527613	0.004004	0.001217	0.007659
B	3.032605	4.845282	3.711007	-0.003973	0.001214	-0.007647
B	-0.579463	8.956318	2.655782	-0.004050	0.001131	-0.007640
B	-0.983708	0.054306	1.827988	0.007311	-0.004859	-0.010892
B	3.436850	13.747295	4.538802	0.007332	-0.004815	-0.010813
B	5.591279	6.955106	1.355407	-0.007305	-0.004813	0.010839
B	-3.138137	6.846495	5.011383	-0.007329	-0.004860	0.010882
Si	0.631772	3.486686	4.508512	0.002922	0.000381	-0.000211
Si	1.821370	10.314915	1.858278	0.002850	0.000347	-0.000267
Si	-0.333059	10.387486	5.041673	-0.002860	0.000326	0.000260
Si	2.786201	3.414115	1.325117	-0.002912	0.000397	0.000212
O	0.061445	3.072947	3.041906	-0.063490	0.036742	-0.004953
O	2.391697	10.728653	3.324884	-0.063160	0.036488	-0.004942
O	4.546126	9.973747	0.141489	0.063196	0.036538	0.004945
O	-2.092984	3.827853	6.225301	0.063442	0.036697	0.004946
O	2.197450	3.933608	4.519003	0.020445	-0.020640	0.042095
O	0.255692	9.867992	1.847787	0.020402	-0.020644	0.042109
O	-1.898737	10.834409	5.031182	-0.020392	-0.020609	-0.042091
O	4.351879	2.967192	1.335608	-0.020453	-0.020664	-0.042103

O	-0.212316	4.798696	5.055280	-0.021268	-0.043318	0.015019
O	2.665458	9.002905	1.311510	-0.021138	-0.043131	0.015029
O	0.511030	11.699496	4.494905	0.021144	-0.043125	-0.014991
O	1.942113	2.102105	1.871885	0.021275	-0.043343	-0.015053
O	0.525580	2.169271	5.472081	-0.008068	0.031430	0.021648
O	1.927562	11.632329	0.894709	-0.007966	0.031478	0.021681
O	-0.226867	9.070071	4.078104	0.008004	0.031456	-0.021681
O	2.680009	4.731529	2.288686	0.008048	0.031447	-0.021647
O	0.058846	0.698526	2.444964	0.002212	0.009104	-0.009923
O	2.394296	13.103075	3.921826	0.002218	0.009137	-0.009862
O	4.548725	7.599326	0.738431	-0.002211	0.009105	0.009869
O	-2.095583	6.202275	5.628359	-0.002213	0.009122	0.009916
O	-2.459230	13.184059	5.445139	-0.008769	-0.004184	0.006909
O	4.912372	0.617542	0.921651	-0.008793	-0.004133	0.006900
O	2.757943	6.283259	4.105046	0.008781	-0.004143	-0.006909
O	-0.304801	7.518342	2.261744	0.008784	-0.004155	-0.006897
O	-0.175430	2.374756	0.744070	0.016753	-0.002545	0.009451
O	2.628573	11.426844	5.622720	0.016636	-0.002517	0.009419
O	4.783002	9.275557	2.439325	-0.016681	-0.002516	-0.009444
O	-2.329859	4.526044	3.927465	-0.016724	-0.002549	-0.009428
O	-1.223866	12.517207	2.155216	-0.009076	0.001302	0.003116
O	3.677009	1.284394	4.211574	-0.009092	0.001356	0.003092
O	5.831438	5.616407	1.028179	0.009079	0.001355	-0.003103
O	-3.378295	8.185194	5.338611	0.009082	0.001306	-0.003111
H	-0.637445	12.195109	2.878812	0.039986	-0.023105	-0.047426
H	3.090587	1.606491	3.487978	0.040208	-0.023204	-0.047718
H	5.245016	5.294309	0.304583	-0.040270	-0.023152	0.047719
H	-2.791874	8.507292	6.062207	-0.039979	-0.023132	0.047444

83 f = 18.334452 THz 115.198760 2PiTHz 611.571472 cm-1 75.825226 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.046730	-0.046678	0.018165
Li	-1.316675	4.156264	2.365404	0.046645	-0.046589	0.018213
Li	-3.471104	2.744536	5.548798	0.046721	0.046646	0.018184
Li	5.924247	11.057064	0.817991	0.046671	0.046626	0.018202

Na	2.049025	6.784862	1.629696	-0.001071	-0.006326	0.000592
Na	0.404117	7.016739	4.737094	-0.001071	-0.006312	0.000579
Na	2.558546	13.685662	1.553699	-0.001071	0.006318	0.000579
Na	-0.105403	0.115939	4.813091	-0.001072	0.006319	0.000591
B	4.155007	8.978944	1.168663	0.006753	-0.003232	-0.017536
B	-1.701865	4.822656	5.198127	0.006777	-0.003248	-0.017441
B	0.452564	2.078144	2.014732	0.006771	0.003224	-0.017465
B	2.000578	11.723457	4.352058	0.006753	0.003246	-0.017515
B	-2.733891	11.746082	5.839177	-0.016975	-0.014361	0.016016
B	5.187034	2.055518	0.527613	-0.016929	-0.014320	0.015990
B	3.032605	4.845282	3.711007	-0.016918	0.014300	0.015987
B	-0.579463	8.956318	2.655782	-0.016994	0.014390	0.016021
B	-0.983708	0.054306	1.827988	0.013164	0.000127	0.004696
B	3.436850	13.747295	4.538802	0.013200	0.000114	0.004718
B	5.591279	6.955106	1.355407	0.013216	-0.000127	0.004717
B	-3.138137	6.846495	5.011383	0.013154	-0.000112	0.004697
Si	0.631772	3.486686	4.508512	-0.002172	-0.002537	-0.010112
Si	1.821370	10.314915	1.858278	-0.002153	-0.002502	-0.010126
Si	-0.333059	10.387486	5.041673	-0.002189	0.002514	-0.010138
Si	2.786201	3.414115	1.325117	-0.002130	0.002518	-0.010098
O	0.061445	3.072947	3.041906	-0.061406	0.023764	-0.010849
O	2.391697	10.728653	3.324884	-0.061482	0.023753	-0.010830
O	4.546126	9.973747	0.141489	-0.061448	-0.023727	-0.010840
O	-2.092984	3.827853	6.225301	-0.061469	-0.023801	-0.010834
O	2.197450	3.933608	4.519003	0.013336	-0.020251	0.035130
O	0.255692	9.867992	1.847787	0.013360	-0.020314	0.035163
O	-1.898737	10.834409	5.031182	0.013373	0.020323	0.035194
O	4.351879	2.967192	1.335608	0.013331	0.020244	0.035106
O	-0.212316	4.798696	5.055280	0.036217	0.048342	-0.002181
O	2.665458	9.002905	1.311510	0.036275	0.048376	-0.002123
O	0.511030	11.699496	4.494905	0.036261	-0.048391	-0.002141
O	1.942113	2.102105	1.871885	0.036211	-0.048308	-0.002168
O	0.525580	2.169271	5.472081	0.015987	-0.019388	-0.009910
O	1.927562	11.632329	0.894709	0.016029	-0.019419	-0.009933
O	-0.226867	9.070071	4.078104	0.016044	0.019392	-0.009920
O	2.680009	4.731529	2.288686	0.015968	0.019409	-0.009923

O	0.058846	0.698526	2.444964	0.008127	0.017276	-0.004012
O	2.394296	13.103075	3.921826	0.008133	0.017342	-0.004034
O	4.548725	7.599326	0.738431	0.008137	-0.017342	-0.004015
O	-2.095583	6.202275	5.628359	0.008126	-0.017285	-0.004037
O	-2.459230	13.184059	5.445139	-0.003279	-0.026032	0.000398
O	4.912372	0.617542	0.921651	-0.003298	-0.025988	0.000388
O	2.757943	6.283259	4.105046	-0.003297	0.025978	0.000387
O	-0.304801	7.518342	2.261744	-0.003288	0.026057	0.000402
O	-0.175430	2.374756	0.744070	-0.015022	0.002150	0.007641
O	2.628573	11.426844	5.622720	-0.015033	0.002141	0.007591
O	4.783002	9.275557	2.439325	-0.015083	-0.002149	0.007625
O	-2.329859	4.526044	3.927465	-0.014970	-0.002136	0.007606
O	-1.223866	12.517207	2.155216	-0.007647	0.000201	-0.010463
O	3.677009	1.284394	4.211574	-0.007668	0.000193	-0.010478
O	5.831438	5.616407	1.028179	-0.007665	-0.000218	-0.010484
O	-3.378295	8.185194	5.338611	-0.007654	-0.000174	-0.010455
H	-0.637445	12.195109	2.878812	-0.054445	-0.021540	0.017170
H	3.090587	1.606491	3.487978	-0.054547	-0.021636	0.017180
H	5.245016	5.294309	0.304583	-0.054509	0.021623	0.017140
H	-2.791874	8.507292	6.062207	-0.054465	0.021570	0.017188

84 f = 18.157304 THz 114.085705 2PiTHz 605.662443 cm-1 75.092599 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.044570	0.047995	-0.005578
Li	-1.316675	4.156264	2.365404	0.044635	-0.048056	0.005612
Li	-3.471104	2.744536	5.548798	0.044635	0.048054	0.005618
Li	5.924247	11.057064	0.817991	-0.044574	-0.047986	-0.005589
Na	2.049025	6.784862	1.629696	0.001673	0.001641	0.000480
Na	0.404117	7.016739	4.737094	-0.001676	-0.001648	-0.000473
Na	2.558546	13.685662	1.553699	-0.001675	0.001648	-0.000473
Na	-0.105403	0.115939	4.813091	0.001674	-0.001637	0.000480
B	4.155007	8.978944	1.168663	-0.003048	-0.000009	0.012564
B	-1.701865	4.822656	5.198127	0.003048	0.000011	-0.012609
B	0.452564	2.078144	2.014732	0.003042	-0.000026	-0.012600
B	2.000578	11.723457	4.352058	-0.003041	0.000003	0.012570

B	-2.733891	11.746082	5.839177	0.017222	0.016799	-0.013245
B	5.187034	2.055518	0.527613	-0.017245	-0.016812	0.013258
B	3.032605	4.845282	3.711007	-0.017261	0.016830	0.013265
B	-0.579463	8.956318	2.655782	0.017221	-0.016800	-0.013239
B	-0.983708	0.054306	1.827988	0.018727	-0.004364	-0.001731
B	3.436850	13.747295	4.538802	-0.018720	0.004359	0.001733
B	5.591279	6.955106	1.355407	-0.018713	-0.004355	0.001736
B	-3.138137	6.846495	5.011383	0.018744	0.004367	-0.001725
Si	0.631772	3.486686	4.508512	-0.002528	-0.000006	-0.010751
Si	1.821370	10.314915	1.858278	0.002527	-0.000003	0.010747
Si	-0.333059	10.387486	5.041673	0.002529	0.000006	0.010740
Si	2.786201	3.414115	1.325117	-0.002523	-0.000001	-0.010758
O	0.061445	3.072947	3.041906	-0.060712	0.022919	-0.009135
O	2.391697	10.728653	3.324884	0.060649	-0.022878	0.009109
O	4.546126	9.973747	0.141489	0.060652	0.022882	0.009107
O	-2.092984	3.827853	6.225301	-0.060734	-0.022915	-0.009130
O	2.197450	3.933608	4.519003	0.017489	-0.024552	0.040100
O	0.255692	9.867992	1.847787	-0.017468	0.024517	-0.040060
O	-1.898737	10.834409	5.031182	-0.017476	-0.024529	-0.040063
O	4.351879	2.967192	1.335608	0.017494	0.024544	0.040104
O	-0.212316	4.798696	5.055280	0.034591	0.046761	-0.002895
O	2.665458	9.002905	1.311510	-0.034541	-0.046697	0.002900
O	0.511030	11.699496	4.494905	-0.034532	0.046693	0.002909
O	1.942113	2.102105	1.871885	0.034569	-0.046745	-0.002894
O	0.525580	2.169271	5.472081	0.016290	-0.021142	-0.013142
O	1.927562	11.632329	0.894709	-0.016271	0.021121	0.013132
O	-0.226867	9.070071	4.078104	-0.016264	-0.021124	0.013139
O	2.680009	4.731529	2.288686	0.016296	0.021133	-0.013136
O	0.058846	0.698526	2.444964	0.007559	0.018303	-0.001046
O	2.394296	13.103075	3.921826	-0.007562	-0.018288	0.001033
O	4.548725	7.599326	0.738431	-0.007561	0.018280	0.001033
O	-2.095583	6.202275	5.628359	0.007564	-0.018327	-0.001049
O	-2.459230	13.184059	5.445139	0.005213	0.024206	-0.000358
O	4.912372	0.617542	0.921651	-0.005204	-0.024213	0.000363
O	2.757943	6.283259	4.105046	-0.005207	0.024238	0.000370
O	-0.304801	7.518342	2.261744	0.005222	-0.024205	-0.000354

O	-0.175430	2.374756	0.744070	-0.017298	0.001652	0.009708
O	2.628573	11.426844	5.622720	0.017274	-0.001650	-0.009704
O	4.783002	9.275557	2.439325	0.017271	0.001652	-0.009707
O	-2.329859	4.526044	3.927465	-0.017307	-0.001648	0.009708
O	-1.223866	12.517207	2.155216	-0.006466	0.005536	-0.004337
O	3.677009	1.284394	4.211574	0.006467	-0.005539	0.004330
O	5.831438	5.616407	1.028179	0.006458	0.005541	0.004327
O	-3.378295	8.185194	5.338611	-0.006477	-0.005537	-0.004346
H	-0.637445	12.195109	2.878812	-0.026671	-0.017273	0.001426
H	3.090587	1.606491	3.487978	0.026598	0.017256	-0.001380
H	5.245016	5.294309	0.304583	0.026603	-0.017236	-0.001403
H	-2.791874	8.507292	6.062207	-0.026706	0.017299	0.001425

85 f = 17.995664 THz 113.070089 2PiTHz 600.270707 cm-1 74.424109 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.033242	0.022366	0.008163
Li	-1.316675	4.156264	2.365404	0.033149	-0.022361	-0.008174
Li	-3.471104	2.744536	5.548798	-0.033152	-0.022341	0.008186
Li	5.924247	11.057064	0.817991	0.033252	0.022407	-0.008146
Na	2.049025	6.784862	1.629696	0.000072	0.004247	0.000100
Na	0.404117	7.016739	4.737094	-0.000069	-0.004249	-0.000098
Na	2.558546	13.685662	1.553699	0.000069	-0.004247	0.000098
Na	-0.105403	0.115939	4.813091	-0.000073	0.004250	-0.000100
B	4.155007	8.978944	1.168663	-0.012628	0.022877	0.030923
B	-1.701865	4.822656	5.198127	0.012618	-0.022838	-0.030878
B	0.452564	2.078144	2.014732	-0.012626	-0.022857	0.030876
B	2.000578	11.723457	4.352058	0.012620	0.022864	-0.030933
B	-2.733891	11.746082	5.839177	-0.034880	-0.036441	0.008601
B	5.187034	2.055518	0.527613	0.034810	0.036375	-0.008581
B	3.032605	4.845282	3.711007	-0.034802	0.036382	0.008582
B	-0.579463	8.956318	2.655782	0.034885	-0.036434	-0.008598
B	-0.983708	0.054306	1.827988	-0.032842	-0.003261	-0.016873
B	3.436850	13.747295	4.538802	0.032865	0.003266	0.016914
B	5.591279	6.955106	1.355407	-0.032858	0.003280	-0.016906
B	-3.138137	6.846495	5.011383	0.032837	-0.003254	0.016882

Si	0.631772	3.486686	4.508512	-0.001888	-0.006159	0.010803
Si	1.821370	10.314915	1.858278	0.001874	0.006167	-0.010820
Si	-0.333059	10.387486	5.041673	-0.001883	0.006162	0.010815
Si	2.786201	3.414115	1.325117	0.001880	-0.006163	-0.010809
O	0.061445	3.072947	3.041906	0.007304	0.030821	-0.005239
O	2.391697	10.728653	3.324884	-0.007292	-0.030869	0.005232
O	4.546126	9.973747	0.141489	0.007255	-0.030880	-0.005241
O	-2.092984	3.827853	6.225301	-0.007313	0.030823	0.005234
O	2.197450	3.933608	4.519003	-0.005913	-0.018519	-0.006011
O	0.255692	9.867992	1.847787	0.005922	0.018548	0.006036
O	-1.898737	10.834409	5.031182	-0.005899	0.018572	-0.005985
O	4.351879	2.967192	1.335608	0.005926	-0.018508	0.006037
O	-0.212316	4.798696	5.055280	0.039531	0.014691	0.007670
O	2.665458	9.002905	1.311510	-0.039556	-0.014663	-0.007695
O	0.511030	11.699496	4.494905	0.039565	-0.014692	0.007694
O	1.942113	2.102105	1.871885	-0.039531	0.014680	-0.007667
O	0.525580	2.169271	5.472081	-0.014323	-0.012770	-0.008398
O	1.927562	11.632329	0.894709	0.014369	0.012749	0.008390
O	-0.226867	9.070071	4.078104	-0.014360	0.012784	-0.008415
O	2.680009	4.731529	2.288686	0.014326	-0.012749	0.008382
O	0.058846	0.698526	2.444964	-0.009476	-0.043384	-0.007035
O	2.394296	13.103075	3.921826	0.009494	0.043429	0.007051
O	4.548725	7.599326	0.738431	-0.009492	0.043418	-0.007054
O	-2.095583	6.202275	5.628359	0.009473	-0.043387	0.007032
O	-2.459230	13.184059	5.445139	-0.008245	-0.051678	0.008944
O	4.912372	0.617542	0.921651	0.008238	0.051598	-0.008951
O	2.757943	6.283259	4.105046	-0.008228	0.051600	0.008950
O	-0.304801	7.518342	2.261744	0.008259	-0.051680	-0.008937
O	-0.175430	2.374756	0.744070	0.031964	-0.005451	0.004427
O	2.628573	11.426844	5.622720	-0.032030	0.005469	-0.004437
O	4.783002	9.275557	2.439325	0.032038	0.005462	0.004423
O	-2.329859	4.526044	3.927465	-0.031961	-0.005458	-0.004431
O	-1.223866	12.517207	2.155216	0.016182	-0.004769	0.019055
O	3.677009	1.284394	4.211574	-0.016200	0.004780	-0.019095
O	5.831438	5.616407	1.028179	0.016184	0.004790	0.019087
O	-3.378295	8.185194	5.338611	-0.016185	-0.004766	-0.019056

H	-0.637445	12.195109	2.878812	0.080273	0.038099	-0.012281
H	3.090587	1.606491	3.487978	-0.080475	-0.038178	0.012340
H	5.245016	5.294309	0.304583	0.080428	-0.038148	-0.012333
H	-2.791874	8.507292	6.062207	-0.080289	0.038112	0.012284

86 f = 17.851447 THz 112.163952 2PiTHz 595.460172 cm-1 73.827679 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.025392	-0.010212	0.023478
Li	-1.316675	4.156264	2.365404	0.025384	-0.010195	0.023456
Li	-3.471104	2.744536	5.548798	-0.025438	-0.010209	-0.023500
Li	5.924247	11.057064	0.817991	-0.025355	-0.010206	-0.023465
Na	2.049025	6.784862	1.629696	-0.002747	0.001141	-0.000547
Na	0.404117	7.016739	4.737094	-0.002751	0.001145	-0.000555
Na	2.558546	13.685662	1.553699	0.002751	0.001139	0.000555
Na	-0.105403	0.115939	4.813091	0.002748	0.001147	0.000548
B	4.155007	8.978944	1.168663	0.007335	-0.029939	-0.033509
B	-1.701865	4.822656	5.198127	0.007336	-0.029961	-0.033532
B	0.452564	2.078144	2.014732	-0.007359	-0.029987	0.033552
B	2.000578	11.723457	4.352058	-0.007321	-0.029925	0.033501
B	-2.733891	11.746082	5.839177	0.031828	0.035348	-0.017762
B	5.187034	2.055518	0.527613	0.031898	0.035405	-0.017814
B	3.032605	4.845282	3.711007	-0.031892	0.035383	0.017785
B	-0.579463	8.956318	2.655782	-0.031841	0.035369	0.017782
B	-0.983708	0.054306	1.827988	-0.032011	-0.003929	-0.018929
B	3.436850	13.747295	4.538802	-0.031929	-0.003927	-0.018904
B	5.591279	6.955106	1.355407	0.031947	-0.003930	0.018906
B	-3.138137	6.846495	5.011383	0.031987	-0.003927	0.018923
Si	0.631772	3.486686	4.508512	-0.003836	-0.001536	0.008550
Si	1.821370	10.314915	1.858278	-0.003826	-0.001528	0.008535
Si	-0.333059	10.387486	5.041673	0.003822	-0.001526	-0.008541
Si	2.786201	3.414115	1.325117	0.003842	-0.001539	-0.008549
O	0.061445	3.072947	3.041906	0.003149	0.029614	-0.003081
O	2.391697	10.728653	3.324884	0.003102	0.029593	-0.003082
O	4.546126	9.973747	0.141489	-0.003115	0.029589	0.003079
O	-2.092984	3.827853	6.225301	-0.003119	0.029630	0.003087

O	2.197450	3.933608	4.519003	-0.004314	-0.020122	-0.008793
O	0.255692	9.867992	1.847787	-0.004333	-0.020071	-0.008842
O	-1.898737	10.834409	5.031182	0.004323	-0.020070	0.008815
O	4.351879	2.967192	1.335608	0.004332	-0.020115	0.008828
O	-0.212316	4.798696	5.055280	0.025776	0.013105	0.008309
O	2.665458	9.002905	1.311510	0.025739	0.013093	0.008291
O	0.511030	11.699496	4.494905	-0.025720	0.013084	-0.008287
O	1.942113	2.102105	1.871885	-0.025797	0.013122	-0.008309
O	0.525580	2.169271	5.472081	-0.019916	-0.019217	-0.023110
O	1.927562	11.632329	0.894709	-0.019890	-0.019198	-0.023074
O	-0.226867	9.070071	4.078104	0.019902	-0.019227	0.023101
O	2.680009	4.731529	2.288686	0.019903	-0.019181	0.023071
O	0.058846	0.698526	2.444964	-0.007424	-0.049533	0.004194
O	2.394296	13.103075	3.921826	-0.007403	-0.049432	0.004184
O	4.548725	7.599326	0.738431	0.007408	-0.049457	-0.004189
O	-2.095583	6.202275	5.628359	0.007417	-0.049494	-0.004178
O	-2.459230	13.184059	5.445139	0.000740	0.047863	-0.010268
O	4.912372	0.617542	0.921651	0.000759	0.047973	-0.010289
O	2.757943	6.283259	4.105046	-0.000747	0.047941	0.010277
O	-0.304801	7.518342	2.261744	-0.000757	0.047899	0.010268
O	-0.175430	2.374756	0.744070	0.024374	0.001891	0.014216
O	2.628573	11.426844	5.622720	0.024335	0.001889	0.014205
O	4.783002	9.275557	2.439325	-0.024344	0.001889	-0.014199
O	-2.329859	4.526044	3.927465	-0.024383	0.001887	-0.014209
O	-1.223866	12.517207	2.155216	0.013648	-0.002510	0.020348
O	3.677009	1.284394	4.211574	0.013613	-0.002503	0.020315
O	5.831438	5.616407	1.028179	-0.013613	-0.002513	-0.020314
O	-3.378295	8.185194	5.338611	-0.013637	-0.002510	-0.020338
H	-0.637445	12.195109	2.878812	0.102919	0.051727	-0.025672
H	3.090587	1.606491	3.487978	0.102770	0.051627	-0.025660
H	5.245016	5.294309	0.304583	-0.102799	0.051646	0.025670
H	-2.791874	8.507292	6.062207	-0.102854	0.051688	0.025656

87 f = 17.703343 THz 111.233387 2PiTHz 590.519953 cm-1 73.215169
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.040424	0.016167	0.046183
Li	-1.316675	4.156264	2.365404	0.040422	0.016130	0.046125
Li	-3.471104	2.744536	5.548798	0.040372	-0.016179	0.046161
Li	5.924247	11.057064	0.817991	0.040464	-0.016122	0.046161
Na	2.049025	6.784862	1.629696	-0.002635	0.005680	-0.001624
Na	0.404117	7.016739	4.737094	-0.002638	0.005679	-0.001625
Na	2.558546	13.685662	1.553699	-0.002637	-0.005683	-0.001625
Na	-0.105403	0.115939	4.813091	-0.002634	-0.005676	-0.001624
B	4.155007	8.978944	1.168663	0.022821	-0.023185	-0.014906
B	-1.701865	4.822656	5.198127	0.022824	-0.023159	-0.014928
B	0.452564	2.078144	2.014732	0.022814	0.023167	-0.014912
B	2.000578	11.723457	4.352058	0.022837	0.023173	-0.014916
B	-2.733891	11.746082	5.839177	-0.003375	-0.016393	0.025139
B	5.187034	2.055518	0.527613	-0.003374	-0.016382	0.025146
B	3.032605	4.845282	3.711007	-0.003394	0.016393	0.025136
B	-0.579463	8.956318	2.655782	-0.003369	0.016388	0.025156
B	-0.983708	0.054306	1.827988	0.014075	-0.000595	0.005036
B	3.436850	13.747295	4.538802	0.014081	-0.000584	0.005037
B	5.591279	6.955106	1.355407	0.014087	0.000598	0.005027
B	-3.138137	6.846495	5.011383	0.014080	0.000579	0.005042
Si	0.631772	3.486686	4.508512	-0.002480	-0.008680	-0.000446
Si	1.821370	10.314915	1.858278	-0.002498	-0.008692	-0.000442
Si	-0.333059	10.387486	5.041673	-0.002481	0.008699	-0.000441
Si	2.786201	3.414115	1.325117	-0.002498	0.008677	-0.000452
O	0.061445	3.072947	3.041906	-0.003701	0.003328	-0.002801
O	2.391697	10.728653	3.324884	-0.003707	0.003334	-0.002804
O	4.546126	9.973747	0.141489	-0.003730	-0.003355	-0.002810
O	-2.092984	3.827853	6.225301	-0.003683	-0.003301	-0.002798
O	2.197450	3.933608	4.519003	-0.030496	0.025187	-0.055741
O	0.255692	9.867992	1.847787	-0.030504	0.025201	-0.055770
O	-1.898737	10.834409	5.031182	-0.030519	-0.025218	-0.055765
O	4.351879	2.967192	1.335608	-0.030484	-0.025181	-0.055726
O	-0.212316	4.798696	5.055280	0.012385	-0.001358	0.000680
O	2.665458	9.002905	1.311510	0.012377	-0.001335	0.000658
O	0.511030	11.699496	4.494905	0.012389	0.001352	0.000660
O	1.942113	2.102105	1.871885	0.012365	0.001351	0.000678

O	0.525580	2.169271	5.472081	0.004944	0.047304	0.045613
O	1.927562	11.632329	0.894709	0.004944	0.047334	0.045627
O	-0.226867	9.070071	4.078104	0.004942	-0.047338	0.045647
O	2.680009	4.731529	2.288686	0.004951	-0.047317	0.045609
O	0.058846	0.698526	2.444964	0.000486	0.032603	-0.012459
O	2.394296	13.103075	3.921826	0.000491	0.032610	-0.012445
O	4.548725	7.599326	0.738431	0.000488	-0.032624	-0.012471
O	-2.095583	6.202275	5.628359	0.000493	-0.032600	-0.012431
O	-2.459230	13.184059	5.445139	-0.009655	-0.026700	0.013152
O	4.912372	0.617542	0.921651	-0.009639	-0.026684	0.013145
O	2.757943	6.283259	4.105046	-0.009650	0.026708	0.013144
O	-0.304801	7.518342	2.261744	-0.009652	0.026698	0.013149
O	-0.175430	2.374756	0.744070	0.008835	-0.002002	-0.002984
O	2.628573	11.426844	5.622720	0.008826	-0.002006	-0.002969
O	4.783002	9.275557	2.439325	0.008842	0.002011	-0.002976
O	-2.329859	4.526044	3.927465	0.008802	0.001995	-0.002969
O	-1.223866	12.517207	2.155216	-0.011531	-0.003040	-0.013513
O	3.677009	1.284394	4.211574	-0.011544	-0.003035	-0.013526
O	5.831438	5.616407	1.028179	-0.011538	0.003038	-0.013517
O	-3.378295	8.185194	5.338611	-0.011536	0.003028	-0.013522
H	-0.637445	12.195109	2.878812	-0.051992	-0.021992	0.009343
H	3.090587	1.606491	3.487978	-0.052002	-0.022008	0.009319
H	5.245016	5.294309	0.304583	-0.052012	0.022005	0.009342
H	-2.791874	8.507292	6.062207	-0.051996	0.022003	0.009324

88 f = 17.524064 THz 110.106941 2PiTHz 584.539834 cm-1 72.473729
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.042271	0.008745	0.034503
Li	-1.316675	4.156264	2.365404	-0.042321	-0.008756	-0.034585
Li	-3.471104	2.744536	5.548798	-0.042312	0.008771	-0.034536
Li	5.924247	11.057064	0.817991	0.042279	-0.008738	0.034572
Na	2.049025	6.784862	1.629696	0.001421	-0.005962	0.001047
Na	0.404117	7.016739	4.737094	-0.001418	0.005948	-0.001056
Na	2.558546	13.685662	1.553699	-0.001421	-0.005955	-0.001056
Na	-0.105403	0.115939	4.813091	0.001418	0.005955	0.001047

B	4.155007	8.978944	1.168663	0.023849	-0.024739	-0.014379
B	-1.701865	4.822656	5.198127	-0.023894	0.024798	0.014413
B	0.452564	2.078144	2.014732	-0.023886	-0.024774	0.014388
B	2.000578	11.723457	4.352058	0.023864	0.024772	-0.014415
B	-2.733891	11.746082	5.839177	-0.005630	-0.019571	0.024179
B	5.187034	2.055518	0.527613	0.005628	0.019536	-0.024183
B	3.032605	4.845282	3.711007	0.005638	-0.019555	-0.024195
B	-0.579463	8.956318	2.655782	-0.005621	0.019547	0.024165
B	-0.983708	0.054306	1.827988	-0.014456	-0.002794	-0.008563
B	3.436850	13.747295	4.538802	0.014486	0.002776	0.008567
B	5.591279	6.955106	1.355407	0.014459	-0.002779	0.008546
B	-3.138137	6.846495	5.011383	-0.014477	0.002794	-0.008573
Si	0.631772	3.486686	4.508512	0.005819	0.006786	-0.000332
Si	1.821370	10.314915	1.858278	-0.005804	-0.006773	0.000329
Si	-0.333059	10.387486	5.041673	-0.005820	0.006774	0.000331
Si	2.786201	3.414115	1.325117	0.005807	-0.006785	-0.000328
O	0.061445	3.072947	3.041906	0.006690	-0.003966	0.001433
O	2.391697	10.728653	3.324884	-0.006667	0.003930	-0.001425
O	4.546126	9.973747	0.141489	-0.006668	-0.003960	-0.001432
O	-2.092984	3.827853	6.225301	0.006689	0.003943	0.001428
O	2.197450	3.933608	4.519003	0.027189	-0.018015	0.052491
O	0.255692	9.867992	1.847787	-0.027160	0.018006	-0.052459
O	-1.898737	10.834409	5.031182	-0.027169	-0.017993	-0.052459
O	4.351879	2.967192	1.335608	0.027182	0.018024	0.052477
O	-0.212316	4.798696	5.055280	-0.016385	-0.002131	-0.001032
O	2.665458	9.002905	1.311510	0.016356	0.002116	0.001032
O	0.511030	11.699496	4.494905	0.016369	-0.002118	0.001041
O	1.942113	2.102105	1.871885	-0.016374	0.002125	-0.001024
O	0.525580	2.169271	5.472081	-0.008297	-0.048493	-0.046022
O	1.927562	11.632329	0.894709	0.008310	0.048490	0.046025
O	-0.226867	9.070071	4.078104	0.008295	-0.048481	0.046003
O	2.680009	4.731529	2.288686	-0.008310	0.048509	-0.046045
O	0.058846	0.698526	2.444964	-0.002664	-0.037913	0.013591
O	2.394296	13.103075	3.921826	0.002655	0.037950	-0.013604
O	4.548725	7.599326	0.738431	0.002658	-0.037896	-0.013590
O	-2.095583	6.202275	5.628359	-0.002661	0.037954	0.013603

O	-2.459230	13.184059	5.445139	-0.013230	-0.034374	0.008406
O	4.912372	0.617542	0.921651	0.013258	0.034382	-0.008389
O	2.757943	6.283259	4.105046	0.013252	-0.034409	-0.008401
O	-0.304801	7.518342	2.261744	-0.013244	0.034349	0.008387
O	-0.175430	2.374756	0.744070	-0.006376	0.004190	0.001777
O	2.628573	11.426844	5.622720	0.006366	-0.004202	-0.001812
O	4.783002	9.275557	2.439325	0.006357	0.004195	-0.001769
O	-2.329859	4.526044	3.927465	-0.006375	-0.004195	0.001803
O	-1.223866	12.517207	2.155216	0.011493	-0.002166	0.010701
O	3.677009	1.284394	4.211574	-0.011500	0.002164	-0.010714
O	5.831438	5.616407	1.028179	-0.011479	-0.002178	-0.010691
O	-3.378295	8.185194	5.338611	0.011506	0.002160	0.010718
H	-0.637445	12.195109	2.878812	0.044552	0.038261	0.003237
H	3.090587	1.606491	3.487978	-0.044644	-0.038311	-0.003199
H	5.245016	5.294309	0.304583	-0.044542	0.038249	-0.003221
H	-2.791874	8.507292	6.062207	0.044626	-0.038299	0.003219

89 f = 17.168301 THz 107.871618 2PiTHz 572.672869 cm-1 71.002412 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.023633	-0.073935	-0.052425
Li	-1.316675	4.156264	2.365404	-0.023562	0.073930	0.052373
Li	-3.471104	2.744536	5.548798	0.023580	0.073894	-0.052401
Li	5.924247	11.057064	0.817991	-0.023612	-0.073962	0.052389
Na	2.049025	6.784862	1.629696	-0.000324	0.000134	0.001614
Na	0.404117	7.016739	4.737094	0.000329	-0.000132	-0.001601
Na	2.558546	13.685662	1.553699	-0.000327	-0.000134	0.001598
Na	-0.105403	0.115939	4.813091	0.000326	0.000131	-0.001616
B	4.155007	8.978944	1.168663	0.021769	0.028899	0.011027
B	-1.701865	4.822656	5.198127	-0.021746	-0.028879	-0.010982
B	0.452564	2.078144	2.014732	0.021760	-0.028878	0.011007
B	2.000578	11.723457	4.352058	-0.021759	0.028894	-0.010986
B	-2.733891	11.746082	5.839177	-0.004964	0.007502	0.024574
B	5.187034	2.055518	0.527613	0.004920	-0.007514	-0.024532
B	3.032605	4.845282	3.711007	-0.004952	-0.007504	0.024547
B	-0.579463	8.956318	2.655782	0.004935	0.007501	-0.024564

B	-0.983708	0.054306	1.827988	-0.021391	0.014301	0.006271
B	3.436850	13.747295	4.538802	0.021405	-0.014305	-0.006269
B	5.591279	6.955106	1.355407	-0.021418	-0.014319	0.006263
B	-3.138137	6.846495	5.011383	0.021385	0.014289	-0.006265
Si	0.631772	3.486686	4.508512	-0.019093	0.018255	-0.006298
Si	1.821370	10.314915	1.858278	0.019138	-0.018248	0.006298
Si	-0.333059	10.387486	5.041673	-0.019117	-0.018243	-0.006312
Si	2.786201	3.414115	1.325117	0.019111	0.018257	0.006285
O	0.061445	3.072947	3.041906	0.008492	-0.017002	0.008559
O	2.391697	10.728653	3.324884	-0.008484	0.017025	-0.008548
O	4.546126	9.973747	0.141489	0.008536	0.017027	0.008553
O	-2.092984	3.827853	6.225301	-0.008443	-0.016989	-0.008554
O	2.197450	3.933608	4.519003	0.021116	-0.045752	0.020255
O	0.255692	9.867992	1.847787	-0.021129	0.045787	-0.020316
O	-1.898737	10.834409	5.031182	0.021104	0.045770	0.020252
O	4.351879	2.967192	1.335608	-0.021143	-0.045773	-0.020315
O	-0.212316	4.798696	5.055280	-0.022939	-0.000367	0.011588
O	2.665458	9.002905	1.311510	0.022913	0.000288	-0.011590
O	0.511030	11.699496	4.494905	-0.022919	0.000337	0.011593
O	1.942113	2.102105	1.871885	0.022943	-0.000331	-0.011573
O	0.525580	2.169271	5.472081	-0.010859	0.009436	-0.023371
O	1.927562	11.632329	0.894709	0.010858	-0.009368	0.023425
O	-0.226867	9.070071	4.078104	-0.010873	-0.009420	-0.023399
O	2.680009	4.731529	2.288686	0.010858	0.009381	0.023402
O	0.058846	0.698526	2.444964	0.004597	-0.026904	0.025278
O	2.394296	13.103075	3.921826	-0.004581	0.026910	-0.025288
O	4.548725	7.599326	0.738431	0.004589	0.026929	0.025294
O	-2.095583	6.202275	5.628359	-0.004588	-0.026901	-0.025276
O	-2.459230	13.184059	5.445139	0.023048	-0.004862	0.000990
O	4.912372	0.617542	0.921651	-0.023060	0.004820	-0.000989
O	2.757943	6.283259	4.105046	0.023042	0.004842	0.000984
O	-0.304801	7.518342	2.261744	-0.023068	-0.004852	-0.001005
O	-0.175430	2.374756	0.744070	-0.007740	0.019289	0.032495
O	2.628573	11.426844	5.622720	0.007727	-0.019307	-0.032480
O	4.783002	9.275557	2.439325	-0.007757	-0.019290	0.032541
O	-2.329859	4.526044	3.927465	0.007710	0.019301	-0.032453

O	-1.223866	12.517207	2.155216	0.009943	0.010926	-0.003241
O	3.677009	1.284394	4.211574	-0.009965	-0.010908	0.003230
O	5.831438	5.616407	1.028179	0.009974	-0.010936	-0.003240
O	-3.378295	8.185194	5.338611	-0.009942	0.010901	0.003223
H	-0.637445	12.195109	2.878812	0.024673	0.036943	-0.002715
H	3.090587	1.606491	3.487978	-0.024720	-0.036974	0.002698
H	5.245016	5.294309	0.304583	0.024710	-0.037004	-0.002695
H	-2.791874	8.507292	6.062207	-0.024700	0.036941	0.002706

90 f = 16.861711 THz 105.945257 2PiTHz 562.446133 cm-1 69.734458 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.043188	0.028373	0.074255
Li	-1.316675	4.156264	2.365404	-0.043270	0.028383	0.074278
Li	-3.471104	2.744536	5.548798	0.043228	0.028357	-0.074286
Li	5.924247	11.057064	0.817991	0.043209	0.028377	-0.074196
Na	2.049025	6.784862	1.629696	-0.000317	0.003022	-0.000267
Na	0.404117	7.016739	4.737094	-0.000316	0.003017	-0.000276
Na	2.558546	13.685662	1.553699	0.000314	0.003021	0.000275
Na	-0.105403	0.115939	4.813091	0.000317	0.003020	0.000268
B	4.155007	8.978944	1.168663	-0.011545	-0.011385	-0.015363
B	-1.701865	4.822656	5.198127	-0.011553	-0.011354	-0.015358
B	0.452564	2.078144	2.014732	0.011553	-0.011364	0.015359
B	2.000578	11.723457	4.352058	0.011547	-0.011367	0.015332
B	-2.733891	11.746082	5.839177	-0.018060	-0.009211	-0.012002
B	5.187034	2.055518	0.527613	-0.018102	-0.009215	-0.011998
B	3.032605	4.845282	3.711007	0.018103	-0.009216	0.011990
B	-0.579463	8.956318	2.655782	0.018068	-0.009219	0.012010
B	-0.983708	0.054306	1.827988	-0.008779	0.016134	0.009292
B	3.436850	13.747295	4.538802	-0.008792	0.016110	0.009308
B	5.591279	6.955106	1.355407	0.008799	0.016122	-0.009286
B	-3.138137	6.846495	5.011383	0.008776	0.016130	-0.009303
Si	0.631772	3.486686	4.508512	-0.020296	0.015607	-0.011488
Si	1.821370	10.314915	1.858278	-0.020277	0.015597	-0.011487
Si	-0.333059	10.387486	5.041673	0.020256	0.015597	0.011494
Si	2.786201	3.414115	1.325117	0.020301	0.015607	0.011493

O	0.061445	3.072947	3.041906	-0.003229	-0.006570	0.000700
O	2.391697	10.728653	3.324884	-0.003222	-0.006574	0.000698
O	4.546126	9.973747	0.141489	0.003214	-0.006568	-0.000701
O	-2.092984	3.827853	6.225301	0.003235	-0.006556	-0.000695
O	2.197450	3.933608	4.519003	0.000242	-0.007976	0.000395
O	0.255692	9.867992	1.847787	0.000244	-0.007974	0.000393
O	-1.898737	10.834409	5.031182	-0.000258	-0.007983	-0.000403
O	4.351879	2.967192	1.335608	-0.000236	-0.007977	-0.000381
O	-0.212316	4.798696	5.055280	-0.031751	-0.013708	0.004519
O	2.665458	9.002905	1.311510	-0.031707	-0.013686	0.004542
O	0.511030	11.699496	4.494905	0.031704	-0.013694	-0.004538
O	1.942113	2.102105	1.871885	0.031765	-0.013724	-0.004513
O	0.525580	2.169271	5.472081	-0.006203	-0.006471	-0.026621
O	1.927562	11.632329	0.894709	-0.006193	-0.006420	-0.026582
O	-0.226867	9.070071	4.078104	0.006208	-0.006432	0.026598
O	2.680009	4.731529	2.288686	0.006196	-0.006444	0.026602
O	0.058846	0.698526	2.444964	0.016468	-0.020363	0.025724
O	2.394296	13.103075	3.921826	0.016448	-0.020348	0.025702
O	4.548725	7.599326	0.738431	-0.016451	-0.020373	-0.025713
O	-2.095583	6.202275	5.628359	-0.016477	-0.020365	-0.025724
O	-2.459230	13.184059	5.445139	-0.027372	-0.025164	-0.013082
O	4.912372	0.617542	0.921651	-0.027398	-0.025169	-0.013104
O	2.757943	6.283259	4.105046	0.027404	-0.025194	0.013100
O	-0.304801	7.518342	2.261744	0.027388	-0.025149	0.013106
O	-0.175430	2.374756	0.744070	-0.036834	0.020448	0.049236
O	2.628573	11.426844	5.622720	-0.036763	0.020417	0.049159
O	4.783002	9.275557	2.439325	0.036795	0.020422	-0.049203
O	-2.329859	4.526044	3.927465	0.036827	0.020433	-0.049240
O	-1.223866	12.517207	2.155216	0.005420	0.018250	0.000206
O	3.677009	1.284394	4.211574	0.005423	0.018217	0.000218
O	5.831438	5.616407	1.028179	-0.005431	0.018243	-0.000229
O	-3.378295	8.185194	5.338611	-0.005414	0.018243	-0.000204
H	-0.637445	12.195109	2.878812	0.022893	0.007320	-0.022086
H	3.090587	1.606491	3.487978	0.022890	0.007287	-0.022075
H	5.245016	5.294309	0.304583	-0.022937	0.007335	0.022084
H	-2.791874	8.507292	6.062207	-0.022891	0.007297	0.022100

91 f = 16.511276 THz 103.743406 2PiTHz 550.756863 cm-1 68.285173
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.013514	-0.041815	0.060409
Li	-1.316675	4.156264	2.365404	0.013557	0.041734	-0.060378
Li	-3.471104	2.744536	5.548798	-0.013494	0.041748	0.060244
Li	5.924247	11.057064	0.817991	0.013549	-0.041842	-0.060459
Na	2.049025	6.784862	1.629696	-0.000061	-0.003280	0.000109
Na	0.404117	7.016739	4.737094	0.000061	0.003300	-0.000112
Na	2.558546	13.685662	1.553699	-0.000060	0.003290	0.000110
Na	-0.105403	0.115939	4.813091	0.000059	-0.003289	-0.000112
B	4.155007	8.978944	1.168663	0.014236	0.002601	-0.023746
B	-1.701865	4.822656	5.198127	-0.014206	-0.002608	0.023748
B	0.452564	2.078144	2.014732	0.014207	-0.002595	-0.023700
B	2.000578	11.723457	4.352058	-0.014235	0.002626	0.023753
B	-2.733891	11.746082	5.839177	-0.018925	0.001283	0.013427
B	5.187034	2.055518	0.527613	0.018847	-0.001296	-0.013368
B	3.032605	4.845282	3.711007	-0.018885	-0.001289	0.013375
B	-0.579463	8.956318	2.655782	0.018913	0.001277	-0.013419
B	-0.983708	0.054306	1.827988	-0.010832	-0.005285	0.016456
B	3.436850	13.747295	4.538802	0.010876	0.005311	-0.016489
B	5.591279	6.955106	1.355407	-0.010872	0.005297	0.016495
B	-3.138137	6.846495	5.011383	0.010838	-0.005319	-0.016468
Si	0.631772	3.486686	4.508512	0.017238	0.008508	0.007401
Si	1.821370	10.314915	1.858278	-0.017226	-0.008519	-0.007417
Si	-0.333059	10.387486	5.041673	0.017229	-0.008519	0.007415
Si	2.786201	3.414115	1.325117	-0.017204	0.008507	-0.007431
O	0.061445	3.072947	3.041906	0.011892	-0.035146	0.017537
O	2.391697	10.728653	3.324884	-0.011964	0.035246	-0.017559
O	4.546126	9.973747	0.141489	0.011939	0.035230	0.017562
O	-2.092984	3.827853	6.225301	-0.011903	-0.035184	-0.017540
O	2.197450	3.933608	4.519003	0.029042	-0.034093	0.020046
O	0.255692	9.867992	1.847787	-0.029061	0.034140	-0.020084
O	-1.898737	10.834409	5.031182	0.029068	0.034152	0.020085
O	4.351879	2.967192	1.335608	-0.029026	-0.034070	-0.020045

O	-0.212316	4.798696	5.055280	-0.003806	0.004701	0.001744
O	2.665458	9.002905	1.311510	0.003791	-0.004753	-0.001762
O	0.511030	11.699496	4.494905	-0.003778	-0.004767	0.001746
O	1.942113	2.102105	1.871885	0.003800	0.004739	-0.001763
O	0.525580	2.169271	5.472081	-0.000796	0.023270	0.011536
O	1.927562	11.632329	0.894709	0.000819	-0.023273	-0.011527
O	-0.226867	9.070071	4.078104	-0.000818	-0.023278	0.011532
O	2.680009	4.731529	2.288686	0.000793	0.023235	-0.011527
O	0.058846	0.698526	2.444964	-0.019348	0.025786	-0.013372
O	2.394296	13.103075	3.921826	0.019424	-0.025827	0.013397
O	4.548725	7.599326	0.738431	-0.019410	-0.025822	-0.013395
O	-2.095583	6.202275	5.628359	0.019392	0.025836	0.013406
O	-2.459230	13.184059	5.445139	-0.009700	-0.017075	-0.017522
O	4.912372	0.617542	0.921651	0.009656	0.016984	0.017466
O	2.757943	6.283259	4.105046	-0.009699	0.017034	-0.017500
O	-0.304801	7.518342	2.261744	0.009696	-0.017049	0.017517
O	-0.175430	2.374756	0.744070	0.041939	-0.003664	-0.050460
O	2.628573	11.426844	5.622720	-0.042048	0.003639	0.050580
O	4.783002	9.275557	2.439325	0.042033	0.003635	-0.050561
O	-2.329859	4.526044	3.927465	-0.042009	-0.003658	0.050561
O	-1.223866	12.517207	2.155216	0.002283	-0.011288	0.005096
O	3.677009	1.284394	4.211574	-0.002302	0.011363	-0.005075
O	5.831438	5.616407	1.028179	0.002293	0.011355	0.005081
O	-3.378295	8.185194	5.338611	-0.002283	-0.011326	-0.005093
H	-0.637445	12.195109	2.878812	0.002593	-0.024011	-0.002352
H	3.090587	1.606491	3.487978	-0.002529	0.024054	0.002276
H	5.245016	5.294309	0.304583	0.002545	0.024041	-0.002297
H	-2.791874	8.507292	6.062207	-0.002557	-0.024072	0.002327

92 f = 16.409434 THz 103.103518 2PiTHz 547.359800 cm-1 67.863990
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001294	-0.067854	0.021623
Li	-1.316675	4.156264	2.365404	0.001278	-0.067944	0.021672
Li	-3.471104	2.744536	5.548798	-0.001306	-0.067955	-0.021669
Li	5.924247	11.057064	0.817991	-0.001302	-0.067862	-0.021524

Na	2.049025	6.784862	1.629696	-0.000676	0.005344	-0.000285
Na	0.404117	7.016739	4.737094	-0.000682	0.005330	-0.000260
Na	2.558546	13.685662	1.553699	0.000682	0.005339	0.000261
Na	-0.105403	0.115939	4.813091	0.000675	0.005337	0.000285
B	4.155007	8.978944	1.168663	0.028001	0.008259	-0.013453
B	-1.701865	4.822656	5.198127	0.028025	0.008283	-0.013462
B	0.452564	2.078144	2.014732	-0.028022	0.008280	0.013458
B	2.000578	11.723457	4.352058	-0.028006	0.008267	0.013417
B	-2.733891	11.746082	5.839177	-0.014661	-0.004308	0.027612
B	5.187034	2.055518	0.527613	-0.014703	-0.004323	0.027633
B	3.032605	4.845282	3.711007	0.014707	-0.004329	-0.027640
B	-0.579463	8.956318	2.655782	0.014686	-0.004328	-0.027604
B	-0.983708	0.054306	1.827988	0.023781	-0.005665	-0.024601
B	3.436850	13.747295	4.538802	0.023759	-0.005685	-0.024578
B	5.591279	6.955106	1.355407	-0.023762	-0.005662	0.024589
B	-3.138137	6.846495	5.011383	-0.023782	-0.005666	0.024598
Si	0.631772	3.486686	4.508512	-0.001716	-0.023897	-0.002230
Si	1.821370	10.314915	1.858278	-0.001701	-0.023880	-0.002210
Si	-0.333059	10.387486	5.041673	0.001668	-0.023877	0.002235
Si	2.786201	3.414115	1.325117	0.001715	-0.023898	0.002232
O	0.061445	3.072947	3.041906	-0.015486	0.039693	-0.017827
O	2.391697	10.728653	3.324884	-0.015464	0.039629	-0.017797
O	4.546126	9.973747	0.141489	0.015459	0.039636	0.017795
O	-2.092984	3.827853	6.225301	0.015486	0.039704	0.017831
O	2.197450	3.933608	4.519003	-0.032401	0.052783	-0.024565
O	0.255692	9.867992	1.847787	-0.032362	0.052727	-0.024558
O	-1.898737	10.834409	5.031182	0.032353	0.052722	0.024557
O	4.351879	2.967192	1.335608	0.032404	0.052783	0.024574
O	-0.212316	4.798696	5.055280	0.020378	-0.002170	-0.005649
O	2.665458	9.002905	1.311510	0.020373	-0.002159	-0.005638
O	0.511030	11.699496	4.494905	-0.020380	-0.002180	0.005640
O	1.942113	2.102105	1.871885	-0.020365	-0.002187	0.005651
O	0.525580	2.169271	5.472081	0.009939	-0.016579	0.010019
O	1.927562	11.632329	0.894709	0.009938	-0.016552	0.010029
O	-0.226867	9.070071	4.078104	-0.009928	-0.016537	-0.010019
O	2.680009	4.731529	2.288686	-0.009944	-0.016561	-0.010033

O	0.058846	0.698526	2.444964	0.014405	-0.000197	-0.004640
O	2.394296	13.103075	3.921826	0.014364	-0.000159	-0.004666
O	4.548725	7.599326	0.738431	-0.014387	-0.000181	0.004641
O	-2.095583	6.202275	5.628359	-0.014416	-0.000205	0.004636
O	-2.459230	13.184059	5.445139	0.002541	-0.011032	-0.018103
O	4.912372	0.617542	0.921651	0.002511	-0.011067	-0.018134
O	2.757943	6.283259	4.105046	-0.002499	-0.011088	0.018138
O	-0.304801	7.518342	2.261744	-0.002510	-0.011043	0.018124
O	-0.175430	2.374756	0.744070	-0.027539	-0.016308	0.023538
O	2.628573	11.426844	5.622720	-0.027448	-0.016324	0.023429
O	4.783002	9.275557	2.439325	0.027507	-0.016324	-0.023505
O	-2.329859	4.526044	3.927465	0.027542	-0.016316	-0.023545
O	-1.223866	12.517207	2.155216	-0.003388	0.018615	0.006654
O	3.677009	1.284394	4.211574	-0.003384	0.018585	0.006666
O	5.831438	5.616407	1.028179	0.003379	0.018625	-0.006667
O	-3.378295	8.185194	5.338611	0.003391	0.018616	-0.006658
H	-0.637445	12.195109	2.878812	0.000741	0.007670	-0.001772
H	3.090587	1.606491	3.487978	0.000761	0.007627	-0.001782
H	5.245016	5.294309	0.304583	-0.000787	0.007667	0.001798
H	-2.791874	8.507292	6.062207	-0.000767	0.007662	0.001797

93 f = 16.217869 THz 101.899874 2PiTHz 540.969852 cm-1 67.071737 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.034550	0.030253	0.068984
Li	-1.316675	4.156264	2.365404	-0.034584	0.030406	0.069042
Li	-3.471104	2.744536	5.548798	-0.034580	-0.030266	0.069129
Li	5.924247	11.057064	0.817991	-0.034596	-0.030317	0.068986
Na	2.049025	6.784862	1.629696	-0.000098	-0.005685	0.002513
Na	0.404117	7.016739	4.737094	-0.000100	-0.005671	0.002491
Na	2.558546	13.685662	1.553699	-0.000101	0.005675	0.002492
Na	-0.105403	0.115939	4.813091	-0.000097	0.005672	0.002511
B	4.155007	8.978944	1.168663	0.002319	-0.002268	-0.023288
B	-1.701865	4.822656	5.198127	0.002289	-0.002286	-0.023287
B	0.452564	2.078144	2.014732	0.002347	0.002264	-0.023313
B	2.000578	11.723457	4.352058	0.002290	0.002280	-0.023286

B	-2.733891	11.746082	5.839177	0.015538	0.005131	-0.008162
B	5.187034	2.055518	0.527613	0.015571	0.005145	-0.008208
B	3.032605	4.845282	3.711007	0.015556	-0.005137	-0.008149
B	-0.579463	8.956318	2.655782	0.015521	-0.005124	-0.008185
B	-0.983708	0.054306	1.827988	-0.002961	-0.008435	0.009095
B	3.436850	13.747295	4.538802	-0.002925	-0.008431	0.009068
B	5.591279	6.955106	1.355407	-0.002932	0.008423	0.009086
B	-3.138137	6.846495	5.011383	-0.002923	0.008442	0.009058
Si	0.631772	3.486686	4.508512	-0.016247	0.000954	0.018431
Si	1.821370	10.314915	1.858278	-0.016218	0.000936	0.018399
Si	-0.333059	10.387486	5.041673	-0.016221	-0.000952	0.018396
Si	2.786201	3.414115	1.325117	-0.016268	-0.000915	0.018418
O	0.061445	3.072947	3.041906	-0.002279	-0.018475	0.005279
O	2.391697	10.728653	3.324884	-0.002281	-0.018404	0.005259
O	4.546126	9.973747	0.141489	-0.002274	0.018451	0.005271
O	-2.092984	3.827853	6.225301	-0.002312	0.018388	0.005241
O	2.197450	3.933608	4.519003	-0.007985	0.019654	0.008060
O	0.255692	9.867992	1.847787	-0.007995	0.019674	0.008031
O	-1.898737	10.834409	5.031182	-0.007975	-0.019645	0.008042
O	4.351879	2.967192	1.335608	-0.008052	-0.019758	0.008017
O	-0.212316	4.798696	5.055280	0.011170	0.033350	0.004145
O	2.665458	9.002905	1.311510	0.011204	0.033309	0.004157
O	0.511030	11.699496	4.494905	0.011163	-0.033288	0.004158
O	1.942113	2.102105	1.871885	0.011208	-0.033356	0.004135
O	0.525580	2.169271	5.472081	-0.004168	-0.034642	-0.015994
O	1.927562	11.632329	0.894709	-0.004130	-0.034596	-0.015948
O	-0.226867	9.070071	4.078104	-0.004137	0.034591	-0.015966
O	2.680009	4.731529	2.288686	-0.004143	0.034667	-0.015974
O	0.058846	0.698526	2.444964	-0.019157	0.019994	-0.016776
O	2.394296	13.103075	3.921826	-0.019118	0.019957	-0.016748
O	4.548725	7.599326	0.738431	-0.019114	-0.019965	-0.016726
O	-2.095583	6.202275	5.628359	-0.019128	-0.019981	-0.016784
O	-2.459230	13.184059	5.445139	0.022413	0.023051	0.020793
O	4.912372	0.617542	0.921651	0.022419	0.023084	0.020827
O	2.757943	6.283259	4.105046	0.022425	-0.023058	0.020796
O	-0.304801	7.518342	2.261744	0.022393	-0.023033	0.020795

O	-0.175430	2.374756	0.744070	0.036606	0.007412	-0.053047
O	2.628573	11.426844	5.622720	0.036508	0.007398	-0.052940
O	4.783002	9.275557	2.439325	0.036509	-0.007407	-0.052937
O	-2.329859	4.526044	3.927465	0.036536	-0.007404	-0.052979
O	-1.223866	12.517207	2.155216	-0.001623	-0.019515	-0.004232
O	3.677009	1.284394	4.211574	-0.001630	-0.019498	-0.004243
O	5.831438	5.616407	1.028179	-0.001622	0.019481	-0.004241
O	-3.378295	8.185194	5.338611	-0.001635	0.019498	-0.004230
H	-0.637445	12.195109	2.878812	-0.021170	-0.020879	0.011903
H	3.090587	1.606491	3.487978	-0.021219	-0.020852	0.011930
H	5.245016	5.294309	0.304583	-0.021198	0.020863	0.011908
H	-2.791874	8.507292	6.062207	-0.021197	0.020863	0.011915

94 f = 16.157237 THz 101.518914 2PiTHz 538.947399 cm-1 66.820985
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.022604	-0.030115	-0.066097
Li	-1.316675	4.156264	2.365404	-0.022557	0.030049	0.066037
Li	-3.471104	2.744536	5.548798	-0.022557	-0.030052	0.066062
Li	5.924247	11.057064	0.817991	0.022631	0.030065	-0.066187
Na	2.049025	6.784862	1.629696	0.002057	-0.000275	0.001678
Na	0.404117	7.016739	4.737094	-0.002056	0.000278	-0.001675
Na	2.558546	13.685662	1.553699	-0.002056	-0.000273	-0.001675
Na	-0.105403	0.115939	4.813091	0.002057	0.000275	0.001679
B	4.155007	8.978944	1.168663	0.001110	0.003430	0.026038
B	-1.701865	4.822656	5.198127	-0.001099	-0.003422	-0.026006
B	0.452564	2.078144	2.014732	-0.001101	0.003419	-0.026016
B	2.000578	11.723457	4.352058	0.001094	-0.003427	0.026057
B	-2.733891	11.746082	5.839177	-0.016747	-0.005780	0.003077
B	5.187034	2.055518	0.527613	0.016713	0.005751	-0.003056
B	3.032605	4.845282	3.711007	0.016706	-0.005758	-0.003064
B	-0.579463	8.956318	2.655782	-0.016732	0.005775	0.003055
B	-0.983708	0.054306	1.827988	-0.003508	-0.011672	0.010531
B	3.436850	13.747295	4.538802	0.003531	0.011684	-0.010559
B	5.591279	6.955106	1.355407	0.003508	-0.011680	-0.010544
B	-3.138137	6.846495	5.011383	-0.003514	0.011668	0.010532

Si	0.631772	3.486686	4.508512	-0.021114	0.000857	0.020563
Si	1.821370	10.314915	1.858278	0.021140	-0.000867	-0.020600
Si	-0.333059	10.387486	5.041673	0.021162	0.000853	-0.020580
Si	2.786201	3.414115	1.325117	-0.021124	-0.000865	0.020564
O	0.061445	3.072947	3.041906	-0.007788	-0.013223	0.004248
O	2.391697	10.728653	3.324884	0.007786	0.013262	-0.004261
O	4.546126	9.973747	0.141489	0.007800	-0.013231	-0.004240
O	-2.092984	3.827853	6.225301	-0.007787	0.013219	0.004246
O	2.197450	3.933608	4.519003	-0.007320	0.012743	0.010160
O	0.255692	9.867992	1.847787	0.007311	-0.012731	-0.010191
O	-1.898737	10.834409	5.031182	0.007344	0.012774	-0.010169
O	4.351879	2.967192	1.335608	-0.007325	-0.012743	0.010156
O	-0.212316	4.798696	5.055280	0.008027	0.034930	0.001924
O	2.665458	9.002905	1.311510	-0.008016	-0.034962	-0.001928
O	0.511030	11.699496	4.494905	-0.008020	0.034959	-0.001924
O	1.942113	2.102105	1.871885	0.008019	-0.034928	0.001919
O	0.525580	2.169271	5.472081	0.004798	-0.029644	-0.009480
O	1.927562	11.632329	0.894709	-0.004807	0.029673	0.009493
O	-0.226867	9.070071	4.078104	-0.004810	-0.029695	0.009505
O	2.680009	4.731529	2.288686	0.004798	0.029651	-0.009493
O	0.058846	0.698526	2.444964	-0.018415	0.024652	-0.022447
O	2.394296	13.103075	3.921826	0.018455	-0.024680	0.022475
O	4.548725	7.599326	0.738431	0.018431	0.024662	0.022456
O	-2.095583	6.202275	5.628359	-0.018411	-0.024637	-0.022437
O	-2.459230	13.184059	5.445139	-0.022913	-0.018848	-0.017147
O	4.912372	0.617542	0.921651	0.022867	0.018806	0.017112
O	2.757943	6.283259	4.105046	0.022862	-0.018801	0.017113
O	-0.304801	7.518342	2.261744	-0.022906	0.018825	-0.017131
O	-0.175430	2.374756	0.744070	0.039727	0.003883	-0.056944
O	2.628573	11.426844	5.622720	-0.039805	-0.003888	0.057056
O	4.783002	9.275557	2.439325	-0.039756	0.003900	0.056997
O	-2.329859	4.526044	3.927465	0.039710	-0.003892	-0.056929
O	-1.223866	12.517207	2.155216	-0.002281	-0.017392	0.004761
O	3.677009	1.284394	4.211574	0.002280	0.017446	-0.004756
O	5.831438	5.616407	1.028179	0.002287	-0.017428	-0.004749
O	-3.378295	8.185194	5.338611	-0.002281	0.017399	0.004751

H	-0.637445	12.195109	2.878812	-0.001454	-0.025386	0.000414
H	3.090587	1.606491	3.487978	0.001488	0.025421	-0.000448
H	5.245016	5.294309	0.304583	0.001504	-0.025407	-0.000446
H	-2.791874	8.507292	6.062207	-0.001458	0.025374	0.000418

95 f = 15.748946 THz 98.953548 2PiTHz 525.328285 cm-1 65.132430 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.045886	-0.059280	0.029806
Li	-1.316675	4.156264	2.365404	0.045885	-0.059263	0.029833
Li	-3.471104	2.744536	5.548798	0.045873	0.059297	0.029830
Li	5.924247	11.057064	0.817991	0.045892	0.059267	0.029822
Na	2.049025	6.784862	1.629696	-0.001590	0.008663	-0.003016
Na	0.404117	7.016739	4.737094	-0.001589	0.008651	-0.003011
Na	2.558546	13.685662	1.553699	-0.001591	-0.008664	-0.003012
Na	-0.105403	0.115939	4.813091	-0.001589	-0.008654	-0.003015
B	4.155007	8.978944	1.168663	-0.020203	0.001958	-0.013969
B	-1.701865	4.822656	5.198127	-0.020218	0.001948	-0.013973
B	0.452564	2.078144	2.014732	-0.020200	-0.001951	-0.013975
B	2.000578	11.723457	4.352058	-0.020212	-0.001964	-0.013965
B	-2.733891	11.746082	5.839177	0.011299	0.027840	0.010612
B	5.187034	2.055518	0.527613	0.011316	0.027841	0.010611
B	3.032605	4.845282	3.711007	0.011317	-0.027839	0.010634
B	-0.579463	8.956318	2.655782	0.011290	-0.027830	0.010598
B	-0.983708	0.054306	1.827988	0.001338	-0.014003	-0.009410
B	3.436850	13.747295	4.538802	0.001345	-0.013987	-0.009425
B	5.591279	6.955106	1.355407	0.001349	0.013983	-0.009412
B	-3.138137	6.846495	5.011383	0.001348	0.014005	-0.009422
Si	0.631772	3.486686	4.508512	-0.023827	0.001475	0.006651
Si	1.821370	10.314915	1.858278	-0.023814	0.001452	0.006641
Si	-0.333059	10.387486	5.041673	-0.023812	-0.001459	0.006642
Si	2.786201	3.414115	1.325117	-0.023835	-0.001456	0.006649
O	0.061445	3.072947	3.041906	0.000523	0.025607	-0.015859
O	2.391697	10.728653	3.324884	0.000520	0.025602	-0.015860
O	4.546126	9.973747	0.141489	0.000518	-0.025590	-0.015855
O	-2.092984	3.827853	6.225301	0.000518	-0.025633	-0.015874

O	2.197450	3.933608	4.519003	0.002123	-0.027630	0.020831
O	0.255692	9.867992	1.847787	0.002108	-0.027585	0.020821
O	-1.898737	10.834409	5.031182	0.002115	0.027605	0.020828
O	4.351879	2.967192	1.335608	0.002103	0.027593	0.020819
O	-0.212316	4.798696	5.055280	-0.048175	-0.029608	-0.000558
O	2.665458	9.002905	1.311510	-0.048135	-0.029589	-0.000556
O	0.511030	11.699496	4.494905	-0.048148	0.029600	-0.000554
O	1.942113	2.102105	1.871885	-0.048157	0.029600	-0.000563
O	0.525580	2.169271	5.472081	0.037204	0.019269	0.017660
O	1.927562	11.632329	0.894709	0.037206	0.019264	0.017655
O	-0.226867	9.070071	4.078104	0.037195	-0.019253	0.017642
O	2.680009	4.731529	2.288686	0.037222	-0.019271	0.017677
O	0.058846	0.698526	2.444964	-0.001013	-0.008669	-0.011646
O	2.394296	13.103075	3.921826	-0.001001	-0.008686	-0.011637
O	4.548725	7.599326	0.738431	-0.000995	0.008673	-0.011631
O	-2.095583	6.202275	5.628359	-0.001006	0.008675	-0.011652
O	-2.459230	13.184059	5.445139	0.018733	0.012893	-0.003870
O	4.912372	0.617542	0.921651	0.018736	0.012898	-0.003849
O	2.757943	6.283259	4.105046	0.018744	-0.012895	-0.003859
O	-0.304801	7.518342	2.261744	0.018725	-0.012888	-0.003858
O	-0.175430	2.374756	0.744070	0.019404	-0.023987	-0.026532
O	2.628573	11.426844	5.622720	0.019367	-0.023995	-0.026496
O	4.783002	9.275557	2.439325	0.019362	0.023987	-0.026496
O	-2.329859	4.526044	3.927465	0.019389	0.023995	-0.026523
O	-1.223866	12.517207	2.155216	0.002258	-0.016809	0.005311
O	3.677009	1.284394	4.211574	0.002270	-0.016785	0.005315
O	5.831438	5.616407	1.028179	0.002265	0.016779	0.005302
O	-3.378295	8.185194	5.338611	0.002259	0.016804	0.005320
H	-0.637445	12.195109	2.878812	-0.032071	0.005245	0.045974
H	3.090587	1.606491	3.487978	-0.032079	0.005284	0.046001
H	5.245016	5.294309	0.304583	-0.032105	-0.005269	0.045996
H	-2.791874	8.507292	6.062207	-0.032061	-0.005248	0.045975

96 f = 15.705556 THz 98.680916 2PiTHz 523.880930 cm-1 64.952980 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.077056	-0.049019	0.051850
Li	-1.316675	4.156264	2.365404	-0.077028	0.049007	-0.051865
Li	-3.471104	2.744536	5.548798	-0.077034	-0.048993	-0.051836
Li	5.924247	11.057064	0.817991	0.077065	0.049044	0.051891
Na	2.049025	6.784862	1.629696	0.001517	-0.000213	0.001079
Na	0.404117	7.016739	4.737094	-0.001517	0.000208	-0.001060
Na	2.558546	13.685662	1.553699	-0.001518	-0.000213	-0.001061
Na	-0.105403	0.115939	4.813091	0.001517	0.000211	0.001079
B	4.155007	8.978944	1.168663	-0.016288	0.015026	-0.010575
B	-1.701865	4.822656	5.198127	0.016260	-0.015016	0.010573
B	0.452564	2.078144	2.014732	0.016269	0.015019	0.010565
B	2.000578	11.723457	4.352058	-0.016278	-0.015028	-0.010571
B	-2.733891	11.746082	5.839177	0.001130	0.033156	0.008903
B	5.187034	2.055518	0.527613	-0.001115	-0.033154	-0.008903
B	3.032605	4.845282	3.711007	-0.001125	0.033153	-0.008902
B	-0.579463	8.956318	2.655782	0.001118	-0.033151	0.008899
B	-0.983708	0.054306	1.827988	0.000352	0.005894	0.010848
B	3.436850	13.747295	4.538802	-0.000351	-0.005899	-0.010855
B	5.591279	6.955106	1.355407	-0.000342	0.005898	-0.010849
B	-3.138137	6.846495	5.011383	0.000353	-0.005896	0.010844
Si	0.631772	3.486686	4.508512	0.025609	0.001040	0.006598
Si	1.821370	10.314915	1.858278	-0.025604	-0.001039	-0.006592
Si	-0.333059	10.387486	5.041673	-0.025611	0.001041	-0.006595
Si	2.786201	3.414115	1.325117	0.025601	-0.001042	0.006593
O	0.061445	3.072947	3.041906	-0.007007	-0.017911	0.021690
O	2.391697	10.728653	3.324884	0.007007	0.017912	-0.021692
O	4.546126	9.973747	0.141489	0.007000	-0.017918	-0.021698
O	-2.092984	3.827853	6.225301	-0.007018	0.017903	0.021688
O	2.197450	3.933608	4.519003	0.008207	0.018998	-0.020125
O	0.255692	9.867992	1.847787	-0.008195	-0.019011	0.020144
O	-1.898737	10.834409	5.031182	-0.008203	0.019003	0.020140
O	4.351879	2.967192	1.335608	0.008198	-0.019009	-0.020131
O	-0.212316	4.798696	5.055280	0.040496	0.030855	-0.010587
O	2.665458	9.002905	1.311510	-0.040518	-0.030856	0.010577
O	0.511030	11.699496	4.494905	-0.040513	0.030860	0.010583
O	1.942113	2.102105	1.871885	0.040493	-0.030847	-0.010583

O	0.525580	2.169271	5.472081	-0.036683	-0.020844	-0.008888
O	1.927562	11.632329	0.894709	0.036701	0.020852	0.008899
O	-0.226867	9.070071	4.078104	0.036696	-0.020839	0.008885
O	2.680009	4.731529	2.288686	-0.036687	0.020846	-0.008896
O	0.058846	0.698526	2.444964	-0.002072	0.009997	0.000951
O	2.394296	13.103075	3.921826	0.002071	-0.010004	-0.000959
O	4.548725	7.599326	0.738431	0.002082	0.010006	-0.000945
O	-2.095583	6.202275	5.628359	-0.002068	-0.009992	0.000955
O	-2.459230	13.184059	5.445139	0.013869	0.015745	-0.009473
O	4.912372	0.617542	0.921651	-0.013864	-0.015734	0.009476
O	2.757943	6.283259	4.105046	-0.013866	0.015741	0.009465
O	-0.304801	7.518342	2.261744	0.013873	-0.015743	-0.009469
O	-0.175430	2.374756	0.744070	-0.010024	0.020777	0.011313
O	2.628573	11.426844	5.622720	0.010040	-0.020793	-0.011335
O	4.783002	9.275557	2.439325	0.010020	0.020787	-0.011326
O	-2.329859	4.526044	3.927465	-0.010041	-0.020784	0.011335
O	-1.223866	12.517207	2.155216	-0.003473	-0.000687	-0.018436
O	3.677009	1.284394	4.211574	0.003476	0.000685	0.018431
O	5.831438	5.616407	1.028179	0.003467	-0.000688	0.018422
O	-3.378295	8.185194	5.338611	-0.003472	0.000678	-0.018429
H	-0.637445	12.195109	2.878812	-0.067283	0.003247	0.036145
H	3.090587	1.606491	3.487978	0.067259	-0.003235	-0.036118
H	5.245016	5.294309	0.304583	0.067251	0.003250	-0.036136
H	-2.791874	8.507292	6.062207	-0.067269	-0.003252	0.036138

97 f = 15.443210 THz 97.032552 2PiTHz 515.130029 cm-1 63.868007 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.049519	0.031170	0.063530
Li	-1.316675	4.156264	2.365404	-0.049530	-0.031151	-0.063496
Li	-3.471104	2.744536	5.548798	-0.049521	0.031151	-0.063502
Li	5.924247	11.057064	0.817991	0.049504	-0.031193	0.063494
Na	2.049025	6.784862	1.629696	-0.001942	0.001483	0.000093
Na	0.404117	7.016739	4.737094	0.001949	-0.001484	-0.000069
Na	2.558546	13.685662	1.553699	0.001949	0.001489	-0.000067
Na	-0.105403	0.115939	4.813091	-0.001942	-0.001481	0.000094

B	4.155007	8.978944	1.168663	0.018100	0.032583	0.000408
B	-1.701865	4.822656	5.198127	-0.018080	-0.032585	-0.000403
B	0.452564	2.078144	2.014732	-0.018086	0.032579	-0.000400
B	2.000578	11.723457	4.352058	0.018094	-0.032581	0.000400
B	-2.733891	11.746082	5.839177	-0.017221	0.010763	-0.011798
B	5.187034	2.055518	0.527613	0.017207	-0.010769	0.011792
B	3.032605	4.845282	3.711007	0.017212	0.010771	0.011790
B	-0.579463	8.956318	2.655782	-0.017214	-0.010766	-0.011793
B	-0.983708	0.054306	1.827988	0.018075	-0.012615	-0.011658
B	3.436850	13.747295	4.538802	-0.018079	0.012614	0.011662
B	5.591279	6.955106	1.355407	-0.018086	-0.012619	0.011656
B	-3.138137	6.846495	5.011383	0.018075	0.012618	-0.011654
Si	0.631772	3.486686	4.508512	0.005125	0.006888	0.032413
Si	1.821370	10.314915	1.858278	-0.005123	-0.006893	-0.032419
Si	-0.333059	10.387486	5.041673	-0.005114	0.006895	-0.032413
Si	2.786201	3.414115	1.325117	0.005126	-0.006892	0.032414
O	0.061445	3.072947	3.041906	-0.017590	0.027961	0.016253
O	2.391697	10.728653	3.324884	0.017594	-0.027965	-0.016258
O	4.546126	9.973747	0.141489	0.017600	0.027964	-0.016255
O	-2.092984	3.827853	6.225301	-0.017588	-0.027960	0.016254
O	2.197450	3.933608	4.519003	0.024188	-0.031170	-0.000275
O	0.255692	9.867992	1.847787	-0.024198	0.031193	0.000262
O	-1.898737	10.834409	5.031182	-0.024193	-0.031192	0.000266
O	4.351879	2.967192	1.335608	0.024190	0.031177	-0.000272
O	-0.212316	4.798696	5.055280	-0.032490	-0.009420	-0.037156
O	2.665458	9.002905	1.311510	0.032516	0.009433	0.037169
O	0.511030	11.699496	4.494905	0.032516	-0.009430	0.037173
O	1.942113	2.102105	1.871885	-0.032492	0.009416	-0.037163
O	0.525580	2.169271	5.472081	0.013252	0.010583	0.028598
O	1.927562	11.632329	0.894709	-0.013266	-0.010596	-0.028613
O	-0.226867	9.070071	4.078104	-0.013269	0.010591	-0.028600
O	2.680009	4.731529	2.288686	0.013254	-0.010583	0.028599
O	0.058846	0.698526	2.444964	0.004194	0.008309	-0.016366
O	2.394296	13.103075	3.921826	-0.004198	-0.008308	0.016366
O	4.548725	7.599326	0.738431	-0.004200	0.008311	0.016361
O	-2.095583	6.202275	5.628359	0.004193	-0.008311	-0.016367

O	-2.459230	13.184059	5.445139	-0.009019	0.006742	0.000208
O	4.912372	0.617542	0.921651	0.009015	-0.006738	-0.000200
O	2.757943	6.283259	4.105046	0.009015	0.006741	-0.000193
O	-0.304801	7.518342	2.261744	-0.009024	-0.006742	0.000200
O	-0.175430	2.374756	0.744070	0.011968	-0.024498	-0.023758
O	2.628573	11.426844	5.622720	-0.011977	0.024516	0.023769
O	4.783002	9.275557	2.439325	-0.011963	-0.024507	0.023767
O	-2.329859	4.526044	3.927465	0.011973	0.024493	-0.023768
O	-1.223866	12.517207	2.155216	-0.012268	-0.009858	-0.004365
O	3.677009	1.284394	4.211574	0.012269	0.009855	0.004363
O	5.831438	5.616407	1.028179	0.012268	-0.009862	0.004365
O	-3.378295	8.185194	5.338611	-0.012274	0.009866	-0.004374
H	-0.637445	12.195109	2.878812	-0.023929	-0.009256	0.003604
H	3.090587	1.606491	3.487978	0.023938	0.009251	-0.003614
H	5.245016	5.294309	0.304583	0.023949	-0.009265	-0.003619
H	-2.791874	8.507292	6.062207	-0.023943	0.009264	0.003602

98 f = 15.315343 THz 96.229141 2PiTHz 510.864851 cm-1 63.339192

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.081494	0.007160	0.073881
Li	-1.316675	4.156264	2.365404	0.081510	0.007153	0.073877
Li	-3.471104	2.744536	5.548798	0.081504	-0.007166	0.073882
Li	5.924247	11.057064	0.817991	0.081505	-0.007151	0.073880
Na	2.049025	6.784862	1.629696	-0.000974	-0.002304	-0.002003
Na	0.404117	7.016739	4.737094	-0.000978	-0.002304	-0.001982
Na	2.558546	13.685662	1.553699	-0.000977	0.002308	-0.001982
Na	-0.105403	0.115939	4.813091	-0.000974	0.002302	-0.002003
B	4.155007	8.978944	1.168663	0.005543	0.033181	0.002212
B	-1.701865	4.822656	5.198127	0.005543	0.033192	0.002221
B	0.452564	2.078144	2.014732	0.005541	-0.033188	0.002215
B	2.000578	11.723457	4.352058	0.005543	-0.033181	0.002223
B	-2.733891	11.746082	5.839177	-0.012757	0.018218	-0.013188
B	5.187034	2.055518	0.527613	-0.012756	0.018220	-0.013181
B	3.032605	4.845282	3.711007	-0.012762	-0.018223	-0.013190
B	-0.579463	8.956318	2.655782	-0.012750	-0.018219	-0.013181

B	-0.983708	0.054306	1.827988	-0.014360	0.002587	0.003350
B	3.436850	13.747295	4.538802	-0.014362	0.002588	0.003343
B	5.591279	6.955106	1.355407	-0.014358	-0.002582	0.003346
B	-3.138137	6.846495	5.011383	-0.014364	-0.002592	0.003352
Si	0.631772	3.486686	4.508512	-0.008477	-0.003775	-0.033450
Si	1.821370	10.314915	1.858278	-0.008475	-0.003778	-0.033440
Si	-0.333059	10.387486	5.041673	-0.008470	0.003784	-0.033443
Si	2.786201	3.414115	1.325117	-0.008477	0.003767	-0.033449
O	0.061445	3.072947	3.041906	0.018602	-0.011960	-0.023675
O	2.391697	10.728653	3.324884	0.018583	-0.011953	-0.023671
O	4.546126	9.973747	0.141489	0.018592	0.011953	-0.023676
O	-2.092984	3.827853	6.225301	0.018600	0.011965	-0.023671
O	2.197450	3.933608	4.519003	-0.021745	0.024086	0.005794
O	0.255692	9.867992	1.847787	-0.021741	0.024082	0.005789
O	-1.898737	10.834409	5.031182	-0.021741	-0.024088	0.005794
O	4.351879	2.967192	1.335608	-0.021742	-0.024080	0.005793
O	-0.212316	4.798696	5.055280	0.008005	-0.009397	0.037340
O	2.665458	9.002905	1.311510	0.007999	-0.009403	0.037339
O	0.511030	11.699496	4.494905	0.008008	0.009396	0.037341
O	1.942113	2.102105	1.871885	0.008002	0.009405	0.037348
O	0.525580	2.169271	5.472081	-0.006414	-0.003667	-0.028022
O	1.927562	11.632329	0.894709	-0.006429	-0.003680	-0.028028
O	-0.226867	9.070071	4.078104	-0.006425	0.003675	-0.028019
O	2.680009	4.731529	2.288686	-0.006423	0.003671	-0.028033
O	0.058846	0.698526	2.444964	-0.003188	-0.021686	0.021702
O	2.394296	13.103075	3.921826	-0.003185	-0.021690	0.021694
O	4.548725	7.599326	0.738431	-0.003192	0.021683	0.021690
O	-2.095583	6.202275	5.628359	-0.003182	0.021696	0.021711
O	-2.459230	13.184059	5.445139	0.001050	0.016964	0.003562
O	4.912372	0.617542	0.921651	0.001060	0.016964	0.003567
O	2.757943	6.283259	4.105046	0.001054	-0.016967	0.003564
O	-0.304801	7.518342	2.261744	0.001063	-0.016966	0.003568
O	-0.175430	2.374756	0.744070	-0.009867	0.019567	0.020120
O	2.628573	11.426844	5.622720	-0.009865	0.019563	0.020118
O	4.783002	9.275557	2.439325	-0.009859	-0.019566	0.020109
O	-2.329859	4.526044	3.927465	-0.009869	-0.019567	0.020129

O	-1.223866	12.517207	2.155216	0.008365	-0.003173	-0.003169
O	3.677009	1.284394	4.211574	0.008363	-0.003171	-0.003163
O	5.831438	5.616407	1.028179	0.008357	0.003179	-0.003168
O	-3.378295	8.185194	5.338611	0.008371	0.003167	-0.003163
H	-0.637445	12.195109	2.878812	0.006859	0.025181	0.010622
H	3.090587	1.606491	3.487978	0.006866	0.025201	0.010632
H	5.245016	5.294309	0.304583	0.006844	-0.025183	0.010634
H	-2.791874	8.507292	6.062207	0.006876	-0.025199	0.010626

99 f = 14.756371 THz 92.717012 2PiTHz 492.219530 cm-1 61.027466 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.090298	-0.046476	0.076964
Li	-1.316675	4.156264	2.365404	-0.090270	0.046451	-0.076948
Li	-3.471104	2.744536	5.548798	0.090277	0.046459	0.076960
Li	5.924247	11.057064	0.817991	-0.090293	-0.046441	-0.076950
Na	2.049025	6.784862	1.629696	0.000214	-0.006730	0.001364
Na	0.404117	7.016739	4.737094	-0.000220	0.006722	-0.001392
Na	2.558546	13.685662	1.553699	0.000221	0.006736	0.001393
Na	-0.105403	0.115939	4.813091	-0.000212	-0.006719	-0.001364
B	4.155007	8.978944	1.168663	0.000952	0.005693	0.025179
B	-1.701865	4.822656	5.198127	-0.000960	-0.005680	-0.025187
B	0.452564	2.078144	2.014732	0.000962	-0.005690	0.025197
B	2.000578	11.723457	4.352058	-0.000964	0.005695	-0.025176
B	-2.733891	11.746082	5.839177	-0.006211	-0.002558	-0.016774
B	5.187034	2.055518	0.527613	0.006197	0.002547	0.016789
B	3.032605	4.845282	3.711007	-0.006200	0.002543	-0.016788
B	-0.579463	8.956318	2.655782	0.006211	-0.002558	0.016773
B	-0.983708	0.054306	1.827988	-0.006609	0.012583	-0.021832
B	3.436850	13.747295	4.538802	0.006601	-0.012591	0.021827
B	5.591279	6.955106	1.355407	-0.006600	-0.012583	-0.021837
B	-3.138137	6.846495	5.011383	0.006604	0.012589	0.021829
Si	0.631772	3.486686	4.508512	0.005373	-0.011729	0.011582
Si	1.821370	10.314915	1.858278	-0.005358	0.011736	-0.011570
Si	-0.333059	10.387486	5.041673	0.005355	0.011730	0.011583
Si	2.786201	3.414115	1.325117	-0.005372	-0.011732	-0.011589

O	0.061445	3.072947	3.041906	-0.008716	0.011487	0.004577
O	2.391697	10.728653	3.324884	0.008734	-0.011462	-0.004575
O	4.546126	9.973747	0.141489	-0.008721	-0.011478	0.004576
O	-2.092984	3.827853	6.225301	0.008736	0.011487	-0.004582
O	2.197450	3.933608	4.519003	-0.000984	0.014983	0.002704
O	0.255692	9.867992	1.847787	0.000993	-0.014991	-0.002702
O	-1.898737	10.834409	5.031182	-0.000990	-0.014980	0.002696
O	4.351879	2.967192	1.335608	0.000980	0.014986	-0.002718
O	-0.212316	4.798696	5.055280	-0.012667	-0.025374	0.013530
O	2.665458	9.002905	1.311510	0.012653	0.025369	-0.013544
O	0.511030	11.699496	4.494905	-0.012678	0.025390	0.013551
O	1.942113	2.102105	1.871885	0.012669	-0.025366	-0.013520
O	0.525580	2.169271	5.472081	-0.000306	0.016947	0.032022
O	1.927562	11.632329	0.894709	0.000300	-0.016948	-0.032011
O	-0.226867	9.070071	4.078104	-0.000296	-0.016947	0.032011
O	2.680009	4.731529	2.288686	0.000300	0.016938	-0.032023
O	0.058846	0.698526	2.444964	0.003916	-0.003533	-0.016009
O	2.394296	13.103075	3.921826	-0.003913	0.003516	0.015997
O	4.548725	7.599326	0.738431	0.003913	0.003525	-0.016010
O	-2.095583	6.202275	5.628359	-0.003920	-0.003522	0.016013
O	-2.459230	13.184059	5.445139	0.016443	0.004600	0.026939
O	4.912372	0.617542	0.921651	-0.016463	-0.004610	-0.026941
O	2.757943	6.283259	4.105046	0.016465	-0.004613	0.026938
O	-0.304801	7.518342	2.261744	-0.016438	0.004587	-0.026938
O	-0.175430	2.374756	0.744070	0.008464	-0.022944	0.022874
O	2.628573	11.426844	5.622720	-0.008462	0.022934	-0.022873
O	4.783002	9.275557	2.439325	0.008465	0.022954	0.022861
O	-2.329859	4.526044	3.927465	-0.008472	-0.022952	-0.022856
O	-1.223866	12.517207	2.155216	0.010111	0.028311	0.019133
O	3.677009	1.284394	4.211574	-0.010123	-0.028308	-0.019139
O	5.831438	5.616407	1.028179	0.010118	-0.028306	0.019137
O	-3.378295	8.185194	5.338611	-0.010110	0.028313	-0.019136
H	-0.637445	12.195109	2.878812	0.059869	0.037730	-0.018227
H	3.090587	1.606491	3.487978	-0.059872	-0.037730	0.018210
H	5.245016	5.294309	0.304583	0.059877	-0.037730	-0.018220
H	-2.791874	8.507292	6.062207	-0.059873	0.037720	0.018233

100 f = 14.315915 THz 89.949547 2PiTHz 477.527510 cm-1 59.205887
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.115073	-0.039846	0.078029
Li	-1.316675	4.156264	2.365404	0.115089	-0.039855	0.078063
Li	-3.471104	2.744536	5.548798	-0.115069	-0.039835	-0.078031
Li	5.924247	11.057064	0.817991	-0.115078	-0.039832	-0.078030
Na	2.049025	6.784862	1.629696	-0.000804	0.000349	-0.000702
Na	0.404117	7.016739	4.737094	-0.000804	0.000350	-0.000720
Na	2.558546	13.685662	1.553699	0.000805	0.000352	0.000719
Na	-0.105403	0.115939	4.813091	0.000805	0.000348	0.000703
B	4.155007	8.978944	1.168663	0.004404	0.004927	0.024753
B	-1.701865	4.822656	5.198127	0.004410	0.004923	0.024751
B	0.452564	2.078144	2.014732	-0.004425	0.004937	-0.024750
B	2.000578	11.723457	4.352058	-0.004405	0.004929	-0.024753
B	-2.733891	11.746082	5.839177	-0.016562	-0.008313	-0.014054
B	5.187034	2.055518	0.527613	-0.016563	-0.008324	-0.014074
B	3.032605	4.845282	3.711007	0.016560	-0.008302	0.014045
B	-0.579463	8.956318	2.655782	0.016562	-0.008316	0.014061
B	-0.983708	0.054306	1.827988	0.011294	0.001966	0.023099
B	3.436850	13.747295	4.538802	0.011292	0.001967	0.023090
B	5.591279	6.955106	1.355407	-0.011293	0.001970	-0.023099
B	-3.138137	6.846495	5.011383	-0.011286	0.001972	-0.023080
Si	0.631772	3.486686	4.508512	-0.001876	0.007837	-0.014513
Si	1.821370	10.314915	1.858278	-0.001893	0.007827	-0.014508
Si	-0.333059	10.387486	5.041673	0.001890	0.007833	0.014514
Si	2.786201	3.414115	1.325117	0.001903	0.007815	0.014507
O	0.061445	3.072947	3.041906	0.005639	-0.016694	-0.001547
O	2.391697	10.728653	3.324884	0.005643	-0.016688	-0.001554
O	4.546126	9.973747	0.141489	-0.005640	-0.016698	0.001553
O	-2.092984	3.827853	6.225301	-0.005650	-0.016697	0.001557
O	2.197450	3.933608	4.519003	0.002006	-0.010492	-0.005423
O	0.255692	9.867992	1.847787	0.002001	-0.010513	-0.005417
O	-1.898737	10.834409	5.031182	-0.002001	-0.010504	0.005419
O	4.351879	2.967192	1.335608	-0.001989	-0.010507	0.005415

O	-0.212316	4.798696	5.055280	0.016608	0.024164	-0.014814
O	2.665458	9.002905	1.311510	0.016598	0.024172	-0.014832
O	0.511030	11.699496	4.494905	-0.016606	0.024180	0.014831
O	1.942113	2.102105	1.871885	-0.016620	0.024178	0.014824
O	0.525580	2.169271	5.472081	0.004758	-0.015059	-0.031526
O	1.927562	11.632329	0.894709	0.004775	-0.015063	-0.031512
O	-0.226867	9.070071	4.078104	-0.004770	-0.015062	0.031518
O	2.680009	4.731529	2.288686	-0.004790	-0.015055	0.031501
O	0.058846	0.698526	2.444964	0.004425	0.015694	0.016541
O	2.394296	13.103075	3.921826	0.004418	0.015702	0.016529
O	4.548725	7.599326	0.738431	-0.004422	0.015702	-0.016538
O	-2.095583	6.202275	5.628359	-0.004409	0.015700	-0.016536
O	-2.459230	13.184059	5.445139	0.015174	-0.000032	0.015799
O	4.912372	0.617542	0.921651	0.015174	-0.000035	0.015814
O	2.757943	6.283259	4.105046	-0.015178	-0.000032	-0.015788
O	-0.304801	7.518342	2.261744	-0.015173	-0.000037	-0.015806
O	-0.175430	2.374756	0.744070	-0.016445	0.009430	-0.021088
O	2.628573	11.426844	5.622720	-0.016433	0.009429	-0.021081
O	4.783002	9.275557	2.439325	0.016434	0.009438	0.021079
O	-2.329859	4.526044	3.927465	0.016430	0.009422	0.021079
O	-1.223866	12.517207	2.155216	-0.004824	-0.000633	-0.000143
O	3.677009	1.284394	4.211574	-0.004825	-0.000628	-0.000133
O	5.831438	5.616407	1.028179	0.004823	-0.000626	0.000133
O	-3.378295	8.185194	5.338611	0.004819	-0.000620	0.000131
H	-0.637445	12.195109	2.878812	-0.009233	-0.034500	-0.012889
H	3.090587	1.606491	3.487978	-0.009230	-0.034486	-0.012877
H	5.245016	5.294309	0.304583	0.009223	-0.034491	0.012886
H	-2.791874	8.507292	6.062207	0.009198	-0.034472	0.012895

101 f = 14.188759 THz 89.150603 2PiTHz 473.286047 cm-1 58.680012 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.021802	-0.029798	0.045582
Li	-1.316675	4.156264	2.365404	0.021553	-0.029698	0.045375
Li	-3.471104	2.744536	5.548798	0.021551	0.029759	0.045348
Li	5.924247	11.057064	0.817991	0.021882	0.029780	0.045642

Na	2.049025	6.784862	1.629696	0.001713	0.000623	0.000334
Na	0.404117	7.016739	4.737094	0.001717	0.000590	0.000376
Na	2.558546	13.685662	1.553699	0.001717	-0.000592	0.000375
Na	-0.105403	0.115939	4.813091	0.001714	-0.000619	0.000335
B	4.155007	8.978944	1.168663	-0.027617	-0.027312	0.003492
B	-1.701865	4.822656	5.198127	-0.027480	-0.027204	0.003473
B	0.452564	2.078144	2.014732	-0.027483	0.027209	0.003480
B	2.000578	11.723457	4.352058	-0.027612	0.027313	0.003510
B	-2.733891	11.746082	5.839177	-0.001561	-0.022769	-0.030882
B	5.187034	2.055518	0.527613	-0.001542	-0.022661	-0.030698
B	3.032605	4.845282	3.711007	-0.001539	0.022646	-0.030705
B	-0.579463	8.956318	2.655782	-0.001573	0.022779	-0.030884
B	-0.983708	0.054306	1.827988	0.015558	-0.008195	0.018902
B	3.436850	13.747295	4.538802	0.015635	-0.008215	0.019031
B	5.591279	6.955106	1.355407	0.015653	0.008204	0.019035
B	-3.138137	6.846495	5.011383	0.015546	0.008219	0.018921
Si	0.631772	3.486686	4.508512	0.033563	0.032707	0.003316
Si	1.821370	10.314915	1.858278	0.033668	0.032896	0.003349
Si	-0.333059	10.387486	5.041673	0.033675	-0.032897	0.003340
Si	2.786201	3.414115	1.325117	0.033548	-0.032717	0.003298
O	0.061445	3.072947	3.041906	-0.012764	0.008300	0.020441
O	2.391697	10.728653	3.324884	-0.012817	0.008331	0.020541
O	4.546126	9.973747	0.141489	-0.012824	-0.008321	0.020544
O	-2.092984	3.827853	6.225301	-0.012761	-0.008285	0.020431
O	2.197450	3.933608	4.519003	0.024408	0.007979	-0.016350
O	0.255692	9.867992	1.847787	0.024471	0.008070	-0.016445
O	-1.898737	10.834409	5.031182	0.024479	-0.008063	-0.016452
O	4.351879	2.967192	1.335608	0.024396	-0.007989	-0.016350
O	-0.212316	4.798696	5.055280	-0.032604	-0.017995	-0.007243
O	2.665458	9.002905	1.311510	-0.032777	-0.018057	-0.007248
O	0.511030	11.699496	4.494905	-0.032763	0.018043	-0.007255
O	1.942113	2.102105	1.871885	-0.032615	0.018002	-0.007237
O	0.525580	2.169271	5.472081	-0.030960	0.002268	-0.024301
O	1.927562	11.632329	0.894709	-0.031114	0.002244	-0.024469
O	-0.226867	9.070071	4.078104	-0.031102	-0.002245	-0.024479
O	2.680009	4.731529	2.288686	-0.030973	-0.002276	-0.024306

O	0.058846	0.698526	2.444964	0.019313	-0.002291	0.002657
O	2.394296	13.103075	3.921826	0.019434	-0.002307	0.002679
O	4.548725	7.599326	0.738431	0.019446	0.002293	0.002693
O	-2.095583	6.202275	5.628359	0.019293	0.002292	0.002661
O	-2.459230	13.184059	5.445139	0.003450	0.000053	0.031792
O	4.912372	0.617542	0.921651	0.003417	0.000042	0.031624
O	2.757943	6.283259	4.105046	0.003427	-0.000042	0.031638
O	-0.304801	7.518342	2.261744	0.003464	-0.000050	0.031790
O	-0.175430	2.374756	0.744070	-0.020386	0.009937	-0.010191
O	2.628573	11.426844	5.622720	-0.020478	0.009997	-0.010244
O	4.783002	9.275557	2.439325	-0.020487	-0.009982	-0.010262
O	-2.329859	4.526044	3.927465	-0.020386	-0.009983	-0.010187
O	-1.223866	12.517207	2.155216	-0.007748	-0.017648	-0.018730
O	3.677009	1.284394	4.211574	-0.007823	-0.017696	-0.018766
O	5.831438	5.616407	1.028179	-0.007816	0.017677	-0.018764
O	-3.378295	8.185194	5.338611	-0.007752	0.017684	-0.018722
H	-0.637445	12.195109	2.878812	-0.068766	-0.037392	0.023195
H	3.090587	1.606491	3.487978	-0.068825	-0.037617	0.023059
H	5.245016	5.294309	0.304583	-0.068846	0.037606	0.023078
H	-2.791874	8.507292	6.062207	-0.068748	0.037439	0.023184

102 f = 14.176299 THz 89.072316 2PiTHz 472.870435 cm-1 58.628483 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.059962	-0.013596	0.049578
Li	-1.316675	4.156264	2.365404	-0.060027	0.013739	-0.049808
Li	-3.471104	2.744536	5.548798	-0.060081	-0.013760	-0.049819
Li	5.924247	11.057064	0.817991	0.059913	0.013590	0.049566
Na	2.049025	6.784862	1.629696	0.000244	0.005347	-0.004453
Na	0.404117	7.016739	4.737094	-0.000250	-0.005339	0.004469
Na	2.558546	13.685662	1.553699	-0.000249	0.005349	0.004470
Na	-0.105403	0.115939	4.813091	0.000245	-0.005342	-0.004454
B	4.155007	8.978944	1.168663	-0.026421	-0.021494	0.005443
B	-1.701865	4.822656	5.198127	0.026568	0.021637	-0.005455
B	0.452564	2.078144	2.014732	0.026565	-0.021639	-0.005469
B	2.000578	11.723457	4.352058	-0.026423	0.021504	0.005438

B	-2.733891	11.746082	5.839177	-0.004565	-0.024590	-0.035030
B	5.187034	2.055518	0.527613	0.004569	0.024709	0.035187
B	3.032605	4.845282	3.711007	0.004577	-0.024708	0.035192
B	-0.579463	8.956318	2.655782	-0.004559	0.024576	-0.035029
B	-0.983708	0.054306	1.827988	-0.017912	-0.000808	-0.022406
B	3.436850	13.747295	4.538802	0.017831	0.000850	0.022334
B	5.591279	6.955106	1.355407	0.017828	-0.000846	0.022327
B	-3.138137	6.846495	5.011383	-0.017918	0.000804	-0.022420
Si	0.631772	3.486686	4.508512	-0.021283	-0.035782	-0.008374
Si	1.821370	10.314915	1.858278	0.021121	0.035613	0.008342
Si	-0.333059	10.387486	5.041673	0.021119	-0.035615	0.008332
Si	2.786201	3.414115	1.325117	-0.021286	0.035789	-0.008362
O	0.061445	3.072947	3.041906	0.009321	-0.008064	-0.020129
O	2.391697	10.728653	3.324884	-0.009273	0.008008	0.020027
O	4.546126	9.973747	0.141489	-0.009282	-0.008002	0.020023
O	-2.092984	3.827853	6.225301	0.009319	0.008050	-0.020127
O	2.197450	3.933608	4.519003	-0.013407	-0.015937	0.021278
O	0.255692	9.867992	1.847787	0.013292	0.015891	-0.021176
O	-1.898737	10.834409	5.031182	0.013288	-0.015903	-0.021181
O	4.351879	2.967192	1.335608	-0.013412	0.015936	0.021279
O	-0.212316	4.798696	5.055280	0.032374	0.009681	0.002741
O	2.665458	9.002905	1.311510	-0.032194	-0.009581	-0.002720
O	0.511030	11.699496	4.494905	-0.032207	0.009598	-0.002706
O	1.942113	2.102105	1.871885	0.032365	-0.009673	0.002747
O	0.525580	2.169271	5.472081	0.027935	0.004700	0.032201
O	1.927562	11.632329	0.894709	-0.027776	-0.004716	-0.032086
O	-0.226867	9.070071	4.078104	-0.027776	0.004699	-0.032076
O	2.680009	4.731529	2.288686	0.027939	-0.004700	0.032215
O	0.058846	0.698526	2.444964	-0.027252	0.001370	-0.004648
O	2.394296	13.103075	3.921826	0.027151	-0.001350	0.004644
O	4.548725	7.599326	0.738431	0.027142	0.001352	0.004646
O	-2.095583	6.202275	5.628359	-0.027255	-0.001367	-0.004658
O	-2.459230	13.184059	5.445139	0.006232	0.001638	0.030039
O	4.912372	0.617542	0.921651	-0.006245	-0.001637	-0.030182
O	2.757943	6.283259	4.105046	-0.006259	0.001637	-0.030194
O	-0.304801	7.518342	2.261744	0.006236	-0.001638	0.030028

O	-0.175430	2.374756	0.744070	0.019175	-0.004013	0.012304
O	2.628573	11.426844	5.622720	-0.019069	0.003976	-0.012267
O	4.783002	9.275557	2.439325	-0.019066	-0.003983	-0.012255
O	-2.329859	4.526044	3.927465	0.019181	0.004024	0.012316
O	-1.223866	12.517207	2.155216	0.014029	0.001865	0.007215
O	3.677009	1.284394	4.211574	-0.013997	-0.001786	-0.007122
O	5.831438	5.616407	1.028179	-0.013984	0.001790	-0.007115
O	-3.378295	8.185194	5.338611	0.014034	-0.001873	0.007217
H	-0.637445	12.195109	2.878812	0.009809	0.036716	0.028250
H	3.090587	1.606491	3.487978	-0.009457	-0.036546	-0.028383
H	5.245016	5.294309	0.304583	-0.009436	0.036534	-0.028375
H	-2.791874	8.507292	6.062207	0.009825	-0.036735	0.028248

103 f = 13.807800 THz 86.756967 2PiTHz 460.578621 cm-1 57.104492
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.048231	0.073782	0.058919
Li	-1.316675	4.156264	2.365404	-0.047994	-0.073660	-0.058942
Li	-3.471104	2.744536	5.548798	0.048195	-0.073781	0.058965
Li	5.924247	11.057064	0.817991	-0.048036	0.073672	-0.058907
Na	2.049025	6.784862	1.629696	0.000492	-0.003998	0.001092
Na	0.404117	7.016739	4.737094	-0.000491	0.003980	-0.001063
Na	2.558546	13.685662	1.553699	0.000489	0.003995	0.001065
Na	-0.105403	0.115939	4.813091	-0.000492	-0.003982	-0.001089
B	4.155007	8.978944	1.168663	0.011020	0.001089	-0.002423
B	-1.701865	4.822656	5.198127	-0.011077	-0.001106	0.002446
B	0.452564	2.078144	2.014732	0.011027	-0.001097	-0.002414
B	2.000578	11.723457	4.352058	-0.011066	0.001103	0.002442
B	-2.733891	11.746082	5.839177	-0.015138	-0.009707	0.007865
B	5.187034	2.055518	0.527613	0.015098	0.009662	-0.007920
B	3.032605	4.845282	3.711007	-0.015136	0.009713	0.007872
B	-0.579463	8.956318	2.655782	0.015111	-0.009673	-0.007903
B	-0.983708	0.054306	1.827988	-0.023655	-0.024366	0.015535
B	3.436850	13.747295	4.538802	0.023720	0.024481	-0.015560
B	5.591279	6.955106	1.355407	-0.023669	0.024415	0.015545
B	-3.138137	6.846495	5.011383	0.023721	-0.024464	-0.015555

Si	0.631772	3.486686	4.508512	-0.028888	0.014133	-0.014350
Si	1.821370	10.314915	1.858278	0.028863	-0.014088	0.014433
Si	-0.333059	10.387486	5.041673	-0.028886	-0.014136	-0.014367
Si	2.786201	3.414115	1.325117	0.028852	0.014073	0.014449
O	0.061445	3.072947	3.041906	-0.002941	-0.004148	-0.015030
O	2.391697	10.728653	3.324884	0.002945	0.004145	0.015087
O	4.546126	9.973747	0.141489	-0.002942	0.004127	-0.015047
O	-2.092984	3.827853	6.225301	0.002955	-0.004158	0.015091
O	2.197450	3.933608	4.519003	-0.018443	0.002200	0.000962
O	0.255692	9.867992	1.847787	0.018420	-0.002180	-0.000999
O	-1.898737	10.834409	5.031182	-0.018441	-0.002209	0.000973
O	4.351879	2.967192	1.335608	0.018410	0.002164	-0.001006
O	-0.212316	4.798696	5.055280	-0.025454	-0.012510	0.011141
O	2.665458	9.002905	1.311510	0.025388	0.012554	-0.011194
O	0.511030	11.699496	4.494905	-0.025455	0.012524	0.011151
O	1.942113	2.102105	1.871885	0.025377	-0.012564	-0.011204
O	0.525580	2.169271	5.472081	-0.001589	0.010779	-0.000860
O	1.927562	11.632329	0.894709	0.001605	-0.010839	0.000792
O	-0.226867	9.070071	4.078104	-0.001586	-0.010795	-0.000846
O	2.680009	4.731529	2.288686	0.001614	0.010846	0.000789
O	0.058846	0.698526	2.444964	-0.027228	-0.001751	-0.002383
O	2.394296	13.103075	3.921826	0.027334	0.001758	0.002398
O	4.548725	7.599326	0.738431	-0.027247	0.001764	-0.002393
O	-2.095583	6.202275	5.628359	0.027343	-0.001744	0.002389
O	-2.459230	13.184059	5.445139	0.006704	0.000635	-0.014188
O	4.912372	0.617542	0.921651	-0.006702	-0.000608	0.014171
O	2.757943	6.283259	4.105046	0.006701	-0.000624	-0.014182
O	-0.304801	7.518342	2.261744	-0.006702	0.000623	0.014181
O	-0.175430	2.374756	0.744070	0.003262	0.050487	0.013672
O	2.628573	11.426844	5.622720	-0.003298	-0.050605	-0.013690
O	4.783002	9.275557	2.439325	0.003262	-0.050537	0.013681
O	-2.329859	4.526044	3.927465	-0.003308	0.050600	-0.013682
O	-1.223866	12.517207	2.155216	0.001330	-0.040136	0.008170
O	3.677009	1.284394	4.211574	-0.001314	0.040284	-0.008198
O	5.831438	5.616407	1.028179	0.001308	0.040188	0.008180
O	-3.378295	8.185194	5.338611	-0.001330	-0.040277	-0.008188

H	-0.637445	12.195109	2.878812	0.023048	-0.038062	-0.005966
H	3.090587	1.606491	3.487978	-0.023113	0.038188	0.005994
H	5.245016	5.294309	0.304583	0.023037	0.038117	-0.005967
H	-2.791874	8.507292	6.062207	-0.023118	-0.038166	0.005985

104 f = 13.778004 THz 86.569753 2PiTHz 459.584731 cm-1 56.981265 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.067203	0.045755	0.001719
Li	-1.316675	4.156264	2.365404	0.067339	0.045904	0.001860
Li	-3.471104	2.744536	5.548798	0.067206	-0.045782	0.001731
Li	5.924247	11.057064	0.817991	0.067332	-0.045979	0.001918
Na	2.049025	6.784862	1.629696	-0.000470	-0.007106	0.001623
Na	0.404117	7.016739	4.737094	-0.000468	-0.007101	0.001592
Na	2.558546	13.685662	1.553699	-0.000469	0.007104	0.001589
Na	-0.105403	0.115939	4.813091	-0.000470	0.007106	0.001625
B	4.155007	8.978944	1.168663	-0.012064	0.002714	0.009947
B	-1.701865	4.822656	5.198127	-0.012030	0.002722	0.009934
B	0.452564	2.078144	2.014732	-0.012063	-0.002717	0.009937
B	2.000578	11.723457	4.352058	-0.012027	-0.002714	0.009933
B	-2.733891	11.746082	5.839177	-0.015018	-0.012390	-0.009111
B	5.187034	2.055518	0.527613	-0.015062	-0.012412	-0.009077
B	3.032605	4.845282	3.711007	-0.015027	0.012387	-0.009098
B	-0.579463	8.956318	2.655782	-0.015065	0.012418	-0.009085
B	-0.983708	0.054306	1.827988	0.017836	0.033109	-0.012421
B	3.436850	13.747295	4.538802	0.017768	0.033047	-0.012362
B	5.591279	6.955106	1.355407	0.017836	-0.033131	-0.012416
B	-3.138137	6.846495	5.011383	0.017781	-0.033062	-0.012382
Si	0.631772	3.486686	4.508512	-0.018758	0.013390	0.031123
Si	1.821370	10.314915	1.858278	-0.018830	0.013438	0.031081
Si	-0.333059	10.387486	5.041673	-0.018729	-0.013401	0.031130
Si	2.786201	3.414115	1.325117	-0.018804	-0.013421	0.031101
O	0.061445	3.072947	3.041906	0.009361	0.002423	0.015309
O	2.391697	10.728653	3.324884	0.009350	0.002400	0.015273
O	4.546126	9.973747	0.141489	0.009359	-0.002414	0.015328
O	-2.092984	3.827853	6.225301	0.009365	-0.002399	0.015286

O	2.197450	3.933608	4.519003	-0.016637	0.010392	-0.012200
O	0.255692	9.867992	1.847787	-0.016679	0.010394	-0.012193
O	-1.898737	10.834409	5.031182	-0.016618	-0.010397	-0.012207
O	4.351879	2.967192	1.335608	-0.016656	-0.010373	-0.012186
O	-0.212316	4.798696	5.055280	-0.017920	0.021099	-0.017769
O	2.665458	9.002905	1.311510	-0.018007	0.021065	-0.017763
O	0.511030	11.699496	4.494905	-0.017922	-0.021108	-0.017793
O	1.942113	2.102105	1.871885	-0.017986	-0.021061	-0.017757
O	0.525580	2.169271	5.472081	0.014766	-0.022084	-0.018898
O	1.927562	11.632329	0.894709	0.014739	-0.022055	-0.018909
O	-0.226867	9.070071	4.078104	0.014752	0.022081	-0.018905
O	2.680009	4.731529	2.288686	0.014756	0.022057	-0.018895
O	0.058846	0.698526	2.444964	0.032287	-0.000848	-0.000348
O	2.394296	13.103075	3.921826	0.032219	-0.000849	-0.000353
O	4.548725	7.599326	0.738431	0.032306	0.000850	-0.000355
O	-2.095583	6.202275	5.628359	0.032235	0.000855	-0.000356
O	-2.459230	13.184059	5.445139	-0.002677	0.006177	-0.009923
O	4.912372	0.617542	0.921651	-0.002649	0.006180	-0.009982
O	2.757943	6.283259	4.105046	-0.002676	-0.006171	-0.009951
O	-0.304801	7.518342	2.261744	-0.002655	-0.006184	-0.009977
O	-0.175430	2.374756	0.744070	-0.010268	-0.038406	-0.001760
O	2.628573	11.426844	5.622720	-0.010253	-0.038262	-0.001736
O	4.783002	9.275557	2.439325	-0.010259	0.038440	-0.001779
O	-2.329859	4.526044	3.927465	-0.010249	0.038309	-0.001741
O	-1.223866	12.517207	2.155216	0.002428	0.050469	-0.004405
O	3.677009	1.284394	4.211574	0.002427	0.050360	-0.004384
O	5.831438	5.616407	1.028179	0.002423	-0.050496	-0.004396
O	-3.378295	8.185194	5.338611	0.002429	-0.050387	-0.004387
H	-0.637445	12.195109	2.878812	-0.010818	0.044212	0.002953
H	3.090587	1.606491	3.487978	-0.010768	0.044094	0.002935
H	5.245016	5.294309	0.304583	-0.010822	-0.044222	0.002952
H	-2.791874	8.507292	6.062207	-0.010762	-0.044126	0.002931

105 f = 13.559958 THz 85.199728 2PiTHz 452.311494 cm-1 56.079498 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.003152	0.068288	0.064612
Li	-1.316675	4.156264	2.365404	-0.003127	0.068284	0.064686
Li	-3.471104	2.744536	5.548798	0.003193	0.068239	-0.064684
Li	5.924247	11.057064	0.817991	0.003186	0.068263	-0.064643
Na	2.049025	6.784862	1.629696	-0.000171	-0.001280	-0.000386
Na	0.404117	7.016739	4.737094	-0.000177	-0.001276	-0.000356
Na	2.558546	13.685662	1.553699	0.000172	-0.001280	0.000354
Na	-0.105403	0.115939	4.813091	0.000175	-0.001265	0.000390
B	4.155007	8.978944	1.168663	0.007270	-0.001954	-0.003973
B	-1.701865	4.822656	5.198127	0.007276	-0.001924	-0.003972
B	0.452564	2.078144	2.014732	-0.007275	-0.001942	0.003993
B	2.000578	11.723457	4.352058	-0.007278	-0.001947	0.003964
B	-2.733891	11.746082	5.839177	-0.011216	-0.002107	0.004693
B	5.187034	2.055518	0.527613	-0.011250	-0.002146	0.004697
B	3.032605	4.845282	3.711007	0.011210	-0.002114	-0.004705
B	-0.579463	8.956318	2.655782	0.011236	-0.002126	-0.004687
B	-0.983708	0.054306	1.827988	0.014033	0.028012	-0.013634
B	3.436850	13.747295	4.538802	0.014001	0.027930	-0.013587
B	5.591279	6.955106	1.355407	-0.014014	0.027986	0.013611
B	-3.138137	6.846495	5.011383	-0.013997	0.027911	0.013584
Si	0.631772	3.486686	4.508512	0.037101	-0.009570	0.019085
Si	1.821370	10.314915	1.858278	0.037137	-0.009575	0.019010
Si	-0.333059	10.387486	5.041673	-0.037121	-0.009579	-0.019046
Si	2.786201	3.414115	1.325117	-0.037154	-0.009573	-0.019007
O	0.061445	3.072947	3.041906	0.007568	-0.007120	0.021416
O	2.391697	10.728653	3.324884	0.007537	-0.007132	0.021382
O	4.546126	9.973747	0.141489	-0.007554	-0.007147	-0.021403
O	-2.092984	3.827853	6.225301	-0.007529	-0.007112	-0.021384
O	2.197450	3.933608	4.519003	0.025783	-0.004405	0.000680
O	0.255692	9.867992	1.847787	0.025815	-0.004402	0.000717
O	-1.898737	10.834409	5.031182	-0.025800	-0.004395	-0.000708
O	4.351879	2.967192	1.335608	-0.025832	-0.004426	-0.000703
O	-0.212316	4.798696	5.055280	0.017086	0.002073	-0.007401
O	2.665458	9.002905	1.311510	0.017098	0.002022	-0.007352
O	0.511030	11.699496	4.494905	-0.017096	0.002037	0.007371
O	1.942113	2.102105	1.871885	-0.017103	0.002023	0.007358

O	0.525580	2.169271	5.472081	-0.001644	-0.003299	0.007278
O	1.927562	11.632329	0.894709	-0.001697	-0.003243	0.007296
O	-0.226867	9.070071	4.078104	0.001690	-0.003273	-0.007285
O	2.680009	4.731529	2.288686	0.001679	-0.003239	-0.007304
O	0.058846	0.698526	2.444964	0.022981	-0.001972	-0.001087
O	2.394296	13.103075	3.921826	0.022928	-0.001984	-0.001076
O	4.548725	7.599326	0.738431	-0.022952	-0.001972	0.001080
O	-2.095583	6.202275	5.628359	-0.022919	-0.001984	0.001085
O	-2.459230	13.184059	5.445139	0.002571	-0.003119	-0.020735
O	4.912372	0.617542	0.921651	0.002543	-0.003119	-0.020778
O	2.757943	6.283259	4.105046	-0.002556	-0.003130	0.020719
O	-0.304801	7.518342	2.261744	-0.002560	-0.003110	0.020764
O	-0.175430	2.374756	0.744070	0.005161	-0.053095	-0.016695
O	2.628573	11.426844	5.622720	0.005174	-0.053007	-0.016704
O	4.783002	9.275557	2.439325	-0.005165	-0.053062	0.016703
O	-2.329859	4.526044	3.927465	-0.005181	-0.052993	0.016706
O	-1.223866	12.517207	2.155216	0.001084	0.041450	0.000408
O	3.677009	1.284394	4.211574	0.001068	0.041333	0.000428
O	5.831438	5.616407	1.028179	-0.001082	0.041407	-0.000424
O	-3.378295	8.185194	5.338611	-0.001068	0.041300	-0.000415
H	-0.637445	12.195109	2.878812	0.018243	0.033674	-0.017594
H	3.090587	1.606491	3.487978	0.018235	0.033571	-0.017569
H	5.245016	5.294309	0.304583	-0.018276	0.033647	0.017597
H	-2.791874	8.507292	6.062207	-0.018195	0.033521	0.017559

106 f = 13.446140 THz 84.484591 2PiTHz 448.514946 cm-1 55.608786 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.011105	0.004467	0.003275
Li	-1.316675	4.156264	2.365404	-0.011173	-0.004284	-0.003096
Li	-3.471104	2.744536	5.548798	-0.011125	0.004383	-0.003214
Li	5.924247	11.057064	0.817991	0.011143	-0.004291	0.003096
Na	2.049025	6.784862	1.629696	-0.002888	0.002529	-0.001150
Na	0.404117	7.016739	4.737094	0.002889	-0.002520	0.001093
Na	2.558546	13.685662	1.553699	0.002888	0.002527	0.001095
Na	-0.105403	0.115939	4.813091	-0.002890	-0.002523	-0.001148

B	4.155007	8.978944	1.168663	0.005182	0.010704	0.010531
B	-1.701865	4.822656	5.198127	-0.005159	-0.010717	-0.010532
B	0.452564	2.078144	2.014732	-0.005172	0.010710	-0.010527
B	2.000578	11.723457	4.352058	0.005155	-0.010711	0.010535
B	-2.733891	11.746082	5.839177	-0.016755	-0.015385	-0.003005
B	5.187034	2.055518	0.527613	0.016739	0.015385	0.003014
B	3.032605	4.845282	3.711007	0.016745	-0.015384	0.003003
B	-0.579463	8.956318	2.655782	-0.016735	0.015386	-0.003025
B	-0.983708	0.054306	1.827988	-0.015475	-0.043406	0.018849
B	3.436850	13.747295	4.538802	0.015500	0.043447	-0.018862
B	5.591279	6.955106	1.355407	0.015460	-0.043402	-0.018829
B	-3.138137	6.846495	5.011383	-0.015485	0.043433	0.018862
Si	0.631772	3.486686	4.508512	0.020797	0.000712	-0.032416
Si	1.821370	10.314915	1.858278	-0.020727	-0.000720	0.032444
Si	-0.333059	10.387486	5.041673	-0.020802	0.000688	0.032406
Si	2.786201	3.414115	1.325117	0.020746	-0.000727	-0.032442
O	0.061445	3.072947	3.041906	-0.018673	0.007197	-0.013553
O	2.391697	10.728653	3.324884	0.018673	-0.007218	0.013595
O	4.546126	9.973747	0.141489	0.018663	0.007210	0.013555
O	-2.092984	3.827853	6.225301	-0.018684	-0.007205	-0.013580
O	2.197450	3.933608	4.519003	0.019993	-0.009754	0.010967
O	0.255692	9.867992	1.847787	-0.019948	0.009769	-0.010963
O	-1.898737	10.834409	5.031182	-0.019995	-0.009757	-0.010969
O	4.351879	2.967192	1.335608	0.019959	0.009749	0.010968
O	-0.212316	4.798696	5.055280	0.001690	-0.022416	0.016037
O	2.665458	9.002905	1.311510	-0.001661	0.022422	-0.016057
O	0.511030	11.699496	4.494905	-0.001701	-0.022428	-0.016053
O	1.942113	2.102105	1.871885	0.001673	0.022409	0.016046
O	0.525580	2.169271	5.472081	-0.011909	0.027768	0.010918
O	1.927562	11.632329	0.894709	0.011902	-0.027774	-0.010912
O	-0.226867	9.070071	4.078104	0.011912	0.027769	-0.010935
O	2.680009	4.731529	2.288686	-0.011915	-0.027768	0.010903
O	0.058846	0.698526	2.444964	-0.026583	-0.002004	-0.003339
O	2.394296	13.103075	3.921826	0.026624	0.001998	0.003343
O	4.548725	7.599326	0.738431	0.026575	-0.002006	0.003342
O	-2.095583	6.202275	5.628359	-0.026607	0.001997	-0.003329

O	-2.459230	13.184059	5.445139	-0.005189	0.002759	-0.022307
O	4.912372	0.617542	0.921651	0.005204	-0.002758	0.022281
O	2.757943	6.283259	4.105046	0.005199	0.002754	0.022308
O	-0.304801	7.518342	2.261744	-0.005213	-0.002765	-0.022259
O	-0.175430	2.374756	0.744070	0.007585	0.048069	-0.004321
O	2.628573	11.426844	5.622720	-0.007579	-0.048148	0.004300
O	4.783002	9.275557	2.439325	-0.007581	0.048048	0.004325
O	-2.329859	4.526044	3.927465	0.007576	-0.048139	-0.004303
O	-1.223866	12.517207	2.155216	-0.005931	-0.060889	0.008565
O	3.677009	1.284394	4.211574	0.005924	0.060951	-0.008563
O	5.831438	5.616407	1.028179	0.005924	-0.060876	-0.008560
O	-3.378295	8.185194	5.338611	-0.005928	0.060931	0.008555
H	-0.637445	12.195109	2.878812	-0.017220	-0.060426	0.020252
H	3.090587	1.606491	3.487978	0.017254	0.060464	-0.020293
H	5.245016	5.294309	0.304583	0.017231	-0.060402	-0.020264
H	-2.791874	8.507292	6.062207	-0.017248	0.060443	0.020278

107 f = 12.789200 THz 80.356912 2PiTHz 426.601773 cm-1 52.891898 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001474	0.002322	-0.015545
Li	-1.316675	4.156264	2.365404	-0.000472	0.000347	0.017604
Li	-3.471104	2.744536	5.548798	0.000445	0.000397	-0.017618
Li	5.924247	11.057064	0.817991	-0.001503	0.002341	0.015619
Na	2.049025	6.784862	1.629696	0.001705	0.008021	-0.006442
Na	0.404117	7.016739	4.737094	-0.002017	-0.008067	0.006157
Na	2.558546	13.685662	1.553699	0.002017	-0.008072	-0.006152
Na	-0.105403	0.115939	4.813091	-0.001704	0.008017	0.006444
B	4.155007	8.978944	1.168663	0.017390	-0.028523	0.006519
B	-1.701865	4.822656	5.198127	-0.018203	0.030747	-0.006912
B	0.452564	2.078144	2.014732	0.018215	0.030733	0.006916
B	2.000578	11.723457	4.352058	-0.017394	-0.028529	-0.006514
B	-2.733891	11.746082	5.839177	-0.013638	0.025808	-0.012419
B	5.187034	2.055518	0.527613	0.014445	-0.027648	0.013637
B	3.032605	4.845282	3.711007	-0.014450	-0.027636	-0.013628
B	-0.579463	8.956318	2.655782	0.013625	0.025822	0.012410

B	-0.983708	0.054306	1.827988	-0.014901	-0.004021	-0.011317
B	3.436850	13.747295	4.538802	0.014222	0.002812	0.010847
B	5.591279	6.955106	1.355407	-0.014224	0.002826	-0.010864
B	-3.138137	6.846495	5.011383	0.014908	-0.004032	0.011307
Si	0.631772	3.486686	4.508512	-0.016644	-0.000717	0.033715
Si	1.821370	10.314915	1.858278	0.015718	0.000703	-0.031592
Si	-0.333059	10.387486	5.041673	-0.015714	0.000697	0.031609
Si	2.786201	3.414115	1.325117	0.016627	-0.000702	-0.033700
O	0.061445	3.072947	3.041906	0.022878	0.040376	0.003573
O	2.391697	10.728653	3.324884	-0.021125	-0.036770	-0.003764
O	4.546126	9.973747	0.141489	0.021159	-0.036787	0.003766
O	-2.092984	3.827853	6.225301	-0.022856	0.040372	-0.003578
O	2.197450	3.933608	4.519003	-0.004146	-0.038740	-0.011130
O	0.255692	9.867992	1.847787	0.003920	0.036551	0.010429
O	-1.898737	10.834409	5.031182	-0.003911	0.036577	-0.010460
O	4.351879	2.967192	1.335608	0.004133	-0.038739	0.011127
O	-0.212316	4.798696	5.055280	-0.018805	0.025071	-0.032837
O	2.665458	9.002905	1.311510	0.018072	-0.023018	0.030457
O	0.511030	11.699496	4.494905	-0.018065	-0.023026	-0.030447
O	1.942113	2.102105	1.871885	0.018820	0.025064	0.032848
O	0.525580	2.169271	5.472081	0.029946	-0.021117	0.009647
O	1.927562	11.632329	0.894709	-0.027901	0.019489	-0.009173
O	-0.226867	9.070071	4.078104	0.027883	0.019503	0.009161
O	2.680009	4.731529	2.288686	-0.029951	-0.021094	-0.009646
O	0.058846	0.698526	2.444964	-0.008023	0.015409	-0.042530
O	2.394296	13.103075	3.921826	0.007899	-0.015157	0.039680
O	4.548725	7.599326	0.738431	-0.007903	-0.015152	-0.039712
O	-2.095583	6.202275	5.628359	0.008021	0.015405	0.042533
O	-2.459230	13.184059	5.445139	0.041067	0.016696	-0.004613
O	4.912372	0.617542	0.921651	-0.043398	-0.018399	0.005376
O	2.757943	6.283259	4.105046	0.043398	-0.018405	-0.005377
O	-0.304801	7.518342	2.261744	-0.041072	0.016713	0.004595
O	-0.175430	2.374756	0.744070	0.011751	0.004353	0.002741
O	2.628573	11.426844	5.622720	-0.011359	-0.003684	-0.002389
O	4.783002	9.275557	2.439325	0.011341	-0.003680	0.002400
O	-2.329859	4.526044	3.927465	-0.011747	0.004373	-0.002738

O	-1.223866	12.517207	2.155216	-0.006915	-0.004965	-0.008565
O	3.677009	1.284394	4.211574	0.005888	0.003425	0.008081
O	5.831438	5.616407	1.028179	-0.005879	0.003434	-0.008072
O	-3.378295	8.185194	5.338611	0.006920	-0.004977	0.008541
H	-0.637445	12.195109	2.878812	-0.004994	-0.009327	-0.010363
H	3.090587	1.606491	3.487978	0.003541	0.007891	0.010149
H	5.245016	5.294309	0.304583	-0.003519	0.007895	-0.010145
H	-2.791874	8.507292	6.062207	0.004962	-0.009336	0.010370

108 f = 12.784160 THz 80.325249 2PiTHz 426.433677 cm-1 52.871057 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.013640	0.036611	0.028547
Li	-1.316675	4.156264	2.365404	0.013701	0.036683	0.027381
Li	-3.471104	2.744536	5.548798	-0.013690	0.036675	-0.027390
Li	5.924247	11.057064	0.817991	-0.013648	0.036618	-0.028594
Na	2.049025	6.784862	1.629696	-0.004154	-0.001039	-0.002625
Na	0.404117	7.016739	4.737094	-0.004028	-0.000448	-0.003045
Na	2.558546	13.685662	1.553699	0.004027	-0.000449	0.003042
Na	-0.105403	0.115939	4.813091	0.004153	-0.001035	0.002625
B	4.155007	8.978944	1.168663	-0.011928	0.031246	-0.005951
B	-1.701865	4.822656	5.198127	-0.010617	0.029066	-0.005436
B	0.452564	2.078144	2.014732	0.010610	0.029066	0.005437
B	2.000578	11.723457	4.352058	0.011940	0.031245	0.005949
B	-2.733891	11.746082	5.839177	0.011564	-0.025888	0.017125
B	5.187034	2.055518	0.527613	0.010543	-0.023935	0.016166
B	3.032605	4.845282	3.711007	-0.010543	-0.023935	-0.016159
B	-0.579463	8.956318	2.655782	-0.011558	-0.025891	-0.017119
B	-0.983708	0.054306	1.827988	-0.008628	-0.015615	-0.005913
B	3.436850	13.747295	4.538802	-0.009706	-0.015818	-0.006740
B	5.591279	6.955106	1.355407	0.009710	-0.015840	0.006750
B	-3.138137	6.846495	5.011383	0.008627	-0.015608	0.005915
Si	0.631772	3.486686	4.508512	-0.011843	-0.000251	0.027494
Si	1.821370	10.314915	1.858278	-0.013022	-0.000325	0.029897
Si	-0.333059	10.387486	5.041673	0.013018	-0.000313	-0.029910
Si	2.786201	3.414115	1.325117	0.011835	-0.000244	-0.027482

O	0.061445	3.072947	3.041906	0.022515	0.047443	-0.002610
O	2.391697	10.728653	3.324884	0.024123	0.050257	-0.002335
O	4.546126	9.973747	0.141489	-0.024145	0.050270	0.002330
O	-2.092984	3.827853	6.225301	-0.022508	0.047434	0.002609
O	2.197450	3.933608	4.519003	-0.002863	-0.028625	-0.009320
O	0.255692	9.867992	1.847787	-0.003149	-0.031397	-0.010090
O	-1.898737	10.834409	5.031182	0.003142	-0.031414	0.010112
O	4.351879	2.967192	1.335608	0.002858	-0.028618	0.009317
O	-0.212316	4.798696	5.055280	-0.009620	0.026766	-0.031628
O	2.665458	9.002905	1.311510	-0.010992	0.028504	-0.033995
O	0.511030	11.699496	4.494905	0.010997	0.028510	0.033998
O	1.942113	2.102105	1.871885	0.009615	0.026766	0.031623
O	0.525580	2.169271	5.472081	0.027019	-0.021274	0.006277
O	1.927562	11.632329	0.894709	0.029102	-0.022773	0.006984
O	-0.226867	9.070071	4.078104	-0.029098	-0.022773	-0.006978
O	2.680009	4.731529	2.288686	-0.027013	-0.021265	-0.006273
O	0.058846	0.698526	2.444964	-0.001164	0.003166	-0.037044
O	2.394296	13.103075	3.921826	-0.001749	0.004307	-0.040049
O	4.548725	7.599326	0.738431	0.001758	0.004302	0.040071
O	-2.095583	6.202275	5.628359	0.001162	0.003169	0.037042
O	-2.459230	13.184059	5.445139	-0.033495	-0.023556	0.010520
O	4.912372	0.617542	0.921651	-0.030384	-0.022300	0.010163
O	2.757943	6.283259	4.105046	0.030388	-0.022295	-0.010165
O	-0.304801	7.518342	2.261744	0.033502	-0.023574	-0.010512
O	-0.175430	2.374756	0.744070	0.005071	0.008536	0.004770
O	2.628573	11.426844	5.622720	0.005932	0.008828	0.004968
O	4.783002	9.275557	2.439325	-0.005917	0.008836	-0.004975
O	-2.329859	4.526044	3.927465	-0.005071	0.008540	-0.004771
O	-1.223866	12.517207	2.155216	-0.013689	-0.019966	-0.006282
O	3.677009	1.284394	4.211574	-0.014163	-0.020218	-0.006924
O	5.831438	5.616407	1.028179	0.014146	-0.020239	0.006905
O	-3.378295	8.185194	5.338611	0.013685	-0.019962	0.006289
H	-0.637445	12.195109	2.878812	-0.019141	-0.018579	-0.003022
H	3.090587	1.606491	3.487978	-0.019476	-0.019175	-0.003802
H	5.245016	5.294309	0.304583	0.019428	-0.019176	0.003798
H	-2.791874	8.507292	6.062207	0.019150	-0.018569	0.003015

109 f = 12.563899 THz 78.941304 2PiTHz 419.086538 cm-1 51.960127
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.015759	-0.065778	-0.060629
Li	-1.316675	4.156264	2.365404	0.015566	-0.065792	-0.060386
Li	-3.471104	2.744536	5.548798	-0.015663	-0.065710	0.060468
Li	5.924247	11.057064	0.817991	-0.015671	-0.065844	0.060506
Na	2.049025	6.784862	1.629696	-0.001150	0.004955	-0.001145
Na	0.404117	7.016739	4.737094	-0.001148	0.004925	-0.001110
Na	2.558546	13.685662	1.553699	0.001151	0.004944	0.001112
Na	-0.105403	0.115939	4.813091	0.001147	0.004938	0.001143
B	4.155007	8.978944	1.168663	-0.020443	0.002731	-0.007593
B	-1.701865	4.822656	5.198127	-0.020435	0.002742	-0.007619
B	0.452564	2.078144	2.014732	0.020436	0.002752	0.007612
B	2.000578	11.723457	4.352058	0.020443	0.002716	0.007598
B	-2.733891	11.746082	5.839177	-0.000851	-0.017131	-0.007061
B	5.187034	2.055518	0.527613	-0.000830	-0.017124	-0.007056
B	3.032605	4.845282	3.711007	0.000841	-0.017130	0.007050
B	-0.579463	8.956318	2.655782	0.000840	-0.017127	0.007074
B	-0.983708	0.054306	1.827988	-0.001412	0.048918	-0.010246
B	3.436850	13.747295	4.538802	-0.001409	0.048926	-0.010234
B	5.591279	6.955106	1.355407	0.001428	0.048948	0.010228
B	-3.138137	6.846495	5.011383	0.001397	0.048888	0.010251
Si	0.631772	3.486686	4.508512	-0.017598	-0.002660	0.004522
Si	1.821370	10.314915	1.858278	-0.017671	-0.002649	0.004495
Si	-0.333059	10.387486	5.041673	0.017626	-0.002641	-0.004468
Si	2.786201	3.414115	1.325117	0.017630	-0.002664	-0.004550
O	0.061445	3.072947	3.041906	-0.003757	-0.009681	0.002368
O	2.391697	10.728653	3.324884	-0.003770	-0.009685	0.002331
O	4.546126	9.973747	0.141489	0.003808	-0.009722	-0.002354
O	-2.092984	3.827853	6.225301	0.003718	-0.009643	-0.002348
O	2.197450	3.933608	4.519003	-0.000034	-0.045787	-0.016786
O	0.255692	9.867992	1.847787	-0.000087	-0.045791	-0.016845
O	-1.898737	10.834409	5.031182	0.000052	-0.045791	0.016825
O	4.351879	2.967192	1.335608	0.000061	-0.045794	0.016815

O	-0.212316	4.798696	5.055280	-0.014708	0.000443	-0.000574
O	2.665458	9.002905	1.311510	-0.014702	0.000471	-0.000506
O	0.511030	11.699496	4.494905	0.014699	0.000438	0.000505
O	1.942113	2.102105	1.871885	0.014708	0.000472	0.000568
O	0.525580	2.169271	5.472081	0.013688	-0.014648	-0.006804
O	1.927562	11.632329	0.894709	0.013741	-0.014662	-0.006840
O	-0.226867	9.070071	4.078104	-0.013720	-0.014617	0.006828
O	2.680009	4.731529	2.288686	-0.013700	-0.014693	0.006821
O	0.058846	0.698526	2.444964	0.009967	0.019442	-0.001753
O	2.394296	13.103075	3.921826	0.009980	0.019423	-0.001721
O	4.548725	7.599326	0.738431	-0.009961	0.019459	0.001739
O	-2.095583	6.202275	5.628359	-0.009983	0.019406	0.001748
O	-2.459230	13.184059	5.445139	-0.027167	0.019394	0.001045
O	4.912372	0.617542	0.921651	-0.027170	0.019396	0.001040
O	2.757943	6.283259	4.105046	0.027163	0.019377	-0.001050
O	-0.304801	7.518342	2.261744	0.027178	0.019407	-0.001030
O	-0.175430	2.374756	0.744070	0.003707	-0.025061	0.005230
O	2.628573	11.426844	5.622720	0.003675	-0.025077	0.005248
O	4.783002	9.275557	2.439325	-0.003680	-0.025080	-0.005241
O	-2.329859	4.526044	3.927465	-0.003698	-0.025056	-0.005236
O	-1.223866	12.517207	2.155216	0.003308	0.055213	-0.019853
O	3.677009	1.284394	4.211574	0.003295	0.055218	-0.019875
O	5.831438	5.616407	1.028179	-0.003309	0.055250	0.019827
O	-3.378295	8.185194	5.338611	-0.003293	0.055173	0.019884
H	-0.637445	12.195109	2.878812	-0.001601	0.062880	-0.014069
H	3.090587	1.606491	3.487978	-0.001600	0.062894	-0.014100
H	5.245016	5.294309	0.304583	0.001559	0.062935	0.014070
H	-2.791874	8.507292	6.062207	0.001660	0.062833	0.014067

110 f = 12.436356 THz 78.139929 2PiTHz 414.832170 cm-1 51.432652 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.068139	0.077606	-0.065037
Li	-1.316675	4.156264	2.365404	-0.068160	-0.077505	0.065130
Li	-3.471104	2.744536	5.548798	-0.068108	0.077627	0.065045
Li	5.924247	11.057064	0.817991	0.068114	-0.077519	-0.065060

Na	2.049025	6.784862	1.629696	-0.000634	0.002453	-0.000887
Na	0.404117	7.016739	4.737094	0.000637	-0.002465	0.000889
Na	2.558546	13.685662	1.553699	0.000636	0.002459	0.000887
Na	-0.105403	0.115939	4.813091	-0.000637	-0.002463	-0.000890
B	4.155007	8.978944	1.168663	-0.007109	0.004314	0.004384
B	-1.701865	4.822656	5.198127	0.007135	-0.004312	-0.004374
B	0.452564	2.078144	2.014732	0.007103	0.004312	-0.004381
B	2.000578	11.723457	4.352058	-0.007130	-0.004314	0.004378
B	-2.733891	11.746082	5.839177	-0.003667	0.002644	0.007912
B	5.187034	2.055518	0.527613	0.003665	-0.002628	-0.007898
B	3.032605	4.845282	3.711007	0.003660	0.002650	-0.007915
B	-0.579463	8.956318	2.655782	-0.003665	-0.002633	0.007904
B	-0.983708	0.054306	1.827988	-0.009236	0.028159	0.002800
B	3.436850	13.747295	4.538802	0.009250	-0.028242	-0.002791
B	5.591279	6.955106	1.355407	0.009251	0.028190	-0.002808
B	-3.138137	6.846495	5.011383	-0.009244	-0.028251	0.002787
Si	0.631772	3.486686	4.508512	0.023200	-0.001097	-0.015676
Si	1.821370	10.314915	1.858278	-0.023193	0.001103	0.015685
Si	-0.333059	10.387486	5.041673	-0.023195	-0.001094	0.015687
Si	2.786201	3.414115	1.325117	0.023168	0.001113	-0.015672
O	0.061445	3.072947	3.041906	-0.023607	-0.031717	0.015376
O	2.391697	10.728653	3.324884	0.023622	0.031765	-0.015395
O	4.546126	9.973747	0.141489	0.023629	-0.031750	-0.015391
O	-2.092984	3.827853	6.225301	-0.023611	0.031760	0.015387
O	2.197450	3.933608	4.519003	0.015941	0.008794	0.015832
O	0.255692	9.867992	1.847787	-0.015939	-0.008766	-0.015827
O	-1.898737	10.834409	5.031182	-0.015932	0.008810	-0.015843
O	4.351879	2.967192	1.335608	0.015932	-0.008735	0.015813
O	-0.212316	4.798696	5.055280	0.004616	-0.021476	0.001846
O	2.665458	9.002905	1.311510	-0.004591	0.021498	-0.001840
O	0.511030	11.699496	4.494905	-0.004611	-0.021488	-0.001857
O	1.942113	2.102105	1.871885	0.004588	0.021484	0.001836
O	0.525580	2.169271	5.472081	-0.014163	0.021867	0.007815
O	1.927562	11.632329	0.894709	0.014151	-0.021865	-0.007811
O	-0.226867	9.070071	4.078104	0.014159	0.021877	-0.007814
O	2.680009	4.731529	2.288686	-0.014163	-0.021839	0.007804

O	0.058846	0.698526	2.444964	-0.007682	0.026300	0.002114
O	2.394296	13.103075	3.921826	0.007683	-0.026350	-0.002112
O	4.548725	7.599326	0.738431	0.007691	0.026324	-0.002117
O	-2.095583	6.202275	5.628359	-0.007677	-0.026348	0.002117
O	-2.459230	13.184059	5.445139	0.012243	-0.010126	0.009774
O	4.912372	0.617542	0.921651	-0.012192	0.010093	-0.009772
O	2.757943	6.283259	4.105046	-0.012233	-0.010128	-0.009785
O	-0.304801	7.518342	2.261744	0.012214	0.010106	0.009770
O	-0.175430	2.374756	0.744070	0.006829	-0.020395	-0.009819
O	2.628573	11.426844	5.622720	-0.006840	0.020430	0.009821
O	4.783002	9.275557	2.439325	-0.006830	-0.020404	0.009822
O	-2.329859	4.526044	3.927465	0.006831	0.020431	-0.009816
O	-1.223866	12.517207	2.155216	0.009331	0.034817	0.016444
O	3.677009	1.284394	4.211574	-0.009343	-0.034913	-0.016435
O	5.831438	5.616407	1.028179	-0.009331	0.034851	-0.016446
O	-3.378295	8.185194	5.338611	0.009341	-0.034924	0.016428
H	-0.637445	12.195109	2.878812	0.029759	0.038574	0.000245
H	3.090587	1.606491	3.487978	-0.029803	-0.038674	-0.000208
H	5.245016	5.294309	0.304583	-0.029789	0.038592	-0.000215
H	-2.791874	8.507292	6.062207	0.029778	-0.038682	0.000219

111 f = 12.338532 THz 77.525286 2PiTHz 411.569130 cm-1 51.028087 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.087038	0.031821	0.084367
Li	-1.316675	4.156264	2.365404	0.086993	-0.032065	-0.084372
Li	-3.471104	2.744536	5.548798	-0.087077	-0.031872	0.084436
Li	5.924247	11.057064	0.817991	0.086994	0.031933	-0.084309
Na	2.049025	6.784862	1.629696	-0.002220	0.002481	-0.001578
Na	0.404117	7.016739	4.737094	0.002218	-0.002492	0.001563
Na	2.558546	13.685662	1.553699	-0.002213	-0.002450	-0.001550
Na	-0.105403	0.115939	4.813091	0.002225	0.002522	0.001588
B	4.155007	8.978944	1.168663	0.012206	0.003004	0.001065
B	-1.701865	4.822656	5.198127	-0.012207	-0.002968	-0.001055
B	0.452564	2.078144	2.014732	0.012234	-0.002993	0.001070
B	2.000578	11.723457	4.352058	-0.012191	0.002980	-0.001043

B	-2.733891	11.746082	5.839177	0.012036	0.013419	0.010646
B	5.187034	2.055518	0.527613	-0.012064	-0.013477	-0.010654
B	3.032605	4.845282	3.711007	0.012038	-0.013448	0.010648
B	-0.579463	8.956318	2.655782	-0.012063	0.013443	-0.010646
B	-0.983708	0.054306	1.827988	-0.003795	0.039507	0.002143
B	3.436850	13.747295	4.538802	0.003797	-0.039465	-0.002198
B	5.591279	6.955106	1.355407	-0.003794	-0.039422	0.002159
B	-3.138137	6.846495	5.011383	0.003804	0.039508	-0.002177
Si	0.631772	3.486686	4.508512	-0.024798	0.000639	-0.013374
Si	1.821370	10.314915	1.858278	0.024762	-0.000694	0.013431
Si	-0.333059	10.387486	5.041673	-0.024789	-0.000685	-0.013383
Si	2.786201	3.414115	1.325117	0.024782	0.000652	0.013404
O	0.061445	3.072947	3.041906	-0.013743	-0.018708	-0.003179
O	2.391697	10.728653	3.324884	0.013866	0.018744	0.003156
O	4.546126	9.973747	0.141489	-0.013755	0.018677	-0.003184
O	-2.092984	3.827853	6.225301	0.013824	-0.018734	0.003165
O	2.197450	3.933608	4.519003	-0.011855	-0.020893	-0.010859
O	0.255692	9.867992	1.847787	0.011852	0.020774	0.010802
O	-1.898737	10.834409	5.031182	-0.011863	0.020839	-0.010883
O	4.351879	2.967192	1.335608	0.011847	-0.020855	0.010801
O	-0.212316	4.798696	5.055280	-0.008361	0.001354	0.003251
O	2.665458	9.002905	1.311510	0.008376	-0.001334	-0.003270
O	0.511030	11.699496	4.494905	-0.008336	-0.001367	0.003322
O	1.942113	2.102105	1.871885	0.008402	0.001340	-0.003201
O	0.525580	2.169271	5.472081	0.012102	-0.008311	-0.016316
O	1.927562	11.632329	0.894709	-0.012177	0.008215	0.016303
O	-0.226867	9.070071	4.078104	0.012141	0.008264	-0.016317
O	2.680009	4.731529	2.288686	-0.012149	-0.008280	0.016307
O	0.058846	0.698526	2.444964	0.006863	0.020782	0.001790
O	2.394296	13.103075	3.921826	-0.006847	-0.020767	-0.001843
O	4.548725	7.599326	0.738431	0.006851	-0.020731	0.001806
O	-2.095583	6.202275	5.628359	-0.006854	0.020794	-0.001802
O	-2.459230	13.184059	5.445139	0.017074	-0.007027	0.008405
O	4.912372	0.617542	0.921651	-0.017122	0.007041	-0.008429
O	2.757943	6.283259	4.105046	0.017114	0.007057	0.008394
O	-0.304801	7.518342	2.261744	-0.017079	-0.006992	-0.008441

O	-0.175430	2.374756	0.744070	-0.013299	-0.013901	0.011147
O	2.628573	11.426844	5.622720	0.013284	0.013906	-0.011114
O	4.783002	9.275557	2.439325	-0.013309	0.013901	0.011150
O	-2.329859	4.526044	3.927465	0.013286	-0.013880	-0.011127
O	-1.223866	12.517207	2.155216	0.010859	0.048832	0.002946
O	3.677009	1.284394	4.211574	-0.010858	-0.048755	-0.002992
O	5.831438	5.616407	1.028179	0.010857	-0.048724	0.002983
O	-3.378295	8.185194	5.338611	-0.010851	0.048816	-0.002965
H	-0.637445	12.195109	2.878812	0.026985	0.038994	-0.015995
H	3.090587	1.606491	3.487978	-0.027016	-0.038902	0.015978
H	5.245016	5.294309	0.304583	0.026985	-0.038883	-0.015954
H	-2.791874	8.507292	6.062207	-0.027004	0.038963	0.016005

112 f = 12.168188 THz 76.454982 2PiTHz 405.887060 cm-1 50.323600
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.022703	-0.056034	0.030212
Li	-1.316675	4.156264	2.365404	-0.022778	-0.055951	0.030194
Li	-3.471104	2.744536	5.548798	-0.022635	0.055990	0.030051
Li	5.924247	11.057064	0.817991	-0.022866	0.056038	0.030391
Na	2.049025	6.784862	1.629696	0.002568	-0.017286	0.004716
Na	0.404117	7.016739	4.737094	0.002575	-0.017233	0.004654
Na	2.558546	13.685662	1.553699	0.002583	0.017299	0.004667
Na	-0.105403	0.115939	4.813091	0.002563	0.017239	0.004706
B	4.155007	8.978944	1.168663	0.006604	0.006883	0.008193
B	-1.701865	4.822656	5.198127	0.006627	0.006873	0.008185
B	0.452564	2.078144	2.014732	0.006603	-0.006879	0.008182
B	2.000578	11.723457	4.352058	0.006627	-0.006862	0.008213
B	-2.733891	11.746082	5.839177	-0.013411	-0.009975	-0.002755
B	5.187034	2.055518	0.527613	-0.013374	-0.009910	-0.002719
B	3.032605	4.845282	3.711007	-0.013396	0.009950	-0.002737
B	-0.579463	8.956318	2.655782	-0.013386	0.009923	-0.002738
B	-0.983708	0.054306	1.827988	0.005527	-0.020608	-0.015086
B	3.436850	13.747295	4.538802	0.005522	-0.020562	-0.015110
B	5.591279	6.955106	1.355407	0.005532	0.020635	-0.015106
B	-3.138137	6.846495	5.011383	0.005507	0.020546	-0.015091

Si	0.631772	3.486686	4.508512	-0.013302	-0.004783	0.025122
Si	1.821370	10.314915	1.858278	-0.013355	-0.004764	0.025163
Si	-0.333059	10.387486	5.041673	-0.013287	0.004754	0.025143
Si	2.786201	3.414115	1.325117	-0.013353	0.004762	0.025120
O	0.061445	3.072947	3.041906	0.051379	0.030965	-0.011002
O	2.391697	10.728653	3.324884	0.051378	0.030987	-0.010985
O	4.546126	9.973747	0.141489	0.051411	-0.030993	-0.010998
O	-2.092984	3.827853	6.225301	0.051343	-0.030953	-0.010992
O	2.197450	3.933608	4.519003	-0.003805	-0.035816	-0.043418
O	0.255692	9.867992	1.847787	-0.003801	-0.035952	-0.043493
O	-1.898737	10.834409	5.031182	-0.003766	0.035899	-0.043503
O	4.351879	2.967192	1.335608	-0.003833	0.035861	-0.043446
O	-0.212316	4.798696	5.055280	0.016163	0.015969	0.020389
O	2.665458	9.002905	1.311510	0.016155	0.016008	0.020407
O	0.511030	11.699496	4.494905	0.016181	-0.015992	0.020418
O	1.942113	2.102105	1.871885	0.016150	-0.015989	0.020419
O	0.525580	2.169271	5.472081	-0.023133	-0.024795	-0.006600
O	1.927562	11.632329	0.894709	-0.023177	-0.024855	-0.006641
O	-0.226867	9.070071	4.078104	-0.023160	0.024804	-0.006618
O	2.680009	4.731529	2.288686	-0.023091	0.024810	-0.006628
O	0.058846	0.698526	2.444964	0.003128	-0.014372	-0.013779
O	2.394296	13.103075	3.921826	0.003150	-0.014332	-0.013822
O	4.548725	7.599326	0.738431	0.003127	0.014371	-0.013805
O	-2.095583	6.202275	5.628359	0.003142	0.014337	-0.013799
O	-2.459230	13.184059	5.445139	0.003523	-0.019301	-0.016361
O	4.912372	0.617542	0.921651	0.003547	-0.019251	-0.016265
O	2.757943	6.283259	4.105046	0.003488	0.019270	-0.016302
O	-0.304801	7.518342	2.261744	0.003574	0.019291	-0.016333
O	-0.175430	2.374756	0.744070	-0.013334	0.002623	0.015269
O	2.628573	11.426844	5.622720	-0.013389	0.002593	0.015326
O	4.783002	9.275557	2.439325	-0.013357	-0.002597	0.015287
O	-2.329859	4.526044	3.927465	-0.013358	-0.002587	0.015293
O	-1.223866	12.517207	2.155216	-0.001384	-0.017674	-0.003654
O	3.677009	1.284394	4.211574	-0.001379	-0.017582	-0.003566
O	5.831438	5.616407	1.028179	-0.001372	0.017677	-0.003567
O	-3.378295	8.185194	5.338611	-0.001370	0.017588	-0.003618

H	-0.637445	12.195109	2.878812	-0.029163	-0.010712	0.022766
H	3.090587	1.606491	3.487978	-0.029011	-0.010634	0.022728
H	5.245016	5.294309	0.304583	-0.029018	0.010702	0.022753
H	-2.791874	8.507292	6.062207	-0.029072	0.010633	0.022736

113 f = 12.044616 THz 75.678557 2PiTHz 401.765144 cm-1 49.812547 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.046630	-0.003025	-0.085929
Li	-1.316675	4.156264	2.365404	-0.046691	0.002928	0.085981
Li	-3.471104	2.744536	5.548798	-0.046758	-0.002894	0.086026
Li	5.924247	11.057064	0.817991	0.046645	0.003028	-0.085901
Na	2.049025	6.784862	1.629696	0.001578	-0.001367	0.002626
Na	0.404117	7.016739	4.737094	-0.001567	0.001339	-0.002562
Na	2.558546	13.685662	1.553699	-0.001568	-0.001335	-0.002563
Na	-0.105403	0.115939	4.813091	0.001581	0.001386	0.002631
B	4.155007	8.978944	1.168663	0.003186	0.000367	-0.009724
B	-1.701865	4.822656	5.198127	-0.003157	-0.000353	0.009733
B	0.452564	2.078144	2.014732	-0.003163	0.000358	0.009746
B	2.000578	11.723457	4.352058	0.003165	-0.000391	-0.009724
B	-2.733891	11.746082	5.839177	0.012017	0.001925	0.001871
B	5.187034	2.055518	0.527613	-0.012060	-0.001937	-0.001882
B	3.032605	4.845282	3.711007	-0.012053	0.001932	-0.001880
B	-0.579463	8.956318	2.655782	0.012030	-0.001907	0.001874
B	-0.983708	0.054306	1.827988	-0.001698	-0.021142	-0.013538
B	3.436850	13.747295	4.538802	0.001708	0.021119	0.013503
B	5.591279	6.955106	1.355407	0.001693	-0.021126	0.013496
B	-3.138137	6.846495	5.011383	-0.001698	0.021152	-0.013538
Si	0.631772	3.486686	4.508512	0.000398	0.002914	0.013151
Si	1.821370	10.314915	1.858278	-0.000411	-0.002938	-0.013124
Si	-0.333059	10.387486	5.041673	-0.000433	0.002931	-0.013100
Si	2.786201	3.414115	1.325117	0.000409	-0.002942	0.013145
O	0.061445	3.072947	3.041906	0.025101	0.027637	-0.005132
O	2.391697	10.728653	3.324884	-0.025015	-0.027598	0.005107
O	4.546126	9.973747	0.141489	-0.025008	0.027590	0.005120
O	-2.092984	3.827853	6.225301	0.025091	-0.027640	-0.005131

O	2.197450	3.933608	4.519003	0.014347	-0.048830	-0.032399
O	0.255692	9.867992	1.847787	-0.014353	0.048798	0.032362
O	-1.898737	10.834409	5.031182	-0.014364	-0.048768	0.032343
O	4.351879	2.967192	1.335608	0.014357	0.048843	-0.032438
O	-0.212316	4.798696	5.055280	0.010896	0.011718	0.010076
O	2.665458	9.002905	1.311510	-0.010856	-0.011707	-0.010053
O	0.511030	11.699496	4.494905	-0.010878	0.011690	-0.010061
O	1.942113	2.102105	1.871885	0.010907	-0.011726	0.010130
O	0.525580	2.169271	5.472081	-0.016173	-0.007243	-0.003782
O	1.927562	11.632329	0.894709	0.016098	0.007203	0.003767
O	-0.226867	9.070071	4.078104	0.016130	-0.007196	0.003772
O	2.680009	4.731529	2.288686	-0.016124	0.007213	-0.003779
O	0.058846	0.698526	2.444964	0.003183	-0.009259	-0.026594
O	2.394296	13.103075	3.921826	-0.003169	0.009220	0.026574
O	4.548725	7.599326	0.738431	-0.003181	-0.009250	0.026540
O	-2.095583	6.202275	5.628359	0.003190	0.009272	-0.026594
O	-2.459230	13.184059	5.445139	-0.003938	0.025832	0.031633
O	4.912372	0.617542	0.921651	0.003943	-0.025844	-0.031662
O	2.757943	6.283259	4.105046	0.003936	0.025850	-0.031658
O	-0.304801	7.518342	2.261744	-0.003972	-0.025808	0.031618
O	-0.175430	2.374756	0.744070	-0.019153	0.005747	0.022021
O	2.628573	11.426844	5.622720	0.019116	-0.005744	-0.021985
O	4.783002	9.275557	2.439325	0.019128	0.005734	-0.021984
O	-2.329859	4.526044	3.927465	-0.019138	-0.005715	0.022005
O	-1.223866	12.517207	2.155216	-0.000150	-0.010055	0.034004
O	3.677009	1.284394	4.211574	0.000162	0.010037	-0.034036
O	5.831438	5.616407	1.028179	0.000166	-0.010054	-0.034006
O	-3.378295	8.185194	5.338611	-0.000155	0.010065	0.034016
H	-0.637445	12.195109	2.878812	0.045355	-0.003408	0.001021
H	3.090587	1.606491	3.487978	-0.045409	0.003405	-0.000991
H	5.245016	5.294309	0.304583	-0.045383	-0.003435	-0.000971
H	-2.791874	8.507292	6.062207	0.045365	0.003410	0.001022

114 f = 11.908810 THz 74.825258 2PiTHz 397.235122 cm-1 49.250896 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.040306	0.079317	-0.068015
Li	-1.316675	4.156264	2.365404	0.040427	0.079516	-0.068134
Li	-3.471104	2.744536	5.548798	-0.040399	0.079417	0.068112
Li	5.924247	11.057064	0.817991	-0.040349	0.079434	0.068055
Na	2.049025	6.784862	1.629696	-0.001041	0.012160	-0.000371
Na	0.404117	7.016739	4.737094	-0.001025	0.012076	-0.000335
Na	2.558546	13.685662	1.553699	0.001031	0.012126	0.000343
Na	-0.105403	0.115939	4.813091	0.001035	0.012103	0.000362
B	4.155007	8.978944	1.168663	0.010618	0.000729	-0.011571
B	-1.701865	4.822656	5.198127	0.010622	0.000738	-0.011594
B	0.452564	2.078144	2.014732	-0.010637	0.000738	0.011600
B	2.000578	11.723457	4.352058	-0.010600	0.000726	0.011561
B	-2.733891	11.746082	5.839177	-0.013959	-0.008682	0.001353
B	5.187034	2.055518	0.527613	-0.013999	-0.008645	0.001348
B	3.032605	4.845282	3.711007	0.014013	-0.008663	-0.001346
B	-0.579463	8.956318	2.655782	0.013949	-0.008663	-0.001351
B	-0.983708	0.054306	1.827988	0.023941	0.002821	0.004408
B	3.436850	13.747295	4.538802	0.023938	0.002796	0.004390
B	5.591279	6.955106	1.355407	-0.023945	0.002790	-0.004397
B	-3.138137	6.846495	5.011383	-0.023941	0.002790	-0.004407
Si	0.631772	3.486686	4.508512	-0.003144	-0.013755	-0.008979
Si	1.821370	10.314915	1.858278	-0.003186	-0.013687	-0.008979
Si	-0.333059	10.387486	5.041673	0.003191	-0.013639	0.008984
Si	2.786201	3.414115	1.325117	0.003158	-0.013777	0.008958
O	0.061445	3.072947	3.041906	-0.009406	0.022433	-0.017515
O	2.391697	10.728653	3.324884	-0.009440	0.022462	-0.017519
O	4.546126	9.973747	0.141489	0.009459	0.022462	0.017507
O	-2.092984	3.827853	6.225301	0.009359	0.022469	0.017535
O	2.197450	3.933608	4.519003	0.003613	-0.009056	0.010454
O	0.255692	9.867992	1.847787	0.003588	-0.009100	0.010303
O	-1.898737	10.834409	5.031182	-0.003590	-0.009096	-0.010299
O	4.351879	2.967192	1.335608	-0.003608	-0.009090	-0.010412
O	-0.212316	4.798696	5.055280	0.015357	-0.002583	-0.002501
O	2.665458	9.002905	1.311510	0.015434	-0.002534	-0.002213
O	0.511030	11.699496	4.494905	-0.015415	-0.002491	0.002243
O	1.942113	2.102105	1.871885	-0.015384	-0.002585	0.002459

O	0.525580	2.169271	5.472081	-0.020931	-0.020166	-0.011595
O	1.927562	11.632329	0.894709	-0.020719	-0.020123	-0.011603
O	-0.226867	9.070071	4.078104	0.020682	-0.020092	0.011610
O	2.680009	4.731529	2.288686	0.020982	-0.020202	0.011599
O	0.058846	0.698526	2.444964	0.031917	-0.022204	0.018920
O	2.394296	13.103075	3.921826	0.031906	-0.022223	0.018934
O	4.548725	7.599326	0.738431	-0.031920	-0.022229	-0.018923
O	-2.095583	6.202275	5.628359	-0.031915	-0.022209	-0.018904
O	-2.459230	13.184059	5.445139	0.021019	0.009763	0.018257
O	4.912372	0.617542	0.921651	0.021053	0.009805	0.018278
O	2.757943	6.283259	4.105046	-0.021060	0.009774	-0.018264
O	-0.304801	7.518342	2.261744	-0.021016	0.009771	-0.018282
O	-0.175430	2.374756	0.744070	-0.020456	0.001544	0.017877
O	2.628573	11.426844	5.622720	-0.020422	0.001376	0.017833
O	4.783002	9.275557	2.439325	0.020425	0.001411	-0.017849
O	-2.329859	4.526044	3.927465	0.020461	0.001553	-0.017874
O	-1.223866	12.517207	2.155216	-0.017408	-0.002758	-0.046399
O	3.677009	1.284394	4.211574	-0.017413	-0.002790	-0.046416
O	5.831438	5.616407	1.028179	0.017390	-0.002800	0.046397
O	-3.378295	8.185194	5.338611	0.017415	-0.002785	0.046380
H	-0.637445	12.195109	2.878812	-0.072876	-0.027364	-0.011582
H	3.090587	1.606491	3.487978	-0.072914	-0.027387	-0.011573
H	5.245016	5.294309	0.304583	0.072904	-0.027392	0.011542
H	-2.791874	8.507292	6.062207	0.072886	-0.027383	0.011555

115 f = 11.803832 THz 74.165663 2PiTHz 393.733439 cm-1 48.816742 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.007347	0.016003	-0.001567
Li	-1.316675	4.156264	2.365404	-0.007343	0.015937	-0.001516
Li	-3.471104	2.744536	5.548798	0.007361	0.015961	0.001539
Li	5.924247	11.057064	0.817991	0.007318	0.016012	0.001557
Na	2.049025	6.784862	1.629696	0.003244	-0.018607	0.004925
Na	0.404117	7.016739	4.737094	0.003221	-0.018473	0.004832
Na	2.558546	13.685662	1.553699	-0.003227	-0.018537	-0.004840
Na	-0.105403	0.115939	4.813091	-0.003237	-0.018530	-0.004912

B	4.155007	8.978944	1.168663	-0.000159	-0.002000	0.005543
B	-1.701865	4.822656	5.198127	-0.000186	-0.002048	0.005582
B	0.452564	2.078144	2.014732	0.000186	-0.002039	-0.005587
B	2.000578	11.723457	4.352058	0.000157	-0.002021	-0.005527
B	-2.733891	11.746082	5.839177	0.006916	-0.003667	0.000052
B	5.187034	2.055518	0.527613	0.006958	-0.003711	0.000063
B	3.032605	4.845282	3.711007	-0.006978	-0.003696	-0.000060
B	-0.579463	8.956318	2.655782	-0.006904	-0.003684	-0.000057
B	-0.983708	0.054306	1.827988	0.004544	-0.008227	0.005787
B	3.436850	13.747295	4.538802	0.004539	-0.008196	0.005798
B	5.591279	6.955106	1.355407	-0.004545	-0.008203	-0.005796
B	-3.138137	6.846495	5.011383	-0.004544	-0.008199	-0.005802
Si	0.631772	3.486686	4.508512	-0.008569	0.030927	-0.008905
Si	1.821370	10.314915	1.858278	-0.008500	0.030784	-0.008847
Si	-0.333059	10.387486	5.041673	0.008493	0.030732	0.008841
Si	2.786201	3.414115	1.325117	0.008560	0.030953	0.008931
O	0.061445	3.072947	3.041906	-0.022242	0.014878	-0.003863
O	2.391697	10.728653	3.324884	-0.022150	0.014823	-0.003832
O	4.546126	9.973747	0.141489	0.022145	0.014837	0.003842
O	-2.092984	3.827853	6.225301	0.022283	0.014846	0.003852
O	2.197450	3.933608	4.519003	-0.001224	-0.005987	-0.029322
O	0.255692	9.867992	1.847787	-0.001193	-0.005915	-0.029074
O	-1.898737	10.834409	5.031182	0.001193	-0.005930	0.029072
O	4.351879	2.967192	1.335608	0.001222	-0.005947	0.029290
O	-0.212316	4.798696	5.055280	0.018715	0.021435	0.060173
O	2.665458	9.002905	1.311510	0.018629	0.021340	0.059799
O	0.511030	11.699496	4.494905	-0.018630	0.021298	-0.059797
O	1.942113	2.102105	1.871885	-0.018704	0.021440	-0.060159
O	0.525580	2.169271	5.472081	0.061375	0.021079	-0.008607
O	1.927562	11.632329	0.894709	0.060915	0.020964	-0.008569
O	-0.226867	9.070071	4.078104	-0.060901	0.020918	0.008569
O	2.680009	4.731529	2.288686	-0.061397	0.021125	0.008600
O	0.058846	0.698526	2.444964	0.013103	-0.016930	0.012457
O	2.394296	13.103075	3.921826	0.013106	-0.016908	0.012410
O	4.548725	7.599326	0.738431	-0.013086	-0.016882	-0.012420
O	-2.095583	6.202275	5.628359	-0.013118	-0.016933	-0.012474

O	-2.459230	13.184059	5.445139	0.002858	-0.006905	0.003836
O	4.912372	0.617542	0.921651	0.002816	-0.006984	0.003796
O	2.757943	6.283259	4.105046	-0.002811	-0.006951	-0.003824
O	-0.304801	7.518342	2.261744	-0.002872	-0.006930	-0.003813
O	-0.175430	2.374756	0.744070	0.003108	-0.039036	-0.003136
O	2.628573	11.426844	5.622720	0.003080	-0.038757	-0.003107
O	4.783002	9.275557	2.439325	-0.003067	-0.038751	0.003118
O	-2.329859	4.526044	3.927465	-0.003132	-0.039059	0.003146
O	-1.223866	12.517207	2.155216	-0.011306	-0.012476	-0.006835
O	3.677009	1.284394	4.211574	-0.011308	-0.012438	-0.006836
O	5.831438	5.616407	1.028179	0.011315	-0.012447	0.006843
O	-3.378295	8.185194	5.338611	0.011302	-0.012450	0.006841
H	-0.637445	12.195109	2.878812	-0.017554	-0.018259	-0.002555
H	3.090587	1.606491	3.487978	-0.017555	-0.018217	-0.002546
H	5.245016	5.294309	0.304583	0.017570	-0.018236	0.002549
H	-2.791874	8.507292	6.062207	0.017533	-0.018235	0.002576

116 f = 11.758801 THz 73.882726 2PiTHz 392.231372 cm-1 48.630510 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.018035	-0.012802	0.026145
Li	-1.316675	4.156264	2.365404	0.017744	0.012685	-0.025703
Li	-3.471104	2.744536	5.548798	-0.017832	0.012754	0.025799
Li	5.924247	11.057064	0.817991	0.017899	-0.012866	-0.025963
Na	2.049025	6.784862	1.629696	-0.004053	0.009531	-0.004538
Na	0.404117	7.016739	4.737094	0.004079	-0.009682	0.004543
Na	2.558546	13.685662	1.553699	-0.004084	-0.009717	-0.004549
Na	-0.105403	0.115939	4.813091	0.004053	0.009530	0.004536
B	4.155007	8.978944	1.168663	-0.002904	-0.006068	0.010929
B	-1.701865	4.822656	5.198127	0.002879	0.006070	-0.010811
B	0.452564	2.078144	2.014732	-0.002862	0.006069	0.010822
B	2.000578	11.723457	4.352058	0.002898	-0.006080	-0.010899
B	-2.733891	11.746082	5.839177	0.011314	-0.002353	0.000511
B	5.187034	2.055518	0.527613	-0.011212	0.002340	-0.000507
B	3.032605	4.845282	3.711007	0.011204	0.002364	0.000505
B	-0.579463	8.956318	2.655782	-0.011327	-0.002354	-0.000509

B	-0.983708	0.054306	1.827988	-0.000327	0.006439	0.003797
B	3.436850	13.747295	4.538802	0.000280	-0.006505	-0.003809
B	5.591279	6.955106	1.355407	-0.000257	-0.006534	0.003773
B	-3.138137	6.846495	5.011383	0.000354	0.006402	-0.003814
Si	0.631772	3.486686	4.508512	0.005764	-0.028472	0.006213
Si	1.821370	10.314915	1.858278	-0.005781	0.028704	-0.006217
Si	-0.333059	10.387486	5.041673	0.005795	0.028690	0.006209
Si	2.786201	3.414115	1.325117	-0.005748	-0.028430	-0.006217
O	0.061445	3.072947	3.041906	0.015122	-0.002308	-0.000923
O	2.391697	10.728653	3.324884	-0.015213	0.002344	0.000972
O	4.546126	9.973747	0.141489	0.015204	0.002343	-0.000964
O	-2.092984	3.827853	6.225301	-0.015117	-0.002308	0.000918
O	2.197450	3.933608	4.519003	0.002542	0.005008	0.034490
O	0.255692	9.867992	1.847787	-0.002559	-0.005015	-0.034727
O	-1.898737	10.834409	5.031182	0.002578	-0.004989	0.034719
O	4.351879	2.967192	1.335608	-0.002544	0.005001	-0.034486
O	-0.212316	4.798696	5.055280	-0.013543	-0.016017	-0.059485
O	2.665458	9.002905	1.311510	0.013623	0.016165	0.059852
O	0.511030	11.699496	4.494905	-0.013634	0.016160	-0.059892
O	1.942113	2.102105	1.871885	0.013547	-0.015969	0.059485
O	0.525580	2.169271	5.472081	-0.068617	-0.024187	0.003350
O	1.927562	11.632329	0.894709	0.069094	0.024382	-0.003355
O	-0.226867	9.070071	4.078104	-0.069081	0.024363	0.003353
O	2.680009	4.731529	2.288686	0.068593	-0.024163	-0.003348
O	0.058846	0.698526	2.444964	0.000762	0.007444	-0.005703
O	2.394296	13.103075	3.921826	-0.000798	-0.007475	0.005714
O	4.548725	7.599326	0.738431	0.000832	-0.007455	-0.005709
O	-2.095583	6.202275	5.628359	-0.000749	0.007434	0.005749
O	-2.459230	13.184059	5.445139	-0.007380	-0.008783	-0.002693
O	4.912372	0.617542	0.921651	0.007331	0.008686	0.002609
O	2.757943	6.283259	4.105046	-0.007310	0.008672	-0.002631
O	-0.304801	7.518342	2.261744	0.007387	-0.008786	0.002649
O	-0.175430	2.374756	0.744070	-0.010296	0.041939	0.010705
O	2.628573	11.426844	5.622720	0.010381	-0.042223	-0.010784
O	4.783002	9.275557	2.439325	-0.010411	-0.042184	0.010836
O	-2.329859	4.526044	3.927465	0.010289	0.041991	-0.010698

O	-1.223866	12.517207	2.155216	-0.004121	0.008937	0.002421
O	3.677009	1.284394	4.211574	0.004105	-0.009002	-0.002321
O	5.831438	5.616407	1.028179	-0.004094	-0.009047	0.002305
O	-3.378295	8.185194	5.338611	0.004108	0.008895	-0.002481
H	-0.637445	12.195109	2.878812	0.000840	0.005883	-0.001419
H	3.090587	1.606491	3.487978	-0.000700	-0.005908	0.001425
H	5.245016	5.294309	0.304583	0.000729	-0.005952	-0.001451
H	-2.791874	8.507292	6.062207	-0.000900	0.005864	0.001391

117 f = 11.497788 THz 72.242734 2PiTHz 383.524921 cm-1 47.551047 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.080430	0.008298	-0.104383
Li	-1.316675	4.156264	2.365404	0.080263	0.010487	-0.103688
Li	-3.471104	2.744536	5.548798	0.080156	-0.010441	-0.103633
Li	5.924247	11.057064	0.817991	0.080483	-0.008288	-0.104377
Na	2.049025	6.784862	1.629696	-0.000322	0.000014	0.001380
Na	0.404117	7.016739	4.737094	-0.000252	-0.000276	0.001457
Na	2.558546	13.685662	1.553699	-0.000257	0.000265	0.001450
Na	-0.105403	0.115939	4.813091	-0.000315	0.000012	0.001389
B	4.155007	8.978944	1.168663	-0.006526	-0.001447	-0.006976
B	-1.701865	4.822656	5.198127	-0.006813	-0.001465	-0.006907
B	0.452564	2.078144	2.014732	-0.006816	0.001466	-0.006881
B	2.000578	11.723457	4.352058	-0.006529	0.001445	-0.006993
B	-2.733891	11.746082	5.839177	0.006274	0.005307	-0.004929
B	5.187034	2.055518	0.527613	0.006271	0.005497	-0.004853
B	3.032605	4.845282	3.711007	0.006302	-0.005513	-0.004840
B	-0.579463	8.956318	2.655782	0.006257	-0.005302	-0.004942
B	-0.983708	0.054306	1.827988	-0.012783	-0.023807	0.018801
B	3.436850	13.747295	4.538802	-0.012734	-0.023898	0.018976
B	5.591279	6.955106	1.355407	-0.012759	0.023892	0.018957
B	-3.138137	6.846495	5.011383	-0.012767	0.023811	0.018809
Si	0.631772	3.486686	4.508512	-0.012026	0.018104	0.009485
Si	1.821370	10.314915	1.858278	-0.012204	0.017790	0.009703
Si	-0.333059	10.387486	5.041673	-0.012210	-0.017772	0.009730
Si	2.786201	3.414115	1.325117	-0.012012	-0.018137	0.009456

O	0.061445	3.072947	3.041906	0.007402	0.004604	0.002696
O	2.391697	10.728653	3.324884	0.007968	0.004803	0.002523
O	4.546126	9.973747	0.141489	0.007989	-0.004781	0.002547
O	-2.092984	3.827853	6.225301	0.007380	-0.004621	0.002680
O	2.197450	3.933608	4.519003	-0.008083	0.002178	-0.016726
O	0.255692	9.867992	1.847787	-0.008290	0.002091	-0.017152
O	-1.898737	10.834409	5.031182	-0.008307	-0.002108	-0.017107
O	4.351879	2.967192	1.335608	-0.008061	-0.002154	-0.016795
O	-0.212316	4.798696	5.055280	-0.001699	0.024115	0.010545
O	2.665458	9.002905	1.311510	-0.001350	0.024021	0.011196
O	0.511030	11.699496	4.494905	-0.001378	-0.024014	0.011129
O	1.942113	2.102105	1.871885	-0.001676	-0.024123	0.010622
O	0.525580	2.169271	5.472081	0.004380	-0.001258	-0.006378
O	1.927562	11.632329	0.894709	0.003792	-0.001675	-0.006389
O	-0.226867	9.070071	4.078104	0.003710	0.001700	-0.006386
O	2.680009	4.731529	2.288686	0.004497	0.001213	-0.006375
O	0.058846	0.698526	2.444964	-0.007978	-0.002877	-0.014611
O	2.394296	13.103075	3.921826	-0.008114	-0.002717	-0.014313
O	4.548725	7.599326	0.738431	-0.008141	0.002701	-0.014330
O	-2.095583	6.202275	5.628359	-0.007963	0.002884	-0.014604
O	-2.459230	13.184059	5.445139	-0.007313	-0.002887	0.025914
O	4.912372	0.617542	0.921651	-0.007529	-0.002982	0.025746
O	2.757943	6.283259	4.105046	-0.007514	0.002959	0.025781
O	-0.304801	7.518342	2.261744	-0.007331	0.002912	0.025860
O	-0.175430	2.374756	0.744070	0.004932	0.043365	-0.010702
O	2.628573	11.426844	5.622720	0.005137	0.043455	-0.010990
O	4.783002	9.275557	2.439325	0.005125	-0.043492	-0.010976
O	-2.329859	4.526044	3.927465	0.004962	-0.043326	-0.010726
O	-1.223866	12.517207	2.155216	0.002289	-0.030208	0.030216
O	3.677009	1.284394	4.211574	0.002026	-0.030333	0.030035
O	5.831438	5.616407	1.028179	0.002028	0.030316	0.030064
O	-3.378295	8.185194	5.338611	0.002283	0.030217	0.030201
H	-0.637445	12.195109	2.878812	0.017827	-0.029259	0.017685
H	3.090587	1.606491	3.487978	0.017342	-0.029549	0.017619
H	5.245016	5.294309	0.304583	0.017388	0.029503	0.017628
H	-2.791874	8.507292	6.062207	0.017823	0.029285	0.017656

118 f = 11.484098 THz 72.156717 2PiTHz 383.068269 cm-1 47.494429
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.011922	-0.119920	-0.037851
Li	-1.316675	4.156264	2.365404	-0.013396	0.119834	0.039803
Li	-3.471104	2.744536	5.548798	-0.013405	-0.119878	0.039754
Li	5.924247	11.057064	0.817991	0.011979	0.119836	-0.037906
Na	2.049025	6.784862	1.629696	-0.004423	0.015471	-0.002976
Na	0.404117	7.016739	4.737094	0.004439	-0.015437	0.002934
Na	2.558546	13.685662	1.553699	0.004436	0.015448	0.002929
Na	-0.105403	0.115939	4.813091	-0.004420	-0.015448	-0.002974
B	4.155007	8.978944	1.168663	0.015617	0.000808	-0.005052
B	-1.701865	4.822656	5.198127	-0.015516	-0.000811	0.005193
B	0.452564	2.078144	2.014732	-0.015510	0.000809	0.005187
B	2.000578	11.723457	4.352058	0.015621	-0.000826	-0.005068
B	-2.733891	11.746082	5.839177	-0.001596	-0.011532	-0.005514
B	5.187034	2.055518	0.527613	0.001488	0.011448	0.005605
B	3.032605	4.845282	3.711007	0.001486	-0.011442	0.005604
B	-0.579463	8.956318	2.655782	-0.001612	0.011535	-0.005503
B	-0.983708	0.054306	1.827988	-0.001306	0.005821	-0.008362
B	3.436850	13.747295	4.538802	0.001519	-0.005433	0.008024
B	5.591279	6.955106	1.355407	0.001543	0.005395	0.008024
B	-3.138137	6.846495	5.011383	-0.001276	-0.005847	-0.008361
Si	0.631772	3.486686	4.508512	0.010266	0.018956	-0.013305
Si	1.821370	10.314915	1.858278	-0.010039	-0.019234	0.013142
Si	-0.333059	10.387486	5.041673	-0.010038	0.019298	0.013135
Si	2.786201	3.414115	1.325117	0.010258	-0.018934	-0.013318
O	0.061445	3.072947	3.041906	-0.032046	-0.009994	0.008652
O	2.391697	10.728653	3.324884	0.031893	0.009936	-0.008694
O	4.546126	9.973747	0.141489	0.031907	-0.009953	-0.008716
O	-2.092984	3.827853	6.225301	-0.032074	0.009983	0.008639
O	2.197450	3.933608	4.519003	0.012441	0.004108	0.021208
O	0.255692	9.867992	1.847787	-0.012285	-0.004135	-0.020897
O	-1.898737	10.834409	5.031182	-0.012282	0.004153	-0.020877
O	4.351879	2.967192	1.335608	0.012444	-0.004088	0.021209

O	-0.212316	4.798696	5.055280	-0.017774	0.005931	-0.032507
O	2.665458	9.002905	1.311510	0.017782	-0.006347	0.032327
O	0.511030	11.699496	4.494905	0.017771	0.006380	0.032247
O	1.942113	2.102105	1.871885	-0.017759	-0.005925	-0.032500
O	0.525580	2.169271	5.472081	0.039630	0.025451	0.001291
O	1.927562	11.632329	0.894709	-0.039635	-0.025390	-0.001176
O	-0.226867	9.070071	4.078104	-0.039707	0.025452	-0.001181
O	2.680009	4.731529	2.288686	0.039614	-0.025428	0.001281
O	0.058846	0.698526	2.444964	0.009281	-0.009388	-0.014747
O	2.394296	13.103075	3.921826	-0.009155	0.009431	0.014996
O	4.548725	7.599326	0.738431	-0.009125	-0.009446	0.014991
O	-2.095583	6.202275	5.628359	0.009323	0.009402	-0.014732
O	-2.459230	13.184059	5.445139	0.011551	0.002906	0.005269
O	4.912372	0.617542	0.921651	-0.011419	-0.002890	-0.005756
O	2.757943	6.283259	4.105046	-0.011401	0.002860	-0.005730
O	-0.304801	7.518342	2.261744	0.011566	-0.002939	0.005290
O	-0.175430	2.374756	0.744070	-0.009507	-0.007319	0.015174
O	2.628573	11.426844	5.622720	0.009426	0.006515	-0.014994
O	4.783002	9.275557	2.439325	0.009399	-0.006579	-0.014963
O	-2.329859	4.526044	3.927465	-0.009519	0.007326	0.015187
O	-1.223866	12.517207	2.155216	0.014336	0.006965	0.007394
O	3.677009	1.284394	4.211574	-0.014381	-0.006461	-0.007873
O	5.831438	5.616407	1.028179	-0.014383	0.006422	-0.007916
O	-3.378295	8.185194	5.338611	0.014324	-0.006986	0.007334
H	-0.637445	12.195109	2.878812	0.024717	0.014204	0.001429
H	3.090587	1.606491	3.487978	-0.024984	-0.013681	-0.001713
H	5.245016	5.294309	0.304583	-0.025026	0.013667	-0.001734
H	-2.791874	8.507292	6.062207	0.024644	-0.014186	0.001398

119 f = 11.243610 THz 70.645682 2PiTHz 375.046432 cm-1 46.499848
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.019451	0.127958	0.041562
Li	-1.316675	4.156264	2.365404	-0.019371	0.127861	0.041522
Li	-3.471104	2.744536	5.548798	-0.019487	-0.127845	0.041529
Li	5.924247	11.057064	0.817991	-0.019400	-0.127923	0.041586

Na	2.049025	6.784862	1.629696	-0.001711	0.005100	-0.001801
Na	0.404117	7.016739	4.737094	-0.001721	0.005103	-0.001810
Na	2.558546	13.685662	1.553699	-0.001720	-0.005107	-0.001808
Na	-0.105403	0.115939	4.813091	-0.001710	-0.005084	-0.001801
B	4.155007	8.978944	1.168663	-0.012719	-0.010192	0.005355
B	-1.701865	4.822656	5.198127	-0.012698	-0.010193	0.005354
B	0.452564	2.078144	2.014732	-0.012699	0.010188	0.005365
B	2.000578	11.723457	4.352058	-0.012714	0.010204	0.005352
B	-2.733891	11.746082	5.839177	-0.001754	0.010570	0.011507
B	5.187034	2.055518	0.527613	-0.001772	0.010555	0.011488
B	3.032605	4.845282	3.711007	-0.001759	-0.010565	0.011496
B	-0.579463	8.956318	2.655782	-0.001769	-0.010572	0.011497
B	-0.983708	0.054306	1.827988	0.008315	-0.027108	-0.005891
B	3.436850	13.747295	4.538802	0.008329	-0.027097	-0.005868
B	5.591279	6.955106	1.355407	0.008305	0.027106	-0.005890
B	-3.138137	6.846495	5.011383	0.008337	0.027109	-0.005865
Si	0.631772	3.486686	4.508512	0.000617	0.004999	-0.005446
Si	1.821370	10.314915	1.858278	0.000652	0.004976	-0.005474
Si	-0.333059	10.387486	5.041673	0.000651	-0.005006	-0.005473
Si	2.786201	3.414115	1.325117	0.000641	-0.004981	-0.005464
O	0.061445	3.072947	3.041906	-0.003901	0.034003	-0.015042
O	2.391697	10.728653	3.324884	-0.003943	0.033996	-0.015050
O	4.546126	9.973747	0.141489	-0.003938	-0.033979	-0.015033
O	-2.092984	3.827853	6.225301	-0.003910	-0.034024	-0.015065
O	2.197450	3.933608	4.519003	0.008664	-0.021865	0.002479
O	0.255692	9.867992	1.847787	0.008701	-0.021893	0.002502
O	-1.898737	10.834409	5.031182	0.008689	0.021860	0.002505
O	4.351879	2.967192	1.335608	0.008693	0.021894	0.002471
O	-0.212316	4.798696	5.055280	-0.010286	0.004221	-0.020521
O	2.665458	9.002905	1.311510	-0.010304	0.004190	-0.020580
O	0.511030	11.699496	4.494905	-0.010309	-0.004205	-0.020584
O	1.942113	2.102105	1.871885	-0.010277	-0.004203	-0.020521
O	0.525580	2.169271	5.472081	0.022679	0.001338	-0.002948
O	1.927562	11.632329	0.894709	0.022708	0.001354	-0.002930
O	-0.226867	9.070071	4.078104	0.022715	-0.001378	-0.002935
O	2.680009	4.731529	2.288686	0.022677	-0.001337	-0.002942

O	0.058846	0.698526	2.444964	0.012029	-0.017255	-0.012529
O	2.394296	13.103075	3.921826	0.012048	-0.017258	-0.012524
O	4.548725	7.599326	0.738431	0.012022	0.017253	-0.012534
O	-2.095583	6.202275	5.628359	0.012058	0.017263	-0.012525
O	-2.459230	13.184059	5.445139	0.015737	-0.011277	-0.006316
O	4.912372	0.617542	0.921651	0.015720	-0.011310	-0.006368
O	2.757943	6.283259	4.105046	0.015749	0.011268	-0.006303
O	-0.304801	7.518342	2.261744	0.015703	0.011316	-0.006370
O	-0.175430	2.374756	0.744070	-0.017448	0.021552	0.023373
O	2.628573	11.426844	5.622720	-0.017445	0.021588	0.023372
O	4.783002	9.275557	2.439325	-0.017458	-0.021561	0.023378
O	-2.329859	4.526044	3.927465	-0.017429	-0.021575	0.023357
O	-1.223866	12.517207	2.155216	-0.013257	-0.024506	0.017038
O	3.677009	1.284394	4.211574	-0.013264	-0.024509	0.017004
O	5.831438	5.616407	1.028179	-0.013231	0.024508	0.017053
O	-3.378295	8.185194	5.338611	-0.013277	0.024515	0.017011
H	-0.637445	12.195109	2.878812	-0.006875	-0.015189	0.016715
H	3.090587	1.606491	3.487978	-0.006906	-0.015240	0.016675
H	5.245016	5.294309	0.304583	-0.006819	0.015187	0.016706
H	-2.791874	8.507292	6.062207	-0.006898	0.015241	0.016670

120 f = 10.936499 THz 68.716049 2PiTHz 364.802326 cm-1 45.229740 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.053943	0.107410	-0.041801
Li	-1.316675	4.156264	2.365404	-0.054176	-0.107334	0.042310
Li	-3.471104	2.744536	5.548798	0.053853	-0.107448	-0.041713
Li	5.924247	11.057064	0.817991	-0.054082	0.107480	0.042200
Na	2.049025	6.784862	1.629696	-0.000993	0.000940	-0.000018
Na	0.404117	7.016739	4.737094	0.001001	-0.000828	-0.000030
Na	2.558546	13.685662	1.553699	-0.000989	-0.000982	0.000021
Na	-0.105403	0.115939	4.813091	0.001010	0.000881	0.000036
B	4.155007	8.978944	1.168663	0.010474	-0.000579	0.004793
B	-1.701865	4.822656	5.198127	-0.010477	0.000695	-0.004741
B	0.452564	2.078144	2.014732	0.010471	0.000635	0.004778
B	2.000578	11.723457	4.352058	-0.010507	-0.000706	-0.004731

B	-2.733891	11.746082	5.839177	-0.003330	-0.001967	0.007108
B	5.187034	2.055518	0.527613	0.003330	0.002082	-0.007253
B	3.032605	4.845282	3.711007	-0.003364	0.001968	0.007124
B	-0.579463	8.956318	2.655782	0.003328	-0.002130	-0.007282
B	-0.983708	0.054306	1.827988	-0.000563	0.030178	-0.010985
B	3.436850	13.747295	4.538802	0.000370	-0.030128	0.010687
B	5.591279	6.955106	1.355407	-0.000617	-0.030198	-0.010989
B	-3.138137	6.846495	5.011383	0.000393	0.030097	0.010678
Si	0.631772	3.486686	4.508512	-0.000297	0.001779	0.023568
Si	1.821370	10.314915	1.858278	0.000305	-0.001329	-0.023572
Si	-0.333059	10.387486	5.041673	-0.000271	-0.001826	0.023542
Si	2.786201	3.414115	1.325117	0.000357	0.001395	-0.023644
O	0.061445	3.072947	3.041906	0.002355	-0.030584	0.028164
O	2.391697	10.728653	3.324884	-0.002574	0.030520	-0.027992
O	4.546126	9.973747	0.141489	0.002401	0.030665	0.028184
O	-2.092984	3.827853	6.225301	-0.002542	-0.030571	-0.028075
O	2.197450	3.933608	4.519003	0.000810	-0.006742	0.011342
O	0.255692	9.867992	1.847787	-0.000637	0.006602	-0.011384
O	-1.898737	10.834409	5.031182	0.000843	0.006779	0.011263
O	4.351879	2.967192	1.335608	-0.000610	-0.006628	-0.011338
O	-0.212316	4.798696	5.055280	-0.007335	0.001077	0.007068
O	2.665458	9.002905	1.311510	0.007490	-0.000795	-0.006562
O	0.511030	11.699496	4.494905	-0.007358	-0.001129	0.006970
O	1.942113	2.102105	1.871885	0.007453	0.000915	-0.006640
O	0.525580	2.169271	5.472081	-0.029897	-0.001411	0.010355
O	1.927562	11.632329	0.894709	0.029920	0.001805	-0.010387
O	-0.226867	9.070071	4.078104	-0.029900	0.001349	0.010350
O	2.680009	4.731529	2.288686	0.029899	-0.001799	-0.010387
O	0.058846	0.698526	2.444964	-0.008428	0.010035	0.014680
O	2.394296	13.103075	3.921826	0.008427	-0.010066	-0.015272
O	4.548725	7.599326	0.738431	-0.008469	-0.010033	0.014666
O	-2.095583	6.202275	5.628359	0.008468	0.010067	-0.015268
O	-2.459230	13.184059	5.445139	0.007039	-0.014502	0.006630
O	4.912372	0.617542	0.921651	-0.007568	0.014498	-0.006721
O	2.757943	6.283259	4.105046	0.007062	0.014505	0.006603
O	-0.304801	7.518342	2.261744	-0.007614	-0.014523	-0.006727

O	-0.175430	2.374756	0.744070	0.013733	-0.022692	-0.009907
O	2.628573	11.426844	5.622720	-0.013674	0.022547	0.009880
O	4.783002	9.275557	2.439325	0.013747	0.022643	-0.009896
O	-2.329859	4.526044	3.927465	-0.013692	-0.022514	0.009884
O	-1.223866	12.517207	2.155216	0.007623	0.025236	-0.037680
O	3.677009	1.284394	4.211574	-0.007197	-0.025122	0.038036
O	5.831438	5.616407	1.028179	0.007684	-0.025265	-0.037587
O	-3.378295	8.185194	5.338611	-0.007248	0.025080	0.038011
H	-0.637445	12.195109	2.878812	-0.011512	0.021651	-0.023558
H	3.090587	1.606491	3.487978	0.012391	-0.021034	0.023784
H	5.245016	5.294309	0.304583	-0.011341	-0.021747	-0.023522
H	-2.791874	8.507292	6.062207	0.012267	0.021051	0.023788

121 f = 10.924359 THz 68.639769 2PiTHz 364.397366 cm-1 45.179531 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.021144	0.000430	0.039156
Li	-1.316675	4.156264	2.365404	-0.020657	0.001753	0.038517
Li	-3.471104	2.744536	5.548798	-0.021132	-0.000422	0.039156
Li	5.924247	11.057064	0.817991	-0.020677	-0.001726	0.038519
Na	2.049025	6.784862	1.629696	0.001229	0.009505	0.000186
Na	0.404117	7.016739	4.737094	0.001215	0.009449	0.000194
Na	2.558546	13.685662	1.553699	0.001222	-0.009508	0.000173
Na	-0.105403	0.115939	4.813091	0.001225	-0.009432	0.000209
B	4.155007	8.978944	1.168663	-0.000913	0.008117	0.003937
B	-1.701865	4.822656	5.198127	-0.000775	0.008131	0.003981
B	0.452564	2.078144	2.014732	-0.000908	-0.008100	0.003930
B	2.000578	11.723457	4.352058	-0.000776	-0.008130	0.004000
B	-2.733891	11.746082	5.839177	-0.001310	0.011640	-0.012129
B	5.187034	2.055518	0.527613	-0.001333	0.011582	-0.012039
B	3.032605	4.845282	3.711007	-0.001321	-0.011640	-0.012128
B	-0.579463	8.956318	2.655782	-0.001326	-0.011593	-0.012054
B	-0.983708	0.054306	1.827988	-0.017023	0.005929	-0.024780
B	3.436850	13.747295	4.538802	-0.017095	0.006260	-0.024984
B	5.591279	6.955106	1.355407	-0.017026	-0.005908	-0.024791
B	-3.138137	6.846495	5.011383	-0.017099	-0.006267	-0.024983

Si	0.631772	3.486686	4.508512	0.003164	0.037214	-0.004197
Si	1.821370	10.314915	1.858278	0.003153	0.037291	-0.003893
Si	-0.333059	10.387486	5.041673	0.003150	-0.037251	-0.004205
Si	2.786201	3.414115	1.325117	0.003167	-0.037278	-0.003899
O	0.061445	3.072947	3.041906	-0.013373	-0.003934	0.009904
O	2.391697	10.728653	3.324884	-0.013257	-0.004366	0.010282
O	4.546126	9.973747	0.141489	-0.013368	0.003926	0.009900
O	-2.092984	3.827853	6.225301	-0.013267	0.004392	0.010286
O	2.197450	3.933608	4.519003	0.016052	-0.010800	-0.003781
O	0.255692	9.867992	1.847787	0.016033	-0.010816	-0.003681
O	-1.898737	10.834409	5.031182	0.016056	0.010811	-0.003801
O	4.351879	2.967192	1.335608	0.016028	0.010785	-0.003660
O	-0.212316	4.798696	5.055280	0.010707	0.021221	0.036177
O	2.665458	9.002905	1.311510	0.010578	0.021243	0.036248
O	0.511030	11.699496	4.494905	0.010718	-0.021249	0.036220
O	1.942113	2.102105	1.871885	0.010575	-0.021222	0.036232
O	0.525580	2.169271	5.472081	0.001018	0.034971	-0.002890
O	1.927562	11.632329	0.894709	0.000634	0.035019	-0.002741
O	-0.226867	9.070071	4.078104	0.001006	-0.034998	-0.002900
O	2.680009	4.731529	2.288686	0.000644	-0.035024	-0.002737
O	0.058846	0.698526	2.444964	0.001337	-0.003949	-0.050086
O	2.394296	13.103075	3.921826	0.001128	-0.003810	-0.049959
O	4.548725	7.599326	0.738431	0.001338	0.003972	-0.050104
O	-2.095583	6.202275	5.628359	0.001121	0.003807	-0.049944
O	-2.459230	13.184059	5.445139	-0.044744	0.001919	-0.007195
O	4.912372	0.617542	0.921651	-0.044605	0.001812	-0.006985
O	2.757943	6.283259	4.105046	-0.044742	-0.001917	-0.007208
O	-0.304801	7.518342	2.261744	-0.044595	-0.001812	-0.006998
O	-0.175430	2.374756	0.744070	0.005150	-0.012229	-0.001959
O	2.628573	11.426844	5.622720	0.005313	-0.012506	-0.002062
O	4.783002	9.275557	2.439325	0.005155	0.012244	-0.001959
O	-2.329859	4.526044	3.927465	0.005305	0.012510	-0.002073
O	-1.223866	12.517207	2.155216	0.033848	0.011878	0.030546
O	3.677009	1.284394	4.211574	0.034018	0.012166	0.030191
O	5.831438	5.616407	1.028179	0.033836	-0.011861	0.030561
O	-3.378295	8.185194	5.338611	0.034018	-0.012170	0.030184

H	-0.637445	12.195109	2.878812	0.071359	0.051339	0.018453
H	3.090587	1.606491	3.487978	0.071417	0.051722	0.018243
H	5.245016	5.294309	0.304583	0.071388	-0.051328	0.018438
H	-2.791874	8.507292	6.062207	0.071377	-0.051727	0.018267

122 f = 10.867470 THz 68.282328 2PiTHz 362.499770 cm-1 44.944260 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.024508	-0.051454	-0.042148
Li	-1.316675	4.156264	2.365404	-0.024394	0.051519	0.042049
Li	-3.471104	2.744536	5.548798	-0.024290	-0.051284	0.042470
Li	5.924247	11.057064	0.817991	0.024175	0.051329	-0.042372
Na	2.049025	6.784862	1.629696	0.002380	-0.029781	0.007508
Na	0.404117	7.016739	4.737094	-0.002383	0.029669	-0.007419
Na	2.558546	13.685662	1.553699	-0.002388	-0.029838	-0.007459
Na	-0.105403	0.115939	4.813091	0.002383	0.029753	0.007532
B	4.155007	8.978944	1.168663	-0.004649	0.018126	0.006235
B	-1.701865	4.822656	5.198127	0.004647	-0.018134	-0.006276
B	0.452564	2.078144	2.014732	0.004622	0.018189	-0.006243
B	2.000578	11.723457	4.352058	-0.004622	-0.018174	0.006263
B	-2.733891	11.746082	5.839177	0.007524	0.015796	-0.010145
B	5.187034	2.055518	0.527613	-0.007562	-0.015811	0.010154
B	3.032605	4.845282	3.711007	-0.007550	0.015743	0.010162
B	-0.579463	8.956318	2.655782	0.007587	-0.015735	-0.010150
B	-0.983708	0.054306	1.827988	0.019783	0.000973	0.000573
B	3.436850	13.747295	4.538802	-0.019780	-0.000954	-0.000596
B	5.591279	6.955106	1.355407	-0.019649	0.000989	-0.000447
B	-3.138137	6.846495	5.011383	0.019639	-0.000971	0.000471
Si	0.631772	3.486686	4.508512	0.008051	-0.036360	-0.007928
Si	1.821370	10.314915	1.858278	-0.008049	0.036343	0.007923
Si	-0.333059	10.387486	5.041673	-0.008046	-0.036315	0.007833
Si	2.786201	3.414115	1.325117	0.008068	0.036329	-0.007856
O	0.061445	3.072947	3.041906	-0.005219	0.026027	-0.020989
O	2.391697	10.728653	3.324884	0.005250	-0.026008	0.020980
O	4.546126	9.973747	0.141489	0.005106	0.025801	0.020841
O	-2.092984	3.827853	6.225301	-0.005086	-0.025815	-0.020868

O	2.197450	3.933608	4.519003	-0.000502	0.011520	0.027661
O	0.255692	9.867992	1.847787	0.000487	-0.011460	-0.027608
O	-1.898737	10.834409	5.031182	0.000567	0.011641	-0.027626
O	4.351879	2.967192	1.335608	-0.000557	-0.011640	0.027628
O	-0.212316	4.798696	5.055280	-0.004681	-0.048489	0.001449
O	2.665458	9.002905	1.311510	0.004652	0.048468	-0.001525
O	0.511030	11.699496	4.494905	0.004758	-0.048496	-0.001415
O	1.942113	2.102105	1.871885	-0.004750	0.048552	0.001476
O	0.525580	2.169271	5.472081	-0.009461	-0.026296	0.001584
O	1.927562	11.632329	0.894709	0.009407	0.026283	-0.001583
O	-0.226867	9.070071	4.078104	0.009568	-0.026203	-0.001671
O	2.680009	4.731529	2.288686	-0.009468	0.026208	0.001666
O	0.058846	0.698526	2.444964	0.012941	0.004381	0.011972
O	2.394296	13.103075	3.921826	-0.012940	-0.004373	-0.011985
O	4.548725	7.599326	0.738431	-0.012690	0.004461	-0.011952
O	-2.095583	6.202275	5.628359	0.012691	-0.004457	0.011953
O	-2.459230	13.184059	5.445139	-0.022475	0.012510	0.010481
O	4.912372	0.617542	0.921651	0.022448	-0.012521	-0.010493
O	2.757943	6.283259	4.105046	0.022377	0.012584	-0.010705
O	-0.304801	7.518342	2.261744	-0.022370	-0.012601	0.010742
O	-0.175430	2.374756	0.744070	-0.008817	-0.020866	-0.004758
O	2.628573	11.426844	5.622720	0.008770	0.020880	0.004797
O	4.783002	9.275557	2.439325	0.008787	-0.020881	0.004765
O	-2.329859	4.526044	3.927465	-0.008766	0.020883	-0.004800
O	-1.223866	12.517207	2.155216	-0.025074	0.001017	-0.028761
O	3.677009	1.284394	4.211574	0.025087	-0.001000	0.028728
O	5.831438	5.616407	1.028179	0.024904	0.001039	0.028652
O	-3.378295	8.185194	5.338611	-0.024964	-0.001019	-0.028670
H	-0.637445	12.195109	2.878812	-0.078213	-0.031633	-0.001633
H	3.090587	1.606491	3.487978	0.078222	0.031654	0.001602
H	5.245016	5.294309	0.304583	0.077930	-0.031359	0.001486
H	-2.791874	8.507292	6.062207	-0.078002	0.031402	-0.001505

123 f = 10.832638 THz 68.063473 2PiTHz 361.337907 cm-1 44.800207 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	0.061650	0.000680	0.047641
Li	-1.316675	4.156264	2.365404	-0.061433	-0.000534	-0.047799
Li	-3.471104	2.744536	5.548798	0.061684	-0.000397	0.047504
Li	5.924247	11.057064	0.817991	-0.061633	0.000318	-0.047553
Na	2.049025	6.784862	1.629696	-0.001819	0.016810	-0.007231
Na	0.404117	7.016739	4.737094	0.001830	-0.016800	0.007272
Na	2.558546	13.685662	1.553699	-0.001825	-0.016677	-0.007243
Na	-0.105403	0.115939	4.813091	0.001794	0.016641	0.007194
B	4.155007	8.978944	1.168663	-0.001586	-0.012391	0.001985
B	-1.701865	4.822656	5.198127	0.001563	0.012336	-0.001994
B	0.452564	2.078144	2.014732	-0.001613	0.012287	0.002018
B	2.000578	11.723457	4.352058	0.001599	-0.012269	-0.002011
B	-2.733891	11.746082	5.839177	-0.006431	0.012984	0.003923
B	5.187034	2.055518	0.527613	0.006431	-0.012981	-0.003904
B	3.032605	4.845282	3.711007	-0.006399	-0.013038	0.003884
B	-0.579463	8.956318	2.655782	0.006406	0.013076	-0.003848
B	-0.983708	0.054306	1.827988	0.027493	0.008599	0.022432
B	3.436850	13.747295	4.538802	-0.027444	-0.008650	-0.022376
B	5.591279	6.955106	1.355407	0.027617	-0.008605	0.022466
B	-3.138137	6.846495	5.011383	-0.027566	0.008665	-0.022378
Si	0.631772	3.486686	4.508512	-0.002703	-0.008095	-0.004825
Si	1.821370	10.314915	1.858278	0.002708	0.007992	0.004814
Si	-0.333059	10.387486	5.041673	-0.002690	0.008272	-0.004838
Si	2.786201	3.414115	1.325117	0.002658	-0.008176	0.004897
O	0.061445	3.072947	3.041906	-0.027135	0.029213	-0.013781
O	2.391697	10.728653	3.324884	0.027207	-0.029190	0.013734
O	4.546126	9.973747	0.141489	-0.027216	-0.029319	-0.013853
O	-2.092984	3.827853	6.225301	0.027210	0.029317	0.013870
O	2.197450	3.933608	4.519003	0.012322	-0.031469	0.008820
O	0.255692	9.867992	1.847787	-0.012346	0.031453	-0.008864
O	-1.898737	10.834409	5.031182	0.012306	0.031419	0.008964
O	4.351879	2.967192	1.335608	-0.012348	-0.031396	-0.008973
O	-0.212316	4.798696	5.055280	0.014566	0.008861	0.010427
O	2.665458	9.002905	1.311510	-0.014618	-0.008916	-0.010619
O	0.511030	11.699496	4.494905	0.014563	-0.008651	0.010489
O	1.942113	2.102105	1.871885	-0.014588	0.008656	-0.010572

O	0.525580	2.169271	5.472081	0.002718	-0.021663	-0.013308
O	1.927562	11.632329	0.894709	-0.002708	0.021578	0.013301
O	-0.226867	9.070071	4.078104	0.002635	0.021812	-0.013290
O	2.680009	4.731529	2.288686	-0.002639	-0.021671	0.013294
O	0.058846	0.698526	2.444964	0.045993	-0.009974	0.010808
O	2.394296	13.103075	3.921826	-0.046035	0.009990	-0.010661
O	4.548725	7.599326	0.738431	0.046084	0.009946	0.010906
O	-2.095583	6.202275	5.628359	-0.046100	-0.009968	-0.010756
O	-2.459230	13.184059	5.445139	-0.014840	-0.021179	-0.046382
O	4.912372	0.617542	0.921651	0.015008	0.021142	0.046343
O	2.757943	6.283259	4.105046	-0.015003	0.021120	-0.046305
O	-0.304801	7.518342	2.261744	0.015147	-0.021087	0.046323
O	-0.175430	2.374756	0.744070	0.001139	-0.003359	-0.003113
O	2.628573	11.426844	5.622720	-0.001176	0.003461	0.003156
O	4.783002	9.275557	2.439325	0.001113	0.003470	-0.003155
O	-2.329859	4.526044	3.927465	-0.001142	-0.003562	0.003164
O	-1.223866	12.517207	2.155216	-0.024755	0.005819	-0.030051
O	3.677009	1.284394	4.211574	0.024696	-0.005886	0.030019
O	5.831438	5.616407	1.028179	-0.024902	-0.005827	-0.030210
O	-3.378295	8.185194	5.338611	0.024801	0.005898	0.030163
H	-0.637445	12.195109	2.878812	-0.052758	-0.043765	-0.032497
H	3.090587	1.606491	3.487978	0.052620	0.043636	0.032507
H	5.245016	5.294309	0.304583	-0.053218	0.043962	-0.032503
H	-2.791874	8.507292	6.062207	0.053004	-0.043781	0.032501

124 f = 10.699877 THz 67.229309 2PiTHz 356.909461 cm-1 44.251149 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.095819	-0.052999	0.043573
Li	-1.316675	4.156264	2.365404	-0.095989	-0.053052	0.043663
Li	-3.471104	2.744536	5.548798	0.095908	-0.053142	-0.043626
Li	5.924247	11.057064	0.817991	0.095866	-0.052952	-0.043649
Na	2.049025	6.784862	1.629696	0.003949	0.005527	0.001936
Na	0.404117	7.016739	4.737094	0.003967	0.005549	0.001908
Na	2.558546	13.685662	1.553699	-0.003963	0.005559	-0.001902
Na	-0.105403	0.115939	4.813091	-0.003942	0.005522	-0.001932

B	4.155007	8.978944	1.168663	0.001180	0.008484	0.008126
B	-1.701865	4.822656	5.198127	0.001178	0.008470	0.008142
B	0.452564	2.078144	2.014732	-0.001166	0.008483	-0.008146
B	2.000578	11.723457	4.352058	-0.001191	0.008493	-0.008146
B	-2.733891	11.746082	5.839177	0.007906	0.004185	0.004689
B	5.187034	2.055518	0.527613	0.007899	0.004197	0.004706
B	3.032605	4.845282	3.711007	-0.007913	0.004226	-0.004684
B	-0.579463	8.956318	2.655782	-0.007913	0.004189	-0.004683
B	-0.983708	0.054306	1.827988	0.012887	0.002023	0.022883
B	3.436850	13.747295	4.538802	0.012844	0.001993	0.022885
B	5.591279	6.955106	1.355407	-0.012903	0.002007	-0.022889
B	-3.138137	6.846495	5.011383	-0.012850	0.002032	-0.022885
Si	0.631772	3.486686	4.508512	0.019468	-0.008101	-0.012122
Si	1.821370	10.314915	1.858278	0.019413	-0.008069	-0.012051
Si	-0.333059	10.387486	5.041673	-0.019405	-0.008077	0.012078
Si	2.786201	3.414115	1.325117	-0.019465	-0.008080	0.012105
O	0.061445	3.072947	3.041906	0.003324	0.022472	-0.018750
O	2.391697	10.728653	3.324884	0.003280	0.022403	-0.018654
O	4.546126	9.973747	0.141489	-0.003239	0.022394	0.018665
O	-2.092984	3.827853	6.225301	-0.003305	0.022392	0.018692
O	2.197450	3.933608	4.519003	0.026978	-0.029087	-0.010908
O	0.255692	9.867992	1.847787	0.026919	-0.029043	-0.010873
O	-1.898737	10.834409	5.031182	-0.026929	-0.029076	0.010885
O	4.351879	2.967192	1.335608	-0.026990	-0.029144	0.010969
O	-0.212316	4.798696	5.055280	0.007263	-0.009371	-0.009770
O	2.665458	9.002905	1.311510	0.007276	-0.009292	-0.009694
O	0.511030	11.699496	4.494905	-0.007285	-0.009297	0.009702
O	1.942113	2.102105	1.871885	-0.007265	-0.009329	0.009790
O	0.525580	2.169271	5.472081	0.003451	-0.003945	-0.002450
O	1.927562	11.632329	0.894709	0.003457	-0.003970	-0.002454
O	-0.226867	9.070071	4.078104	-0.003398	-0.003947	0.002444
O	2.680009	4.731529	2.288686	-0.003447	-0.003923	0.002445
O	0.058846	0.698526	2.444964	0.029000	-0.003909	0.005574
O	2.394296	13.103075	3.921826	0.028930	-0.003883	0.005555
O	4.548725	7.599326	0.738431	-0.028964	-0.003890	-0.005632
O	-2.095583	6.202275	5.628359	-0.028939	-0.003875	-0.005578

O	-2.459230	13.184059	5.445139	0.014116	0.026602	0.042291
O	4.912372	0.617542	0.921651	0.014142	0.026622	0.042318
O	2.757943	6.283259	4.105046	-0.014135	0.026639	-0.042299
O	-0.304801	7.518342	2.261744	-0.014199	0.026587	-0.042253
O	-0.175430	2.374756	0.744070	0.009063	0.018099	-0.012360
O	2.628573	11.426844	5.622720	0.009052	0.018138	-0.012361
O	4.783002	9.275557	2.439325	-0.009067	0.018079	0.012356
O	-2.329859	4.526044	3.927465	-0.009075	0.018157	0.012359
O	-1.223866	12.517207	2.155216	-0.023681	0.000596	-0.007469
O	3.677009	1.284394	4.211574	-0.023683	0.000572	-0.007404
O	5.831438	5.616407	1.028179	0.023679	0.000588	0.007441
O	-3.378295	8.185194	5.338611	0.023643	0.000605	0.007416
H	-0.637445	12.195109	2.878812	-0.048829	-0.030828	-0.002357
H	3.090587	1.606491	3.487978	-0.048783	-0.030819	-0.002317
H	5.245016	5.294309	0.304583	0.048863	-0.030834	0.002301
H	-2.791874	8.507292	6.062207	0.048735	-0.030766	0.002324

125 f = 10.549493 THz 66.284418 2PiTHz 351.893189 cm-1 43.629211 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.071418	-0.011373	-0.000317
Li	-1.316675	4.156264	2.365404	0.071283	0.011198	0.000299
Li	-3.471104	2.744536	5.548798	0.071414	-0.011489	0.000275
Li	5.924247	11.057064	0.817991	-0.071399	0.011339	-0.000220
Na	2.049025	6.784862	1.629696	0.002075	-0.016418	0.002725
Na	0.404117	7.016739	4.737094	-0.002070	0.016320	-0.002645
Na	2.558546	13.685662	1.553699	-0.002074	-0.016360	-0.002645
Na	-0.105403	0.115939	4.813091	0.002068	0.016296	0.002698
B	4.155007	8.978944	1.168663	0.014794	0.007165	0.004239
B	-1.701865	4.822656	5.198127	-0.014799	-0.007143	-0.004275
B	0.452564	2.078144	2.014732	-0.014759	0.007131	-0.004244
B	2.000578	11.723457	4.352058	0.014766	-0.007129	0.004284
B	-2.733891	11.746082	5.839177	0.000603	0.004558	0.005211
B	5.187034	2.055518	0.527613	-0.000633	-0.004575	-0.005201
B	3.032605	4.845282	3.711007	-0.000596	0.004591	-0.005199
B	-0.579463	8.956318	2.655782	0.000635	-0.004605	0.005242

B	-0.983708	0.054306	1.827988	-0.017141	-0.002584	-0.004073
B	3.436850	13.747295	4.538802	0.017188	0.002559	0.004100
B	5.591279	6.955106	1.355407	0.017162	-0.002606	0.004070
B	-3.138137	6.846495	5.011383	-0.017178	0.002615	-0.004080
Si	0.631772	3.486686	4.508512	0.013581	-0.025118	0.012360
Si	1.821370	10.314915	1.858278	-0.013572	0.025167	-0.012355
Si	-0.333059	10.387486	5.041673	-0.013538	-0.025117	-0.012430
Si	2.786201	3.414115	1.325117	0.013509	0.025161	0.012397
O	0.061445	3.072947	3.041906	-0.005868	-0.040461	0.028593
O	2.391697	10.728653	3.324884	0.005910	0.040517	-0.028607
O	4.546126	9.973747	0.141489	0.005961	-0.040488	-0.028675
O	-2.092984	3.827853	6.225301	-0.005952	0.040493	0.028632
O	2.197450	3.933608	4.519003	0.011397	-0.019929	-0.012645
O	0.255692	9.867992	1.847787	-0.011378	0.019960	0.012740
O	-1.898737	10.834409	5.031182	-0.011360	-0.019895	0.012586
O	4.351879	2.967192	1.335608	0.011305	0.019890	-0.012658
O	-0.212316	4.798696	5.055280	-0.011418	-0.017389	-0.032136
O	2.665458	9.002905	1.311510	0.011402	0.017478	0.031998
O	0.511030	11.699496	4.494905	0.011372	-0.017347	0.032012
O	1.942113	2.102105	1.871885	-0.011372	0.017414	-0.031958
O	0.525580	2.169271	5.472081	0.005816	-0.026097	0.000520
O	1.927562	11.632329	0.894709	-0.005897	0.026124	-0.000521
O	-0.226867	9.070071	4.078104	-0.005728	-0.026142	-0.000509
O	2.680009	4.731529	2.288686	0.005909	0.026162	0.000516
O	0.058846	0.698526	2.444964	-0.048500	0.024360	0.012993
O	2.394296	13.103075	3.921826	0.048592	-0.024423	-0.012979
O	4.548725	7.599326	0.738431	0.048556	0.024392	-0.013000
O	-2.095583	6.202275	5.628359	-0.048580	-0.024388	0.012988
O	-2.459230	13.184059	5.445139	0.000880	0.020679	0.031253
O	4.912372	0.617542	0.921651	-0.000860	-0.020659	-0.031182
O	2.757943	6.283259	4.105046	-0.000856	0.020696	-0.031233
O	-0.304801	7.518342	2.261744	0.000847	-0.020707	0.031234
O	-0.175430	2.374756	0.744070	-0.009217	0.018613	-0.003051
O	2.628573	11.426844	5.622720	0.009183	-0.018621	0.003097
O	4.783002	9.275557	2.439325	0.009224	0.018610	0.003079
O	-2.329859	4.526044	3.927465	-0.009221	-0.018645	-0.003065

O	-1.223866	12.517207	2.155216	0.015664	-0.004923	0.011289
O	3.677009	1.284394	4.211574	-0.015715	0.004899	-0.011324
O	5.831438	5.616407	1.028179	-0.015644	-0.004944	-0.011339
O	-3.378295	8.185194	5.338611	0.015658	0.004958	0.011307
H	-0.637445	12.195109	2.878812	0.032463	0.009790	0.004150
H	3.090587	1.606491	3.487978	-0.032568	-0.009865	-0.004168
H	5.245016	5.294309	0.304583	-0.032457	0.009778	-0.004189
H	-2.791874	8.507292	6.062207	0.032472	-0.009780	0.004168

126 f = 10.501030 THz 65.979918 2PiTHz 350.276651 cm-1 43.428785 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.019349	0.037212	-0.019978
Li	-1.316675	4.156264	2.365404	-0.019234	-0.037089	0.019804
Li	-3.471104	2.744536	5.548798	0.019083	-0.037127	-0.019912
Li	5.924247	11.057064	0.817991	-0.019246	0.037087	0.019903
Na	2.049025	6.784862	1.629696	0.000855	-0.020589	0.006685
Na	0.404117	7.016739	4.737094	-0.000864	0.020477	-0.006603
Na	2.558546	13.685662	1.553699	0.000868	0.020578	0.006603
Na	-0.105403	0.115939	4.813091	-0.000861	-0.020541	-0.006681
B	4.155007	8.978944	1.168663	0.011041	0.011885	-0.003949
B	-1.701865	4.822656	5.198127	-0.011030	-0.011876	0.003910
B	0.452564	2.078144	2.014732	0.011057	-0.011883	-0.003915
B	2.000578	11.723457	4.352058	-0.011066	0.011892	0.003942
B	-2.733891	11.746082	5.839177	0.002719	-0.017252	-0.011273
B	5.187034	2.055518	0.527613	-0.002720	0.017232	0.011265
B	3.032605	4.845282	3.711007	0.002721	0.017221	-0.011240
B	-0.579463	8.956318	2.655782	-0.002699	-0.017268	0.011281
B	-0.983708	0.054306	1.827988	0.001736	0.014660	-0.002220
B	3.436850	13.747295	4.538802	-0.001742	-0.014690	0.002209
B	5.591279	6.955106	1.355407	0.001734	-0.014674	-0.002180
B	-3.138137	6.846495	5.011383	-0.001711	0.014676	0.002239
Si	0.631772	3.486686	4.508512	0.028228	-0.007757	-0.033108
Si	1.821370	10.314915	1.858278	-0.028290	0.007829	0.033134
Si	-0.333059	10.387486	5.041673	0.028299	0.007846	-0.033156
Si	2.786201	3.414115	1.325117	-0.028260	-0.007854	0.033072

O	0.061445	3.072947	3.041906	0.029817	0.006481	-0.032243
O	2.391697	10.728653	3.324884	-0.029854	-0.006471	0.032277
O	4.546126	9.973747	0.141489	0.029801	-0.006411	-0.032257
O	-2.092984	3.827853	6.225301	-0.029797	0.006344	0.032157
O	2.197450	3.933608	4.519003	0.027819	-0.024966	-0.040223
O	0.255692	9.867992	1.847787	-0.027892	0.025072	0.040320
O	-1.898737	10.834409	5.031182	0.027898	0.025079	-0.040313
O	4.351879	2.967192	1.335608	-0.027857	-0.025069	0.040286
O	-0.212316	4.798696	5.055280	-0.013491	-0.031230	-0.040894
O	2.665458	9.002905	1.311510	0.013472	0.031316	0.040890
O	0.511030	11.699496	4.494905	-0.013513	0.031346	-0.040969
O	1.942113	2.102105	1.871885	0.013500	-0.031273	0.040989
O	0.525580	2.169271	5.472081	0.021838	0.018002	0.003272
O	1.927562	11.632329	0.894709	-0.021850	-0.017954	-0.003268
O	-0.226867	9.070071	4.078104	0.021879	-0.017971	0.003282
O	2.680009	4.731529	2.288686	-0.021808	0.017911	-0.003277
O	0.058846	0.698526	2.444964	0.011657	-0.001799	-0.005054
O	2.394296	13.103075	3.921826	-0.011662	0.001788	0.005039
O	4.548725	7.599326	0.738431	0.011615	0.001767	-0.004975
O	-2.095583	6.202275	5.628359	-0.011517	-0.001728	0.004971
O	-2.459230	13.184059	5.445139	0.006637	-0.018423	-0.012854
O	4.912372	0.617542	0.921651	-0.006677	0.018385	0.012843
O	2.757943	6.283259	4.105046	0.006625	0.018325	-0.012711
O	-0.304801	7.518342	2.261744	-0.006600	-0.018418	0.012841
O	-0.175430	2.374756	0.744070	0.006795	0.004331	0.001532
O	2.628573	11.426844	5.622720	-0.006795	-0.004376	-0.001518
O	4.783002	9.275557	2.439325	0.006800	-0.004406	0.001510
O	-2.329859	4.526044	3.927465	-0.006773	0.004358	-0.001541
O	-1.223866	12.517207	2.155216	0.014710	0.015224	-0.004023
O	3.677009	1.284394	4.211574	-0.014689	-0.015244	0.004057
O	5.831438	5.616407	1.028179	0.014676	-0.015232	-0.004035
O	-3.378295	8.185194	5.338611	-0.014751	0.015226	0.004029
H	-0.637445	12.195109	2.878812	0.023960	0.019184	-0.008553
H	3.090587	1.606491	3.487978	-0.023859	-0.019201	0.008524
H	5.245016	5.294309	0.304583	0.023868	-0.019153	-0.008536
H	-2.791874	8.507292	6.062207	-0.023967	0.019229	0.008514

127 f = 10.396500 THz 65.323135 2PiTHz 346.789898 cm-1 42.996483
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.054453	0.014155	0.027135
Li	-1.316675	4.156264	2.365404	0.054566	0.014199	0.027183
Li	-3.471104	2.744536	5.548798	0.054478	-0.014128	0.027173
Li	5.924247	11.057064	0.817991	0.054518	-0.014082	0.027136
Na	2.049025	6.784862	1.629696	-0.000634	0.001187	-0.000560
Na	0.404117	7.016739	4.737094	-0.000639	0.001225	-0.000556
Na	2.558546	13.685662	1.553699	-0.000644	-0.001194	-0.000550
Na	-0.105403	0.115939	4.813091	-0.000650	-0.001216	-0.000576
B	4.155007	8.978944	1.168663	-0.012596	0.004092	0.006145
B	-1.701865	4.822656	5.198127	-0.012622	0.004066	0.006153
B	0.452564	2.078144	2.014732	-0.012590	-0.004117	0.006118
B	2.000578	11.723457	4.352058	-0.012593	-0.004092	0.006109
B	-2.733891	11.746082	5.839177	0.006093	0.005531	-0.013044
B	5.187034	2.055518	0.527613	0.006077	0.005559	-0.013036
B	3.032605	4.845282	3.711007	0.006095	-0.005483	-0.013069
B	-0.579463	8.956318	2.655782	0.006062	-0.005509	-0.013059
B	-0.983708	0.054306	1.827988	-0.007951	-0.004748	-0.005127
B	3.436850	13.747295	4.538802	-0.007952	-0.004728	-0.005113
B	5.591279	6.955106	1.355407	-0.007966	0.004756	-0.005123
B	-3.138137	6.846495	5.011383	-0.007921	0.004755	-0.005100
Si	0.631772	3.486686	4.508512	0.005624	-0.010029	0.005096
Si	1.821370	10.314915	1.858278	0.005586	-0.010014	0.005136
Si	-0.333059	10.387486	5.041673	0.005566	0.009955	0.005196
Si	2.786201	3.414115	1.325117	0.005535	0.010011	0.005242
O	0.061445	3.072947	3.041906	-0.021814	-0.043845	0.028168
O	2.391697	10.728653	3.324884	-0.021847	-0.043807	0.028187
O	4.546126	9.973747	0.141489	-0.021827	0.043833	0.028250
O	-2.092984	3.827853	6.225301	-0.021917	0.043859	0.028299
O	2.197450	3.933608	4.519003	0.018860	-0.044656	-0.027631
O	0.255692	9.867992	1.847787	0.018818	-0.044617	-0.027580
O	-1.898737	10.834409	5.031182	0.018799	0.044563	-0.027503
O	4.351879	2.967192	1.335608	0.018787	0.044616	-0.027487

O	-0.212316	4.798696	5.055280	-0.003312	-0.000891	-0.017464
O	2.665458	9.002905	1.311510	-0.003275	-0.000857	-0.017350
O	0.511030	11.699496	4.494905	-0.003281	0.000784	-0.017357
O	1.942113	2.102105	1.871885	-0.003262	0.000767	-0.017338
O	0.525580	2.169271	5.472081	-0.019217	-0.002709	0.003717
O	1.927562	11.632329	0.894709	-0.019215	-0.002736	0.003707
O	-0.226867	9.070071	4.078104	-0.019297	0.002718	0.003716
O	2.680009	4.731529	2.288686	-0.019362	0.002781	0.003727
O	0.058846	0.698526	2.444964	-0.041339	0.017018	0.022011
O	2.394296	13.103075	3.921826	-0.041318	0.017033	0.021990
O	4.548725	7.599326	0.738431	-0.041337	-0.017011	0.022003
O	-2.095583	6.202275	5.628359	-0.041349	-0.017037	0.022087
O	-2.459230	13.184059	5.445139	0.021849	-0.017024	-0.044332
O	4.912372	0.617542	0.921651	0.021882	-0.017052	-0.044391
O	2.757943	6.283259	4.105046	0.021927	0.017071	-0.044385
O	-0.304801	7.518342	2.261744	0.021830	0.017073	-0.044376
O	-0.175430	2.374756	0.744070	0.002728	0.005804	-0.001380
O	2.628573	11.426844	5.622720	0.002738	0.005816	-0.001404
O	4.783002	9.275557	2.439325	0.002716	-0.005756	-0.001382
O	-2.329859	4.526044	3.927465	0.002725	-0.005756	-0.001394
O	-1.223866	12.517207	2.155216	0.017623	-0.003170	0.022340
O	3.677009	1.284394	4.211574	0.017606	-0.003159	0.022293
O	5.831438	5.616407	1.028179	0.017596	0.003179	0.022322
O	-3.378295	8.185194	5.338611	0.017567	0.003183	0.022263
H	-0.637445	12.195109	2.878812	0.017445	0.029588	0.038330
H	3.090587	1.606491	3.487978	0.017394	0.029586	0.038300
H	5.245016	5.294309	0.304583	0.017409	-0.029592	0.038326
H	-2.791874	8.507292	6.062207	0.017298	-0.029524	0.038297

128 f = 10.359792 THz 65.092492 2PiTHz 345.565452 cm-1 42.844671 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.036751	0.036536	-0.017823
Li	-1.316675	4.156264	2.365404	0.036800	0.036451	-0.017700
Li	-3.471104	2.744536	5.548798	-0.036862	0.036472	0.017634
Li	5.924247	11.057064	0.817991	-0.036950	0.036591	0.017776

Na	2.049025	6.784862	1.629696	0.004107	-0.006756	0.003721
Na	0.404117	7.016739	4.737094	0.004128	-0.006695	0.003715
Na	2.558546	13.685662	1.553699	-0.004128	-0.006727	-0.003717
Na	-0.105403	0.115939	4.813091	-0.004105	-0.006710	-0.003715
B	4.155007	8.978944	1.168663	-0.007467	-0.017316	0.006835
B	-1.701865	4.822656	5.198127	-0.007495	-0.017334	0.006845
B	0.452564	2.078144	2.014732	0.007509	-0.017323	-0.006859
B	2.000578	11.723457	4.352058	0.007511	-0.017310	-0.006843
B	-2.733891	11.746082	5.839177	-0.004438	0.020517	0.010218
B	5.187034	2.055518	0.527613	-0.004430	0.020536	0.010230
B	3.032605	4.845282	3.711007	0.004416	0.020545	-0.010205
B	-0.579463	8.956318	2.655782	0.004420	0.020533	-0.010185
B	-0.983708	0.054306	1.827988	-0.008133	0.003690	-0.011958
B	3.436850	13.747295	4.538802	-0.008076	0.003648	-0.011920
B	5.591279	6.955106	1.355407	0.008127	0.003639	0.011945
B	-3.138137	6.846495	5.011383	0.008131	0.003686	0.011959
Si	0.631772	3.486686	4.508512	0.020992	-0.007220	-0.041741
Si	1.821370	10.314915	1.858278	0.020965	-0.007180	-0.041758
Si	-0.333059	10.387486	5.041673	-0.020993	-0.007215	0.041741
Si	2.786201	3.414115	1.325117	-0.020996	-0.007242	0.041740
O	0.061445	3.072947	3.041906	0.021168	0.004249	-0.036382
O	2.391697	10.728653	3.324884	0.021152	0.004346	-0.036434
O	4.546126	9.973747	0.141489	-0.021085	0.004203	0.036340
O	-2.092984	3.827853	6.225301	-0.021117	0.004180	0.036343
O	2.197450	3.933608	4.519003	0.014080	-0.006058	-0.042291
O	0.255692	9.867992	1.847787	0.014070	-0.006032	-0.042227
O	-1.898737	10.834409	5.031182	-0.014129	-0.006148	0.042286
O	4.351879	2.967192	1.335608	-0.014111	-0.006133	0.042333
O	-0.212316	4.798696	5.055280	-0.013021	-0.034202	-0.032556
O	2.665458	9.002905	1.311510	-0.012988	-0.034152	-0.032517
O	0.511030	11.699496	4.494905	0.013005	-0.034170	0.032569
O	1.942113	2.102105	1.871885	0.013019	-0.034209	0.032572
O	0.525580	2.169271	5.472081	0.038173	0.022433	-0.000793
O	1.927562	11.632329	0.894709	0.038155	0.022437	-0.000831
O	-0.226867	9.070071	4.078104	-0.038125	0.022426	0.000817
O	2.680009	4.731529	2.288686	-0.038120	0.022432	0.000785

O	0.058846	0.698526	2.444964	-0.003093	-0.004415	-0.016281
O	2.394296	13.103075	3.921826	-0.002991	-0.004480	-0.016271
O	4.548725	7.599326	0.738431	0.003142	-0.004418	0.016226
O	-2.095583	6.202275	5.628359	0.003147	-0.004390	0.016226
O	-2.459230	13.184059	5.445139	-0.010172	0.004910	-0.007603
O	4.912372	0.617542	0.921651	-0.010226	0.004906	-0.007664
O	2.757943	6.283259	4.105046	0.010168	0.004885	0.007736
O	-0.304801	7.518342	2.261744	0.010144	0.004855	0.007739
O	-0.175430	2.374756	0.744070	-0.000117	0.009456	0.007357
O	2.628573	11.426844	5.622720	-0.000136	0.009430	0.007378
O	4.783002	9.275557	2.439325	0.000127	0.009446	-0.007361
O	-2.329859	4.526044	3.927465	0.000103	0.009453	-0.007354
O	-1.223866	12.517207	2.155216	0.019535	0.004075	0.012297
O	3.677009	1.284394	4.211574	0.019454	0.004035	0.012282
O	5.831438	5.616407	1.028179	-0.019512	0.004028	-0.012353
O	-3.378295	8.185194	5.338611	-0.019556	0.004075	-0.012327
H	-0.637445	12.195109	2.878812	0.043605	0.020695	0.000664
H	3.090587	1.606491	3.487978	0.043475	0.020567	0.000646
H	5.245016	5.294309	0.304583	-0.043577	0.020667	-0.000732
H	-2.791874	8.507292	6.062207	-0.043596	0.020743	-0.000741

129 f = 10.246088 THz 64.378070 2PiTHz 341.772698 cm-1 42.374429 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.010850	-0.003883	-0.016758
Li	-1.316675	4.156264	2.365404	-0.011033	0.004050	0.016934
Li	-3.471104	2.744536	5.548798	-0.010994	-0.003704	0.016695
Li	5.924247	11.057064	0.817991	0.010764	0.004164	-0.016863
Na	2.049025	6.784862	1.629696	0.002905	0.013356	-0.011210
Na	0.404117	7.016739	4.737094	-0.002990	-0.013157	0.010981
Na	2.558546	13.685662	1.553699	-0.002973	0.013330	0.011022
Na	-0.105403	0.115939	4.813091	0.002934	-0.013194	-0.011167
B	4.155007	8.978944	1.168663	-0.002705	-0.016402	-0.013199
B	-1.701865	4.822656	5.198127	0.002787	0.016508	0.013357
B	0.452564	2.078144	2.014732	0.002728	-0.016464	0.013224
B	2.000578	11.723457	4.352058	-0.002750	0.016424	-0.013260

B	-2.733891	11.746082	5.839177	-0.011346	-0.011607	0.000471
B	5.187034	2.055518	0.527613	0.011470	0.011708	-0.000424
B	3.032605	4.845282	3.711007	0.011344	-0.011652	-0.000467
B	-0.579463	8.956318	2.655782	-0.011407	0.011611	0.000458
B	-0.983708	0.054306	1.827988	0.026477	-0.000783	0.018847
B	3.436850	13.747295	4.538802	-0.026469	0.000854	-0.018777
B	5.591279	6.955106	1.355407	-0.026408	-0.000849	-0.018779
B	-3.138137	6.846495	5.011383	0.026526	0.000868	0.018833
Si	0.631772	3.486686	4.508512	-0.014867	0.000318	-0.012319
Si	1.821370	10.314915	1.858278	0.014713	-0.000374	0.012324
Si	-0.333059	10.387486	5.041673	0.014784	0.000277	0.012277
Si	2.786201	3.414115	1.325117	-0.014805	-0.000571	-0.012325
O	0.061445	3.072947	3.041906	-0.019054	-0.022685	0.000041
O	2.391697	10.728653	3.324884	0.018932	0.022562	-0.000011
O	4.546126	9.973747	0.141489	0.019038	-0.022660	-0.000077
O	-2.092984	3.827853	6.225301	-0.018900	0.022547	0.000014
O	2.197450	3.933608	4.519003	-0.002617	-0.029297	-0.023246
O	0.255692	9.867992	1.847787	0.002454	0.029237	0.023032
O	-1.898737	10.834409	5.031182	0.002567	-0.029200	0.023079
O	4.351879	2.967192	1.335608	-0.002506	0.029237	-0.023065
O	-0.212316	4.798696	5.055280	0.000302	0.019024	-0.030065
O	2.665458	9.002905	1.311510	-0.000225	-0.018980	0.030223
O	0.511030	11.699496	4.494905	-0.000272	0.018897	0.030009
O	1.942113	2.102105	1.871885	0.000230	-0.019273	-0.030351
O	0.525580	2.169271	5.472081	-0.023390	0.015947	0.007611
O	1.927562	11.632329	0.894709	0.023633	-0.016010	-0.007597
O	-0.226867	9.070071	4.078104	0.023473	0.015891	-0.007601
O	2.680009	4.731529	2.288686	-0.023640	-0.016177	0.007604
O	0.058846	0.698526	2.444964	0.005613	-0.007360	0.061938
O	2.394296	13.103075	3.921826	-0.005633	0.007401	-0.061854
O	4.548725	7.599326	0.738431	-0.005520	-0.007320	-0.061818
O	-2.095583	6.202275	5.628359	0.005727	0.007504	0.061980
O	-2.459230	13.184059	5.445139	-0.063917	-0.007417	0.010279
O	4.912372	0.617542	0.921651	0.063987	0.007574	-0.010169
O	2.757943	6.283259	4.105046	0.063993	-0.007465	-0.010209
O	-0.304801	7.518342	2.261744	-0.063878	0.007402	0.010311

O	-0.175430	2.374756	0.744070	0.009973	-0.006171	0.012161
O	2.628573	11.426844	5.622720	-0.009910	0.006358	-0.012140
O	4.783002	9.275557	2.439325	-0.009925	-0.006273	-0.012096
O	-2.329859	4.526044	3.927465	0.009915	0.006418	0.012262
O	-1.223866	12.517207	2.155216	-0.009775	-0.001344	-0.007928
O	3.677009	1.284394	4.211574	0.009834	0.001383	0.007858
O	5.831438	5.616407	1.028179	0.009782	-0.001382	0.007827
O	-3.378295	8.185194	5.338611	-0.009828	0.001412	-0.007876
H	-0.637445	12.195109	2.878812	-0.036794	-0.026811	0.001213
H	3.090587	1.606491	3.487978	0.036811	0.026756	-0.001277
H	5.245016	5.294309	0.304583	0.036723	-0.026740	-0.001299
H	-2.791874	8.507292	6.062207	-0.036844	0.026878	0.001257

130 f = 10.184432 THz 63.990675 2PiTHz 339.716080 cm-1 42.119441 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.004221	0.052472	0.032856
Li	-1.316675	4.156264	2.365404	-0.004050	0.052538	0.032721
Li	-3.471104	2.744536	5.548798	0.004128	0.052588	-0.032775
Li	5.924247	11.057064	0.817991	0.003894	0.052669	-0.032792
Na	2.049025	6.784862	1.629696	-0.003587	0.023651	-0.007214
Na	0.404117	7.016739	4.737094	-0.003594	0.023702	-0.007227
Na	2.558546	13.685662	1.553699	0.003586	0.023642	0.007144
Na	-0.105403	0.115939	4.813091	0.003551	0.023701	0.007264
B	4.155007	8.978944	1.168663	0.011288	0.008115	0.018433
B	-1.701865	4.822656	5.198127	0.011234	0.007986	0.018348
B	0.452564	2.078144	2.014732	-0.011262	0.008027	-0.018402
B	2.000578	11.723457	4.352058	-0.011234	0.007957	-0.018328
B	-2.733891	11.746082	5.839177	0.017425	0.005497	0.005249
B	5.187034	2.055518	0.527613	0.017320	0.005394	0.005211
B	3.032605	4.845282	3.711007	-0.017375	0.005448	-0.005206
B	-0.579463	8.956318	2.655782	-0.017332	0.005351	-0.005225
B	-0.983708	0.054306	1.827988	-0.008704	0.009956	0.003567
B	3.436850	13.747295	4.538802	-0.008545	0.009991	0.003713
B	5.591279	6.955106	1.355407	0.008737	0.009973	-0.003543
B	-3.138137	6.846495	5.011383	0.008559	0.009950	-0.003648

Si	0.631772	3.486686	4.508512	-0.011693	-0.034899	0.004601
Si	1.821370	10.314915	1.858278	-0.011855	-0.034870	0.004552
Si	-0.333059	10.387486	5.041673	0.011687	-0.035019	-0.004674
Si	2.786201	3.414115	1.325117	0.011763	-0.034888	-0.004538
O	0.061445	3.072947	3.041906	-0.025580	-0.019706	0.007604
O	2.391697	10.728653	3.324884	-0.025689	-0.019810	0.007612
O	4.546126	9.973747	0.141489	0.025615	-0.019716	-0.007665
O	-2.092984	3.827853	6.225301	0.025676	-0.019722	-0.007567
O	2.197450	3.933608	4.519003	-0.018750	-0.004416	-0.020435
O	0.255692	9.867992	1.847787	-0.018852	-0.004534	-0.020597
O	-1.898737	10.834409	5.031182	0.018765	-0.004393	0.020406
O	4.351879	2.967192	1.335608	0.018759	-0.004540	0.020516
O	-0.212316	4.798696	5.055280	0.012402	-0.031208	0.044287
O	2.665458	9.002905	1.311510	0.012419	-0.031042	0.044184
O	0.511030	11.699496	4.494905	-0.012407	-0.031338	-0.044426
O	1.942113	2.102105	1.871885	-0.012426	-0.031152	-0.044268
O	0.525580	2.169271	5.472081	0.031600	-0.034602	0.000996
O	1.927562	11.632329	0.894709	0.031482	-0.034478	0.001074
O	-0.226867	9.070071	4.078104	-0.031519	-0.034719	-0.001031
O	2.680009	4.731529	2.288686	-0.031431	-0.034517	-0.001031
O	0.058846	0.698526	2.444964	-0.018842	0.021568	-0.006250
O	2.394296	13.103075	3.921826	-0.018779	0.021558	-0.005892
O	4.548725	7.599326	0.738431	0.018930	0.021671	0.006287
O	-2.095583	6.202275	5.628359	0.018758	0.021541	0.006027
O	-2.459230	13.184059	5.445139	-0.000852	0.012907	0.005003
O	4.912372	0.617542	0.921651	-0.001226	0.012766	0.004971
O	2.757943	6.283259	4.105046	0.000919	0.012815	-0.004932
O	-0.304801	7.518342	2.261744	0.001236	0.012716	-0.004890
O	-0.175430	2.374756	0.744070	0.006537	0.035996	-0.014560
O	2.628573	11.426844	5.622720	0.006629	0.036044	-0.014477
O	4.783002	9.275557	2.439325	-0.006555	0.036014	0.014626
O	-2.329859	4.526044	3.927465	-0.006602	0.035969	0.014533
O	-1.223866	12.517207	2.155216	0.006170	0.007579	-0.004424
O	3.677009	1.284394	4.211574	0.006099	0.007605	-0.004479
O	5.831438	5.616407	1.028179	-0.006149	0.007608	0.004389
O	-3.378295	8.185194	5.338611	-0.006088	0.007591	0.004416

H	-0.637445	12.195109	2.878812	0.005109	0.004234	-0.003535
H	3.090587	1.606491	3.487978	0.004871	0.004108	-0.003530
H	5.245016	5.294309	0.304583	-0.005101	0.004313	0.003493
H	-2.791874	8.507292	6.062207	-0.004905	0.004136	0.003487

131 f = 10.114521 THz 63.551409 2PiTHz 337.384093 cm-1 41.830311 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.009267	0.039750	0.041026
Li	-1.316675	4.156264	2.365404	0.009321	-0.039827	-0.041042
Li	-3.471104	2.744536	5.548798	-0.009327	-0.039809	0.041088
Li	5.924247	11.057064	0.817991	0.009298	0.039805	-0.041023
Na	2.049025	6.784862	1.629696	0.002741	0.001280	-0.000817
Na	0.404117	7.016739	4.737094	-0.002715	-0.001315	0.000872
Na	2.558546	13.685662	1.553699	0.002730	-0.001283	-0.000837
Na	-0.105403	0.115939	4.813091	-0.002720	0.001239	0.000812
B	4.155007	8.978944	1.168663	0.009851	0.011097	0.015186
B	-1.701865	4.822656	5.198127	-0.009864	-0.011147	-0.015226
B	0.452564	2.078144	2.014732	0.009870	-0.011145	0.015236
B	2.000578	11.723457	4.352058	-0.009856	0.011160	-0.015237
B	-2.733891	11.746082	5.839177	0.017759	0.011716	0.008914
B	5.187034	2.055518	0.527613	-0.017816	-0.011727	-0.008905
B	3.032605	4.845282	3.711007	0.017813	-0.011725	0.008907
B	-0.579463	8.956318	2.655782	-0.017808	0.011770	-0.008909
B	-0.983708	0.054306	1.827988	0.008217	-0.016939	-0.001225
B	3.436850	13.747295	4.538802	-0.008265	0.016945	0.001183
B	5.591279	6.955106	1.355407	0.008174	0.016934	-0.001238
B	-3.138137	6.846495	5.011383	-0.008213	-0.016951	0.001219
Si	0.631772	3.486686	4.508512	0.009890	0.038496	-0.003495
Si	1.821370	10.314915	1.858278	-0.009825	-0.038491	0.003479
Si	-0.333059	10.387486	5.041673	0.009889	-0.038445	-0.003442
Si	2.786201	3.414115	1.325117	-0.009882	0.038514	0.003498
O	0.061445	3.072947	3.041906	0.023731	0.018532	-0.007090
O	2.391697	10.728653	3.324884	-0.023631	-0.018496	0.007064
O	4.546126	9.973747	0.141489	0.023713	-0.018556	-0.007068
O	-2.092984	3.827853	6.225301	-0.023724	0.018541	0.007096

O	2.197450	3.933608	4.519003	0.017545	0.005291	0.028377
O	0.255692	9.867992	1.847787	-0.017512	-0.005233	-0.028342
O	-1.898737	10.834409	5.031182	0.017518	-0.005346	0.028432
O	4.351879	2.967192	1.335608	-0.017545	0.005288	-0.028372
O	-0.212316	4.798696	5.055280	-0.008856	0.035402	-0.032526
O	2.665458	9.002905	1.311510	0.008822	-0.035458	0.032466
O	0.511030	11.699496	4.494905	-0.008832	-0.035350	-0.032406
O	1.942113	2.102105	1.871885	0.008858	0.035416	0.032514
O	0.525580	2.169271	5.472081	-0.023016	0.032462	-0.005633
O	1.927562	11.632329	0.894709	0.023021	-0.032454	0.005624
O	-0.226867	9.070071	4.078104	-0.022941	-0.032365	-0.005649
O	2.680009	4.731529	2.288686	0.023015	0.032475	0.005636
O	0.058846	0.698526	2.444964	0.021651	-0.026677	0.000214
O	2.394296	13.103075	3.921826	-0.021671	0.026679	-0.000297
O	4.548725	7.599326	0.738431	0.021620	0.026633	0.000130
O	-2.095583	6.202275	5.628359	-0.021657	-0.026682	-0.000198
O	-2.459230	13.184059	5.445139	0.000839	0.022104	0.006707
O	4.912372	0.617542	0.921651	-0.000946	-0.022134	-0.006720
O	2.757943	6.283259	4.105046	0.000956	-0.022132	0.006702
O	-0.304801	7.518342	2.261744	-0.001044	0.022134	-0.006682
O	-0.175430	2.374756	0.744070	-0.008880	-0.045683	0.011963
O	2.628573	11.426844	5.622720	0.008845	0.045657	-0.011957
O	4.783002	9.275557	2.439325	-0.008889	0.045653	0.011912
O	-2.329859	4.526044	3.927465	0.008877	-0.045671	-0.011952
O	-1.223866	12.517207	2.155216	-0.006222	-0.013336	0.008535
O	3.677009	1.284394	4.211574	0.006230	0.013341	-0.008520
O	5.831438	5.616407	1.028179	-0.006215	0.013336	0.008511
O	-3.378295	8.185194	5.338611	0.006211	-0.013349	-0.008556
H	-0.637445	12.195109	2.878812	-0.004778	-0.022430	0.004687
H	3.090587	1.606491	3.487978	0.004837	0.022479	-0.004695
H	5.245016	5.294309	0.304583	-0.004764	0.022412	0.004666
H	-2.791874	8.507292	6.062207	0.004755	-0.022425	-0.004709

132 f = 10.038839 THz 63.075886 2PiTHz 334.859618 cm-1 41.517316 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.037442	-0.044994	0.016141
Li	-1.316675	4.156264	2.365404	-0.037375	-0.044960	0.016044
Li	-3.471104	2.744536	5.548798	-0.037382	0.044775	0.016135
Li	5.924247	11.057064	0.817991	-0.037407	0.044867	0.016162
Na	2.049025	6.784862	1.629696	-0.007798	0.001642	-0.006171
Na	0.404117	7.016739	4.737094	-0.007828	0.001680	-0.006122
Na	2.558546	13.685662	1.553699	-0.007834	-0.001735	-0.006136
Na	-0.105403	0.115939	4.813091	-0.007814	-0.001691	-0.006191
B	4.155007	8.978944	1.168663	0.000918	0.021058	0.012749
B	-1.701865	4.822656	5.198127	0.000905	0.020986	0.012699
B	0.452564	2.078144	2.014732	0.000948	-0.021015	0.012757
B	2.000578	11.723457	4.352058	0.000939	-0.021063	0.012771
B	-2.733891	11.746082	5.839177	0.008215	0.018175	0.004266
B	5.187034	2.055518	0.527613	0.008170	0.018113	0.004273
B	3.032605	4.845282	3.711007	0.008219	-0.018140	0.004285
B	-0.579463	8.956318	2.655782	0.008252	-0.018180	0.004274
B	-0.983708	0.054306	1.827988	0.002766	0.004274	0.011559
B	3.436850	13.747295	4.538802	0.002837	0.004283	0.011642
B	5.591279	6.955106	1.355407	0.002813	-0.004290	0.011638
B	-3.138137	6.846495	5.011383	0.002730	-0.004323	0.011560
Si	0.631772	3.486686	4.508512	-0.014432	0.024463	-0.006784
Si	1.821370	10.314915	1.858278	-0.014492	0.024405	-0.006844
Si	-0.333059	10.387486	5.041673	-0.014524	-0.024368	-0.006834
Si	2.786201	3.414115	1.325117	-0.014470	-0.024334	-0.006779
O	0.061445	3.072947	3.041906	0.002964	-0.024058	0.007072
O	2.391697	10.728653	3.324884	0.002902	-0.024185	0.007068
O	4.546126	9.973747	0.141489	0.002836	0.024230	0.007096
O	-2.092984	3.827853	6.225301	0.002862	0.024129	0.007097
O	2.197450	3.933608	4.519003	-0.010395	-0.010478	-0.026524
O	0.255692	9.867992	1.847787	-0.010428	-0.010588	-0.026642
O	-1.898737	10.834409	5.031182	-0.010476	0.010584	-0.026683
O	4.351879	2.967192	1.335608	-0.010460	0.010489	-0.026590
O	-0.212316	4.798696	5.055280	-0.003562	0.045921	-0.048457
O	2.665458	9.002905	1.311510	-0.003568	0.045955	-0.048623
O	0.511030	11.699496	4.494905	-0.003548	-0.045920	-0.048532
O	1.942113	2.102105	1.871885	-0.003520	-0.045805	-0.048326

O	0.525580	2.169271	5.472081	0.035533	0.025471	0.000550
O	1.927562	11.632329	0.894709	0.035480	0.025469	0.000556
O	-0.226867	9.070071	4.078104	0.035569	-0.025437	0.000565
O	2.680009	4.731529	2.288686	0.035640	-0.025342	0.000545
O	0.058846	0.698526	2.444964	0.001773	-0.012075	0.029117
O	2.394296	13.103075	3.921826	0.001750	-0.012065	0.029339
O	4.548725	7.599326	0.738431	0.001700	0.012028	0.029322
O	-2.095583	6.202275	5.628359	0.001706	0.011998	0.029089
O	-2.459230	13.184059	5.445139	0.010712	0.023272	0.018906
O	4.912372	0.617542	0.921651	0.010498	0.023220	0.018919
O	2.757943	6.283259	4.105046	0.010471	-0.023264	0.018932
O	-0.304801	7.518342	2.261744	0.010709	-0.023273	0.018883
O	-0.175430	2.374756	0.744070	-0.001860	0.019385	0.029562
O	2.628573	11.426844	5.622720	-0.001854	0.019467	0.029602
O	4.783002	9.275557	2.439325	-0.001838	-0.019509	0.029589
O	-2.329859	4.526044	3.927465	-0.001844	-0.019510	0.029519
O	-1.223866	12.517207	2.155216	0.010094	-0.002531	-0.015371
O	3.677009	1.284394	4.211574	0.010083	-0.002530	-0.015386
O	5.831438	5.616407	1.028179	0.010096	0.002521	-0.015386
O	-3.378295	8.185194	5.338611	0.010144	0.002491	-0.015374
H	-0.637445	12.195109	2.878812	0.000102	-0.010129	-0.008733
H	3.090587	1.606491	3.487978	0.000011	-0.010188	-0.008719
H	5.245016	5.294309	0.304583	0.000020	0.010179	-0.008711
H	-2.791874	8.507292	6.062207	0.000172	0.010065	-0.008739

133 f = 9.908906 THz 62.259494 2PiTHz 330.525525 cm-1 40.979957 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.009885	0.021581	-0.029771
Li	-1.316675	4.156264	2.365404	-0.009890	0.021531	-0.029819
Li	-3.471104	2.744536	5.548798	-0.009850	-0.021638	-0.029764
Li	5.924247	11.057064	0.817991	-0.009853	-0.021571	-0.029820
Na	2.049025	6.784862	1.629696	-0.007826	0.002074	-0.006393
Na	0.404117	7.016739	4.737094	-0.007860	0.002080	-0.006355
Na	2.558546	13.685662	1.553699	-0.007865	-0.002122	-0.006369
Na	-0.105403	0.115939	4.813091	-0.007831	-0.002046	-0.006385

B	4.155007	8.978944	1.168663	0.008175	0.010485	0.006705
B	-1.701865	4.822656	5.198127	0.008157	0.010429	0.006655
B	0.452564	2.078144	2.014732	0.008168	-0.010439	0.006683
B	2.000578	11.723457	4.352058	0.008169	-0.010479	0.006683
B	-2.733891	11.746082	5.839177	0.007206	0.010550	-0.005120
B	5.187034	2.055518	0.527613	0.007157	0.010502	-0.005131
B	3.032605	4.845282	3.711007	0.007180	-0.010522	-0.005104
B	-0.579463	8.956318	2.655782	0.007195	-0.010528	-0.005138
B	-0.983708	0.054306	1.827988	0.029008	-0.000183	0.010974
B	3.436850	13.747295	4.538802	0.029041	-0.000167	0.011001
B	5.591279	6.955106	1.355407	0.029044	0.000184	0.010991
B	-3.138137	6.846495	5.011383	0.028983	0.000157	0.010977
Si	0.631772	3.486686	4.508512	-0.017300	0.014631	-0.012304
Si	1.821370	10.314915	1.858278	-0.017333	0.014602	-0.012341
Si	-0.333059	10.387486	5.041673	-0.017343	-0.014640	-0.012325
Si	2.786201	3.414115	1.325117	-0.017323	-0.014564	-0.012305
O	0.061445	3.072947	3.041906	-0.025591	0.007757	-0.012941
O	2.391697	10.728653	3.324884	-0.025644	0.007677	-0.012940
O	4.546126	9.973747	0.141489	-0.025649	-0.007677	-0.012920
O	-2.092984	3.827853	6.225301	-0.025612	-0.007725	-0.012942
O	2.197450	3.933608	4.519003	-0.001425	-0.018655	-0.009419
O	0.255692	9.867992	1.847787	-0.001437	-0.018720	-0.009533
O	-1.898737	10.834409	5.031182	-0.001446	0.018694	-0.009470
O	4.351879	2.967192	1.335608	-0.001465	0.018655	-0.009499
O	-0.212316	4.798696	5.055280	0.010611	0.016586	0.030400
O	2.665458	9.002905	1.311510	0.010627	0.016573	0.030414
O	0.511030	11.699496	4.494905	0.010621	-0.016623	0.030396
O	1.942113	2.102105	1.871885	0.010613	-0.016518	0.030449
O	0.525580	2.169271	5.472081	-0.056947	0.028570	0.007674
O	1.927562	11.632329	0.894709	-0.056972	0.028604	0.007708
O	-0.226867	9.070071	4.078104	-0.056972	-0.028608	0.007691
O	2.680009	4.731529	2.288686	-0.056908	-0.028534	0.007701
O	0.058846	0.698526	2.444964	0.033204	-0.016124	0.025758
O	2.394296	13.103075	3.921826	0.033201	-0.016130	0.025847
O	4.548725	7.599326	0.738431	0.033203	0.016143	0.025850
O	-2.095583	6.202275	5.628359	0.033155	0.016076	0.025748

O	-2.459230	13.184059	5.445139	0.047579	0.008241	-0.001347
O	4.912372	0.617542	0.921651	0.047463	0.008181	-0.001344
O	2.757943	6.283259	4.105046	0.047458	-0.008217	-0.001331
O	-0.304801	7.518342	2.261744	0.047551	-0.008191	-0.001374
O	-0.175430	2.374756	0.744070	0.021944	-0.027597	-0.011477
O	2.628573	11.426844	5.622720	0.021991	-0.027547	-0.011478
O	4.783002	9.275557	2.439325	0.021983	0.027615	-0.011465
O	-2.329859	4.526044	3.927465	0.021955	0.027526	-0.011493
O	-1.223866	12.517207	2.155216	-0.011661	0.004676	0.006274
O	3.677009	1.284394	4.211574	-0.011680	0.004690	0.006258
O	5.831438	5.616407	1.028179	-0.011651	-0.004674	0.006266
O	-3.378295	8.185194	5.338611	-0.011645	-0.004696	0.006276
H	-0.637445	12.195109	2.878812	-0.025601	-0.016072	0.006590
H	3.090587	1.606491	3.487978	-0.025639	-0.016084	0.006575
H	5.245016	5.294309	0.304583	-0.025598	0.016087	0.006582
H	-2.791874	8.507292	6.062207	-0.025567	0.016037	0.006582

134 f = 9.758651 THz 61.315412 2PiTHz 325.513548 cm-1 40.358551 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.043290	-0.050387	0.034724
Li	-1.316675	4.156264	2.365404	0.043314	0.050378	-0.034764
Li	-3.471104	2.744536	5.548798	0.043327	-0.050409	-0.034733
Li	5.924247	11.057064	0.817991	-0.043326	0.050374	0.034766
Na	2.049025	6.784862	1.629696	-0.000394	0.001208	0.001985
Na	0.404117	7.016739	4.737094	0.000400	-0.001215	-0.001920
Na	2.558546	13.685662	1.553699	0.000401	0.001199	-0.001924
Na	-0.105403	0.115939	4.813091	-0.000392	-0.001216	0.001985
B	4.155007	8.978944	1.168663	0.001299	-0.008292	-0.002131
B	-1.701865	4.822656	5.198127	-0.001288	0.008275	0.002103
B	0.452564	2.078144	2.014732	-0.001292	-0.008274	0.002117
B	2.000578	11.723457	4.352058	0.001302	0.008278	-0.002119
B	-2.733891	11.746082	5.839177	-0.001436	-0.001585	0.012140
B	5.187034	2.055518	0.527613	0.001412	0.001577	-0.012155
B	3.032605	4.845282	3.711007	0.001420	-0.001584	-0.012142

B	-0.579463	8.956318	2.655782	-0.001416	0.001571	0.012146
B	-0.983708	0.054306	1.827988	0.001617	-0.002740	-0.021332
B	3.436850	13.747295	4.538802	-0.001611	0.002746	0.021309
B	5.591279	6.955106	1.355407	-0.001605	-0.002762	0.021314
B	-3.138137	6.846495	5.011383	0.001615	0.002742	-0.021325
Si	0.631772	3.486686	4.508512	0.000417	0.006769	0.000680
Si	1.821370	10.314915	1.858278	-0.000410	-0.006758	-0.000682
Si	-0.333059	10.387486	5.041673	-0.000409	0.006783	-0.000682
Si	2.786201	3.414115	1.325117	0.000413	-0.006748	0.000676
O	0.061445	3.072947	3.041906	-0.030241	-0.007634	0.006812
O	2.391697	10.728653	3.324884	0.030239	0.007663	-0.006827
O	4.546126	9.973747	0.141489	0.030218	-0.007655	-0.006823
O	-2.092984	3.827853	6.225301	-0.030229	0.007642	0.006802
O	2.197450	3.933608	4.519003	0.016118	-0.018460	0.003291
O	0.255692	9.867992	1.847787	-0.016103	0.018475	-0.003225
O	-1.898737	10.834409	5.031182	-0.016105	-0.018456	-0.003255
O	4.351879	2.967192	1.335608	0.016108	0.018466	0.003254
O	-0.212316	4.798696	5.055280	0.010821	-0.003986	0.056174
O	2.665458	9.002905	1.311510	-0.010811	0.003987	-0.056142
O	0.511030	11.699496	4.494905	-0.010804	-0.003957	-0.056117
O	1.942113	2.102105	1.871885	0.010818	0.004016	0.056193
O	0.525580	2.169271	5.472081	-0.055084	0.015588	0.006850
O	1.927562	11.632329	0.894709	0.054998	-0.015570	-0.006850
O	-0.226867	9.070071	4.078104	0.055026	0.015586	-0.006844
O	2.680009	4.731529	2.288686	-0.055078	-0.015582	0.006863
O	0.058846	0.698526	2.444964	0.000425	-0.008637	-0.013051
O	2.394296	13.103075	3.921826	-0.000397	0.008622	0.013022
O	4.548725	7.599326	0.738431	-0.000402	-0.008645	0.013024
O	-2.095583	6.202275	5.628359	0.000415	0.008629	-0.013047
O	-2.459230	13.184059	5.445139	-0.001472	0.010302	0.028180
O	4.912372	0.617542	0.921651	0.001463	-0.010315	-0.028205
O	2.757943	6.283259	4.105046	0.001473	0.010310	-0.028203
O	-0.304801	7.518342	2.261744	-0.001460	-0.010318	0.028188
O	-0.175430	2.374756	0.744070	0.021957	-0.042577	-0.026888
O	2.628573	11.426844	5.622720	-0.021957	0.042519	0.026867
O	4.783002	9.275557	2.439325	-0.021944	-0.042562	0.026856

O	-2.329859	4.526044	3.927465	0.021960	0.042555	-0.026898
O	-1.223866	12.517207	2.155216	0.011905	0.002034	0.000892
O	3.677009	1.284394	4.211574	-0.011919	-0.002020	-0.000879
O	5.831438	5.616407	1.028179	-0.011907	0.002008	-0.000893
O	-3.378295	8.185194	5.338611	0.011906	-0.002030	0.000889
H	-0.637445	12.195109	2.878812	0.026211	0.016100	-0.001676
H	3.090587	1.606491	3.487978	-0.026214	-0.016066	0.001685
H	5.245016	5.294309	0.304583	-0.026209	0.016066	0.001671
H	-2.791874	8.507292	6.062207	0.026208	-0.016089	-0.001677

135 f = 9.084128 THz 57.077261 2PiTHz 303.013891 cm-1 37.568948
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.030462	-0.009178	0.028015
Li	-1.316675	4.156264	2.365404	0.030752	-0.009020	0.027917
Li	-3.471104	2.744536	5.548798	-0.030711	-0.009033	-0.027927
Li	5.924247	11.057064	0.817991	-0.030461	-0.009162	-0.028022
Na	2.049025	6.784862	1.629696	0.010180	0.003821	0.005109
Na	0.404117	7.016739	4.737094	0.010226	0.003968	0.004991
Na	2.558546	13.685662	1.553699	-0.010227	0.003969	-0.004989
Na	-0.105403	0.115939	4.813091	-0.010177	0.003817	-0.005104
B	4.155007	8.978944	1.168663	-0.023275	-0.005728	-0.004350
B	-1.701865	4.822656	5.198127	-0.023437	-0.005759	-0.004404
B	0.452564	2.078144	2.014732	0.023436	-0.005758	0.004401
B	2.000578	11.723457	4.352058	0.023275	-0.005732	0.004348
B	-2.733891	11.746082	5.839177	0.009425	0.003556	0.024164
B	5.187034	2.055518	0.527613	0.009501	0.003529	0.024321
B	3.032605	4.845282	3.711007	-0.009500	0.003538	-0.024326
B	-0.579463	8.956318	2.655782	-0.009421	0.003545	-0.024165
B	-0.983708	0.054306	1.827988	0.004436	0.001328	0.004212
B	3.436850	13.747295	4.538802	0.004368	0.001328	0.004164
B	5.591279	6.955106	1.355407	-0.004383	0.001329	-0.004172
B	-3.138137	6.846495	5.011383	-0.004436	0.001332	-0.004229
Si	0.631772	3.486686	4.508512	-0.007568	-0.000557	0.017497
Si	1.821370	10.314915	1.858278	-0.007469	-0.000526	0.017401

Si	-0.333059	10.387486	5.041673	0.007469	-0.000539	-0.017402
Si	2.786201	3.414115	1.325117	0.007580	-0.000540	-0.017488
O	0.061445	3.072947	3.041906	0.052999	0.008315	-0.004019
O	2.391697	10.728653	3.324884	0.052731	0.008193	-0.003956
O	4.546126	9.973747	0.141489	-0.052728	0.008199	0.003959
O	-2.092984	3.827853	6.225301	-0.053005	0.008337	0.004035
O	2.197450	3.933608	4.519003	-0.009959	-0.008072	-0.040713
O	0.255692	9.867992	1.847787	-0.009856	-0.008015	-0.040456
O	-1.898737	10.834409	5.031182	0.009854	-0.008030	0.040467
O	4.351879	2.967192	1.335608	0.009971	-0.008070	0.040721
O	-0.212316	4.798696	5.055280	-0.023074	-0.023816	0.026442
O	2.665458	9.002905	1.311510	-0.022924	-0.023716	0.026306
O	0.511030	11.699496	4.494905	0.022925	-0.023725	-0.026299
O	1.942113	2.102105	1.871885	0.023075	-0.023792	-0.026425
O	0.525580	2.169271	5.472081	-0.023610	0.020402	0.034607
O	1.927562	11.632329	0.894709	-0.023437	0.020322	0.034406
O	-0.226867	9.070071	4.078104	0.023438	0.020306	-0.034405
O	2.680009	4.731529	2.288686	0.023590	0.020417	-0.034603
O	0.058846	0.698526	2.444964	-0.013073	0.005032	0.036137
O	2.394296	13.103075	3.921826	-0.013057	0.005022	0.035904
O	4.548725	7.599326	0.738431	0.013057	0.005034	-0.035925
O	-2.095583	6.202275	5.628359	0.013063	0.005030	-0.036145
O	-2.459230	13.184059	5.445139	0.030812	0.000128	-0.016663
O	4.912372	0.617542	0.921651	0.031011	0.000137	-0.016712
O	2.757943	6.283259	4.105046	-0.031008	0.000153	0.016685
O	-0.304801	7.518342	2.261744	-0.030816	0.000111	0.016662
O	-0.175430	2.374756	0.744070	0.012959	-0.000809	0.010721
O	2.628573	11.426844	5.622720	0.012865	-0.000745	0.010639
O	4.783002	9.275557	2.439325	-0.012863	-0.000765	-0.010636
O	-2.329859	4.526044	3.927465	-0.012954	-0.000804	-0.010733
O	-1.223866	12.517207	2.155216	-0.027232	0.000089	-0.023476
O	3.677009	1.284394	4.211574	-0.027030	0.000101	-0.023276
O	5.831438	5.616407	1.028179	0.026994	0.000099	0.023269
O	-3.378295	8.185194	5.338611	0.027234	0.000090	0.023464
H	-0.637445	12.195109	2.878812	-0.039950	-0.022820	-0.025052
H	3.090587	1.606491	3.487978	-0.039438	-0.022605	-0.025001

H	5.245016	5.294309	0.304583	0.039396	-0.022603	0.024995
H	-2.791874	8.507292	6.062207	0.039947	-0.022821	0.025045

136 f = 9.032121 THz 56.750493 2PiTHz 301.279133 cm-1 37.353865 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.040964	-0.021312	0.016180
Li	-1.316675	4.156264	2.365404	0.040761	0.021506	-0.016370
Li	-3.471104	2.744536	5.548798	-0.040745	0.021433	0.016351
Li	5.924247	11.057064	0.817991	0.040959	-0.021394	-0.016205
Na	2.049025	6.784862	1.629696	-0.001598	-0.021520	0.011833
Na	0.404117	7.016739	4.737094	0.001549	0.021272	-0.011769
Na	2.558546	13.685662	1.553699	-0.001532	0.021474	0.011792
Na	-0.105403	0.115939	4.813091	0.001612	-0.021331	-0.011806
B	4.155007	8.978944	1.168663	0.025754	0.003858	0.005701
B	-1.701865	4.822656	5.198127	-0.025595	-0.003781	-0.005705
B	0.452564	2.078144	2.014732	0.025578	-0.003799	0.005695
B	2.000578	11.723457	4.352058	-0.025765	0.003847	-0.005710
B	-2.733891	11.746082	5.839177	-0.010258	0.001973	-0.020933
B	5.187034	2.055518	0.527613	0.010219	-0.001999	0.020805
B	3.032605	4.845282	3.711007	-0.010208	-0.001998	-0.020807
B	-0.579463	8.956318	2.655782	0.010268	0.001991	0.020943
B	-0.983708	0.054306	1.827988	0.011662	-0.000864	0.006958
B	3.436850	13.747295	4.538802	-0.011692	0.000847	-0.006942
B	5.591279	6.955106	1.355407	0.011713	0.000883	0.006973
B	-3.138137	6.846495	5.011383	-0.011666	-0.000831	-0.006959
Si	0.631772	3.486686	4.508512	-0.014860	-0.001161	0.015863
Si	1.821370	10.314915	1.858278	0.014910	0.001138	-0.015995
Si	-0.333059	10.387486	5.041673	-0.014908	0.001135	0.015968
Si	2.786201	3.414115	1.325117	0.014863	-0.001173	-0.015886
O	0.061445	3.072947	3.041906	0.044316	0.019353	-0.010468
O	2.391697	10.728653	3.324884	-0.044739	-0.019414	0.010505
O	4.546126	9.973747	0.141489	0.044708	-0.019420	-0.010524
O	-2.092984	3.827853	6.225301	-0.044354	0.019367	0.010463
O	2.197450	3.933608	4.519003	-0.014755	-0.007524	-0.033526

O	0.255692	9.867992	1.847787	0.014819	0.007559	0.033744
O	-1.898737	10.834409	5.031182	-0.014814	0.007561	-0.033752
O	4.351879	2.967192	1.335608	0.014769	-0.007517	0.033529
O	-0.212316	4.798696	5.055280	-0.022664	-0.013719	0.026391
O	2.665458	9.002905	1.311510	0.022813	0.013844	-0.026609
O	0.511030	11.699496	4.494905	-0.022829	0.013865	0.026593
O	1.942113	2.102105	1.871885	0.022647	-0.013697	-0.026385
O	0.525580	2.169271	5.472081	-0.025707	0.011958	0.027419
O	1.927562	11.632329	0.894709	0.025864	-0.012075	-0.027612
O	-0.226867	9.070071	4.078104	-0.025859	-0.012110	0.027625
O	2.680009	4.731529	2.288686	0.025694	0.011908	-0.027406
O	0.058846	0.698526	2.444964	0.001274	-0.001161	0.032771
O	2.394296	13.103075	3.921826	-0.001206	0.001157	-0.032978
O	4.548725	7.599326	0.738431	0.001218	0.001156	0.033007
O	-2.095583	6.202275	5.628359	-0.001281	-0.001149	-0.032771
O	-2.459230	13.184059	5.445139	-0.032217	-0.002967	0.006356
O	4.912372	0.617542	0.921651	0.032007	0.002969	-0.006202
O	2.757943	6.283259	4.105046	-0.032006	0.002977	0.006193
O	-0.304801	7.518342	2.261744	0.032227	-0.002945	-0.006329
O	-0.175430	2.374756	0.744070	0.011604	-0.006207	0.012118
O	2.628573	11.426844	5.622720	-0.011670	0.006202	-0.012198
O	4.783002	9.275557	2.439325	0.011678	0.006255	0.012181
O	-2.329859	4.526044	3.927465	-0.011592	-0.006164	-0.012140
O	-1.223866	12.517207	2.155216	-0.034196	-0.002167	-0.029590
O	3.677009	1.284394	4.211574	0.034410	0.002152	0.029770
O	5.831438	5.616407	1.028179	-0.034372	0.002181	-0.029738
O	-3.378295	8.185194	5.338611	0.034194	-0.002145	0.029599
H	-0.637445	12.195109	2.878812	-0.082905	-0.034958	-0.006612
H	3.090587	1.606491	3.487978	0.083185	0.035099	0.006828
H	5.245016	5.294309	0.304583	-0.083148	0.035118	-0.006781
H	-2.791874	8.507292	6.062207	0.082904	-0.034949	0.006635

137 f = 8.145723 THz 51.181084 2PiTHz 271.712048 cm-1 33.688013
meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.005832	0.019771	0.008074
Li	-1.316675	4.156264	2.365404	-0.006092	0.019821	0.007945
Li	-3.471104	2.744536	5.548798	0.005890	0.019822	-0.008088
Li	5.924247	11.057064	0.817991	0.006039	0.019759	-0.007944
Na	2.049025	6.784862	1.629696	0.008311	-0.070369	0.023540
Na	0.404117	7.016739	4.737094	0.008311	-0.069684	0.023195
Na	2.558546	13.685662	1.553699	-0.008363	-0.070379	-0.023326
Na	-0.105403	0.115939	4.813091	-0.008259	-0.069678	-0.023414
B	4.155007	8.978944	1.168663	0.011091	0.015665	-0.020088
B	-1.701865	4.822656	5.198127	0.011155	0.015806	-0.020171
B	0.452564	2.078144	2.014732	-0.011156	0.015713	0.020200
B	2.000578	11.723457	4.352058	-0.011097	0.015750	0.020069
B	-2.733891	11.746082	5.839177	0.003659	0.011191	0.012697
B	5.187034	2.055518	0.527613	0.003730	0.011267	0.012728
B	3.032605	4.845282	3.711007	-0.003695	0.011172	-0.012705
B	-0.579463	8.956318	2.655782	-0.003687	0.011283	-0.012719
B	-0.983708	0.054306	1.827988	-0.000484	0.015677	0.006263
B	3.436850	13.747295	4.538802	-0.000476	0.015655	0.006134
B	5.591279	6.955106	1.355407	0.000424	0.015656	-0.006191
B	-3.138137	6.846495	5.011383	0.000535	0.015685	-0.006204
Si	0.631772	3.486686	4.508512	-0.005401	-0.006564	0.003725
Si	1.821370	10.314915	1.858278	-0.005266	-0.006688	0.003790
Si	-0.333059	10.387486	5.041673	0.005382	-0.006567	-0.003703
Si	2.786201	3.414115	1.325117	0.005281	-0.006688	-0.003808
O	0.061445	3.072947	3.041906	-0.039087	-0.005365	0.019957
O	2.391697	10.728653	3.324884	-0.038679	-0.005234	0.019853
O	4.546126	9.973747	0.141489	0.038914	-0.005359	-0.019880
O	-2.092984	3.827853	6.225301	0.038831	-0.005223	-0.019917
O	2.197450	3.933608	4.519003	-0.004724	-0.001294	-0.025488
O	0.255692	9.867992	1.847787	-0.004626	-0.001225	-0.025322
O	-1.898737	10.834409	5.031182	0.004699	-0.001325	0.025533
O	4.351879	2.967192	1.335608	0.004652	-0.001187	0.025267
O	-0.212316	4.798696	5.055280	0.007298	0.014993	-0.031020
O	2.665458	9.002905	1.311510	0.007268	0.014756	-0.030851
O	0.511030	11.699496	4.494905	-0.007272	0.014889	0.030824
O	1.942113	2.102105	1.871885	-0.007298	0.014851	0.031047

O	0.525580	2.169271	5.472081	-0.007114	0.003646	0.015026
O	1.927562	11.632329	0.894709	-0.007339	0.003507	0.015015
O	-0.226867	9.070071	4.078104	0.007213	0.003680	-0.015026
O	2.680009	4.731529	2.288686	0.007248	0.003472	-0.015013
O	0.058846	0.698526	2.444964	-0.012343	0.015626	0.020343
O	2.394296	13.103075	3.921826	-0.012373	0.015639	0.020243
O	4.548725	7.599326	0.738431	0.012217	0.015554	-0.020196
O	-2.095583	6.202275	5.628359	0.012490	0.015720	-0.020373
O	-2.459230	13.184059	5.445139	0.006125	0.014384	0.005458
O	4.912372	0.617542	0.921651	0.006075	0.014468	0.005650
O	2.757943	6.283259	4.105046	-0.006076	0.014391	-0.005502
O	-0.304801	7.518342	2.261744	-0.006116	0.014457	-0.005600
O	-0.175430	2.374756	0.744070	0.004013	0.025283	0.012207
O	2.628573	11.426844	5.622720	0.003932	0.025316	0.012121
O	4.783002	9.275557	2.439325	-0.003956	0.025335	-0.012170
O	-2.329859	4.526044	3.927465	-0.003982	0.025265	-0.012156
O	-1.223866	12.517207	2.155216	0.005257	0.007662	-0.016906
O	3.677009	1.284394	4.211574	0.005061	0.007657	-0.017082
O	5.831438	5.616407	1.028179	-0.005220	0.007666	0.016935
O	-3.378295	8.185194	5.338611	-0.005095	0.007670	0.017030
H	-0.637445	12.195109	2.878812	-0.002562	-0.002090	-0.016660
H	3.090587	1.606491	3.487978	-0.002882	-0.002214	-0.016810
H	5.245016	5.294309	0.304583	0.002638	-0.002067	0.016656
H	-2.791874	8.507292	6.062207	0.002800	-0.002217	0.016797

138 f = 7.904810 THz 49.667385 2PiTHz 263.676066 cm-1 32.691677
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.001840	0.020205	-0.005423
Li	-1.316675	4.156264	2.365404	0.001763	0.020214	-0.005437
Li	-3.471104	2.744536	5.548798	0.001849	-0.020188	-0.005387
Li	5.924247	11.057064	0.817991	0.001718	-0.020228	-0.005470
Na	2.049025	6.784862	1.629696	0.010100	-0.074687	0.017095
Na	0.404117	7.016739	4.737094	0.010053	-0.073987	0.017002
Na	2.558546	13.685662	1.553699	0.010184	0.074788	0.017091

Na	-0.105403	0.115939	4.813091	0.009974	0.073863	0.017007
B	4.155007	8.978944	1.168663	-0.005245	0.024957	-0.002298
B	-1.701865	4.822656	5.198127	-0.005085	0.025087	-0.002366
B	0.452564	2.078144	2.014732	-0.005233	-0.024978	-0.002308
B	2.000578	11.723457	4.352058	-0.005090	-0.025074	-0.002379
B	-2.733891	11.746082	5.839177	0.001063	-0.017235	0.001688
B	5.187034	2.055518	0.527613	0.001041	-0.017231	0.001589
B	3.032605	4.845282	3.711007	0.001092	0.017217	0.001669
B	-0.579463	8.956318	2.655782	0.001052	0.017258	0.001585
B	-0.983708	0.054306	1.827988	-0.011250	-0.025206	0.008464
B	3.436850	13.747295	4.538802	-0.011234	-0.025235	0.008438
B	5.591279	6.955106	1.355407	-0.011248	0.025216	0.008479
B	-3.138137	6.846495	5.011383	-0.011226	0.025226	0.008423
Si	0.631772	3.486686	4.508512	0.003923	0.004714	-0.012188
Si	1.821370	10.314915	1.858278	0.003947	0.004683	-0.012249
Si	-0.333059	10.387486	5.041673	0.003915	-0.004700	-0.012189
Si	2.786201	3.414115	1.325117	0.003954	-0.004693	-0.012258
O	0.061445	3.072947	3.041906	-0.004551	-0.011169	-0.007765
O	2.391697	10.728653	3.324884	-0.004271	-0.011092	-0.007928
O	4.546126	9.973747	0.141489	-0.004595	0.011155	-0.007763
O	-2.092984	3.827853	6.225301	-0.004258	0.011097	-0.007931
O	2.197450	3.933608	4.519003	0.006554	0.004573	-0.004406
O	0.255692	9.867992	1.847787	0.006534	0.004512	-0.004630
O	-1.898737	10.834409	5.031182	0.006539	-0.004573	-0.004412
O	4.351879	2.967192	1.335608	0.006551	-0.004492	-0.004597
O	-0.212316	4.798696	5.055280	-0.003458	0.001307	-0.011884
O	2.665458	9.002905	1.311510	-0.003617	0.000997	-0.011711
O	0.511030	11.699496	4.494905	-0.003468	-0.001289	-0.011887
O	1.942113	2.102105	1.871885	-0.003606	-0.001016	-0.011753
O	0.525580	2.169271	5.472081	0.010992	0.012526	0.000409
O	1.927562	11.632329	0.894709	0.011009	0.012685	0.000526
O	-0.226867	9.070071	4.078104	0.011045	-0.012489	0.000390
O	2.680009	4.731529	2.288686	0.011012	-0.012709	0.000523
O	0.058846	0.698526	2.444964	-0.011779	-0.017702	0.011711
O	2.394296	13.103075	3.921826	-0.011854	-0.017666	0.011808
O	4.548725	7.599326	0.738431	-0.011779	0.017681	0.011696

O	-2.095583	6.202275	5.628359	-0.011880	0.017672	0.011862
O	-2.459230	13.184059	5.445139	-0.018293	-0.015548	0.012100
O	4.912372	0.617542	0.921651	-0.018396	-0.015450	0.012255
O	2.757943	6.283259	4.105046	-0.018241	0.015527	0.012063
O	-0.304801	7.518342	2.261744	-0.018393	0.015481	0.012253
O	-0.175430	2.374756	0.744070	0.005483	-0.050573	-0.009250
O	2.628573	11.426844	5.622720	0.005525	-0.050662	-0.009252
O	4.783002	9.275557	2.439325	0.005482	0.050573	-0.009247
O	-2.329859	4.526044	3.927465	0.005556	0.050655	-0.009253
O	-1.223866	12.517207	2.155216	0.002890	-0.025227	0.002539
O	3.677009	1.284394	4.211574	0.002982	-0.025247	0.002558
O	5.831438	5.616407	1.028179	0.002931	0.025228	0.002612
O	-3.378295	8.185194	5.338611	0.002935	0.025247	0.002475
H	-0.637445	12.195109	2.878812	0.006570	-0.016709	0.005258
H	3.090587	1.606491	3.487978	0.006533	-0.016583	0.005455
H	5.245016	5.294309	0.304583	0.006641	0.016673	0.005325
H	-2.791874	8.507292	6.062207	0.006436	0.016622	0.005392

139 f = 7.414221 THz 46.584922 2PiTHz 247.311770 cm-1 30.662763 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.011777	0.018371	-0.003262
Li	-1.316675	4.156264	2.365404	0.012038	-0.018191	0.003283
Li	-3.471104	2.744536	5.548798	-0.012039	-0.018238	-0.003255
Li	5.924247	11.057064	0.817991	0.011766	0.018329	0.003214
Na	2.049025	6.784862	1.629696	-0.002479	0.008399	-0.017237
Na	0.404117	7.016739	4.737094	0.002430	-0.009250	0.016875
Na	2.558546	13.685662	1.553699	-0.002431	-0.009215	-0.016846
Na	-0.105403	0.115939	4.813091	0.002496	0.008411	0.017220
B	4.155007	8.978944	1.168663	0.008814	0.002699	-0.034111
B	-1.701865	4.822656	5.198127	-0.008879	-0.002558	0.034620
B	0.452564	2.078144	2.014732	0.008879	-0.002695	-0.034618
B	2.000578	11.723457	4.352058	-0.008823	0.002664	0.034126
B	-2.733891	11.746082	5.839177	0.023600	0.001052	-0.000342
B	5.187034	2.055518	0.527613	-0.024110	-0.000931	0.000599

B	3.032605	4.845282	3.711007	0.024091	-0.000794	-0.000609
B	-0.579463	8.956318	2.655782	-0.023587	0.001073	0.000334
B	-0.983708	0.054306	1.827988	0.007853	-0.003151	-0.012769
B	3.436850	13.747295	4.538802	-0.007836	0.003158	0.012678
B	5.591279	6.955106	1.355407	0.007833	0.003187	-0.012672
B	-3.138137	6.846495	5.011383	-0.007939	-0.003037	0.012845
Si	0.631772	3.486686	4.508512	0.006510	0.001003	0.007481
Si	1.821370	10.314915	1.858278	-0.006595	-0.000927	-0.007435
Si	-0.333059	10.387486	5.041673	0.006583	-0.000943	0.007427
Si	2.786201	3.414115	1.325117	-0.006470	0.000984	-0.007524
O	0.061445	3.072947	3.041906	0.040335	-0.000545	-0.009100
O	2.391697	10.728653	3.324884	-0.040176	0.000422	0.009040
O	4.546126	9.973747	0.141489	0.040128	0.000450	-0.009028
O	-2.092984	3.827853	6.225301	-0.040252	-0.000564	0.009014
O	2.197450	3.933608	4.519003	0.011111	-0.003512	-0.003208
O	0.255692	9.867992	1.847787	-0.011088	0.003578	0.002543
O	-1.898737	10.834409	5.031182	0.011081	0.003563	-0.002574
O	4.351879	2.967192	1.335608	-0.011046	-0.003518	0.003161
O	-0.212316	4.798696	5.055280	0.003367	-0.017372	0.065010
O	2.665458	9.002905	1.311510	-0.003238	0.017490	-0.064260
O	0.511030	11.699496	4.494905	0.003236	0.017472	0.064282
O	1.942113	2.102105	1.871885	-0.003340	-0.017436	-0.065076
O	0.525580	2.169271	5.472081	-0.030229	-0.003211	0.000624
O	1.927562	11.632329	0.894709	0.029245	0.003453	-0.000333
O	-0.226867	9.070071	4.078104	-0.029211	0.003451	0.000321
O	2.680009	4.731529	2.288686	0.030271	-0.003192	-0.000667
O	0.058846	0.698526	2.444964	0.034829	-0.011789	-0.053627
O	2.394296	13.103075	3.921826	-0.034246	0.011545	0.052812
O	4.548725	7.599326	0.738431	0.034256	0.011590	-0.052804
O	-2.095583	6.202275	5.628359	-0.034943	-0.011707	0.053773
O	-2.459230	13.184059	5.445139	0.017865	0.003174	-0.011431
O	4.912372	0.617542	0.921651	-0.018463	-0.003003	0.011997
O	2.757943	6.283259	4.105046	0.018309	-0.002893	-0.011885
O	-0.304801	7.518342	2.261744	-0.017851	0.003194	0.011423
O	-0.175430	2.374756	0.744070	-0.027365	0.013571	-0.013168
O	2.628573	11.426844	5.622720	0.026904	-0.013427	0.012939

O	4.783002	9.275557	2.439325	-0.026893	-0.013394	-0.012932
O	-2.329859	4.526044	3.927465	0.027393	0.013931	0.013119
O	-1.223866	12.517207	2.155216	0.013361	0.000762	0.010639
O	3.677009	1.284394	4.211574	-0.013300	-0.000717	-0.010551
O	5.831438	5.616407	1.028179	0.013265	-0.000696	0.010562
O	-3.378295	8.185194	5.338611	-0.013311	0.000923	-0.010655
H	-0.637445	12.195109	2.878812	0.020947	0.012759	0.008647
H	3.090587	1.606491	3.487978	-0.020406	-0.012745	-0.008936
H	5.245016	5.294309	0.304583	0.020371	-0.012713	0.008940
H	-2.791874	8.507292	6.062207	-0.020868	0.012887	-0.008672

140 f = 7.378500 THz 46.360485 2PiTHz 246.120274 cm-1 30.515036 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.015719	-0.005086	0.000246
Li	-1.316675	4.156264	2.365404	-0.015021	-0.005447	0.000675
Li	-3.471104	2.744536	5.548798	0.015484	-0.005447	-0.000318
Li	5.924247	11.057064	0.817991	0.015275	-0.005084	-0.000641
Na	2.049025	6.784862	1.629696	0.005288	0.026745	0.002526
Na	0.404117	7.016739	4.737094	0.005431	0.025199	0.003284
Na	2.558546	13.685662	1.553699	-0.005317	0.026705	-0.002754
Na	-0.105403	0.115939	4.813091	-0.005387	0.025422	-0.002992
B	4.155007	8.978944	1.168663	0.003688	-0.000858	-0.029098
B	-1.701865	4.822656	5.198127	0.003557	-0.000917	-0.028471
B	0.452564	2.078144	2.014732	-0.003533	-0.000918	0.028446
B	2.000578	11.723457	4.352058	-0.003719	-0.000869	0.029127
B	-2.733891	11.746082	5.839177	0.029107	-0.006556	-0.013167
B	5.187034	2.055518	0.527613	0.028570	-0.006852	-0.013176
B	3.032605	4.845282	3.711007	-0.028613	-0.006607	0.013156
B	-0.579463	8.956318	2.655782	-0.029030	-0.006834	0.013190
B	-0.983708	0.054306	1.827988	-0.000357	-0.001945	0.003544
B	3.436850	13.747295	4.538802	-0.000268	-0.001801	0.003853
B	5.591279	6.955106	1.355407	0.000490	-0.001875	-0.003816
B	-3.138137	6.846495	5.011383	0.000135	-0.001858	-0.003640
Si	0.631772	3.486686	4.508512	0.003425	-0.001789	-0.004070

Si	1.821370	10.314915	1.858278	0.002996	-0.001699	-0.004390
Si	-0.333059	10.387486	5.041673	-0.003290	-0.001819	0.004234
Si	2.786201	3.414115	1.325117	-0.003124	-0.001686	0.004226
O	0.061445	3.072947	3.041906	-0.013496	0.004248	0.004150
O	2.391697	10.728653	3.324884	-0.014968	0.003986	0.004431
O	4.546126	9.973747	0.141489	0.014257	0.004299	-0.004283
O	-2.092984	3.827853	6.225301	0.014163	0.003999	-0.004252
O	2.197450	3.933608	4.519003	-0.000375	-0.004218	0.026966
O	0.255692	9.867992	1.847787	-0.000844	-0.004395	0.026490
O	-1.898737	10.834409	5.031182	0.000590	-0.004174	-0.026991
O	4.351879	2.967192	1.335608	0.000627	-0.004452	-0.026458
O	-0.212316	4.798696	5.055280	-0.006007	-0.000217	-0.045112
O	2.665458	9.002905	1.311510	-0.006129	0.000166	-0.046159
O	0.511030	11.699496	4.494905	0.006074	0.000115	0.046369
O	1.942113	2.102105	1.871885	0.006057	-0.000155	0.044933
O	0.525580	2.169271	5.472081	0.051138	-0.008557	-0.014190
O	1.927562	11.632329	0.894709	0.051975	-0.008264	-0.014202
O	-0.226867	9.070071	4.078104	-0.051692	-0.008499	0.014207
O	2.680009	4.731529	2.288686	-0.051385	-0.008374	0.014206
O	0.058846	0.698526	2.444964	-0.031875	0.009487	0.047200
O	2.394296	13.103075	3.921826	-0.032071	0.009623	0.047989
O	4.548725	7.599326	0.738431	0.032538	0.009731	-0.048262
O	-2.095583	6.202275	5.628359	0.031428	0.009416	-0.046989
O	-2.459230	13.184059	5.445139	0.035130	-0.010093	-0.033359
O	4.912372	0.617542	0.921651	0.034603	-0.010366	-0.033313
O	2.757943	6.283259	4.105046	-0.034726	-0.010165	0.033075
O	-0.304801	7.518342	2.261744	-0.034973	-0.010327	0.033539
O	-0.175430	2.374756	0.744070	0.026466	-0.011419	0.013035
O	2.628573	11.426844	5.622720	0.026991	-0.011298	0.013393
O	4.783002	9.275557	2.439325	-0.026989	-0.011698	-0.013272
O	-2.329859	4.526044	3.927465	-0.026445	-0.011082	-0.013144
O	-1.223866	12.517207	2.155216	-0.006505	-0.004866	-0.011514
O	3.677009	1.284394	4.211574	-0.006444	-0.004734	-0.011400
O	5.831438	5.616407	1.028179	0.006730	-0.004878	0.011682
O	-3.378295	8.185194	5.338611	0.006138	-0.004730	0.011168
H	-0.637445	12.195109	2.878812	-0.036136	-0.004523	0.010703

H	3.090587	1.606491	3.487978	-0.036081	-0.004390	0.010876
H	5.245016	5.294309	0.304583	0.036489	-0.004758	-0.010563
H	-2.791874	8.507292	6.062207	0.035601	-0.004151	-0.011047

141 f = 7.279511 THz 45.738516 2PiTHz 242.818339 cm-1 30.105648 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.014970	-0.001661	0.024376
Li	-1.316675	4.156264	2.365404	-0.015107	0.001363	-0.024586
Li	-3.471104	2.744536	5.548798	-0.014957	-0.001688	-0.024405
Li	5.924247	11.057064	0.817991	0.015134	0.001419	0.024574
Na	2.049025	6.784862	1.629696	0.001755	-0.052472	0.024702
Na	0.404117	7.016739	4.737094	-0.001678	0.052951	-0.024715
Na	2.558546	13.685662	1.553699	-0.001804	-0.052439	-0.024630
Na	-0.105403	0.115939	4.813091	0.001674	0.053146	0.024890
B	4.155007	8.978944	1.168663	0.001640	0.013392	-0.000249
B	-1.701865	4.822656	5.198127	-0.001738	-0.013412	-0.000047
B	0.452564	2.078144	2.014732	-0.001618	0.013367	0.000173
B	2.000578	11.723457	4.352058	0.001709	-0.013420	0.000110
B	-2.733891	11.746082	5.839177	-0.003072	-0.021781	-0.002579
B	5.187034	2.055518	0.527613	0.003635	0.021636	0.002151
B	3.032605	4.845282	3.711007	0.003119	-0.021831	0.002588
B	-0.579463	8.956318	2.655782	-0.003647	0.021616	-0.002157
B	-0.983708	0.054306	1.827988	0.019504	0.012582	-0.003962
B	3.436850	13.747295	4.538802	-0.019350	-0.012690	0.003831
B	5.591279	6.955106	1.355407	-0.019461	0.012607	0.003885
B	-3.138137	6.846495	5.011383	0.019326	-0.012689	-0.003858
Si	0.631772	3.486686	4.508512	-0.016529	0.001205	-0.001617
Si	1.821370	10.314915	1.858278	0.016672	-0.001206	0.001590
Si	-0.333059	10.387486	5.041673	0.016545	0.001197	0.001607
Si	2.786201	3.414115	1.325117	-0.016680	-0.001232	-0.001614
O	0.061445	3.072947	3.041906	-0.036752	-0.013400	0.013347
O	2.391697	10.728653	3.324884	0.036883	0.013481	-0.013348
O	4.546126	9.973747	0.141489	0.036815	-0.013350	-0.013361
O	-2.092984	3.827853	6.225301	-0.037003	0.013557	0.013407

O	2.197450	3.933608	4.519003	-0.018051	-0.006009	-0.011789
O	0.255692	9.867992	1.847787	0.018142	0.005918	0.012614
O	-1.898737	10.834409	5.031182	0.018074	-0.005990	0.011807
O	4.351879	2.967192	1.335608	-0.018165	0.005877	-0.012593
O	-0.212316	4.798696	5.055280	-0.005925	-0.005926	0.014826
O	2.665458	9.002905	1.311510	0.005739	0.005730	-0.015204
O	0.511030	11.699496	4.494905	0.005913	-0.005866	-0.014718
O	1.942113	2.102105	1.871885	-0.005745	0.005670	0.015057
O	0.525580	2.169271	5.472081	0.003351	0.009016	0.004644
O	1.927562	11.632329	0.894709	-0.002272	-0.009292	-0.005097
O	-0.226867	9.070071	4.078104	-0.003399	0.008960	-0.004628
O	2.680009	4.731529	2.288686	0.002322	-0.009371	0.005123
O	0.058846	0.698526	2.444964	0.033246	0.002854	-0.026270
O	2.394296	13.103075	3.921826	-0.033483	-0.002824	0.026702
O	4.548725	7.599326	0.738431	-0.033164	0.002912	0.026153
O	-2.095583	6.202275	5.628359	0.033449	-0.002786	-0.026663
O	-2.459230	13.184059	5.445139	-0.023515	-0.015580	0.004301
O	4.912372	0.617542	0.921651	0.024404	0.015319	-0.005203
O	2.757943	6.283259	4.105046	0.023539	-0.015630	-0.004335
O	-0.304801	7.518342	2.261744	-0.024370	0.015322	0.005158
O	-0.175430	2.374756	0.744070	-0.004354	0.051352	0.008855
O	2.628573	11.426844	5.622720	0.004753	-0.051274	-0.008641
O	4.783002	9.275557	2.439325	0.004323	0.051288	-0.008882
O	-2.329859	4.526044	3.927465	-0.004704	-0.051298	0.008680
O	-1.223866	12.517207	2.155216	0.006314	0.021850	0.021064
O	3.677009	1.284394	4.211574	-0.006669	-0.021822	-0.021039
O	5.831438	5.616407	1.028179	-0.006300	0.021859	-0.021106
O	-3.378295	8.185194	5.338611	0.006580	-0.021821	0.020957
H	-0.637445	12.195109	2.878812	0.010629	0.026833	0.020855
H	3.090587	1.606491	3.487978	-0.011483	-0.026818	-0.020450
H	5.245016	5.294309	0.304583	-0.010634	0.026801	-0.020864
H	-2.791874	8.507292	6.062207	0.011366	-0.026786	0.020379

142 f = 7.145537 THz 44.896733 2PiTHz 238.349450 cm-1 29.551576 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.021298	-0.001822	0.003636
Li	-1.316675	4.156264	2.365404	0.021238	0.002152	-0.003146
Li	-3.471104	2.744536	5.548798	0.021288	-0.001946	-0.003599
Li	5.924247	11.057064	0.817991	-0.021246	0.002266	0.003135
Na	2.049025	6.784862	1.629696	-0.008915	0.055543	-0.014984
Na	0.404117	7.016739	4.737094	0.008782	-0.055448	0.015098
Na	2.558546	13.685662	1.553699	0.008937	0.055310	0.014884
Na	-0.105403	0.115939	4.813091	-0.008659	-0.055457	-0.015055
B	4.155007	8.978944	1.168663	0.000045	0.022613	0.001787
B	-1.701865	4.822656	5.198127	0.000233	-0.022708	-0.001797
B	0.452564	2.078144	2.014732	0.000025	0.022605	-0.001829
B	2.000578	11.723457	4.352058	-0.000292	-0.022685	0.001850
B	-2.733891	11.746082	5.839177	-0.000952	-0.011354	-0.000986
B	5.187034	2.055518	0.527613	0.000450	0.011481	0.001557
B	3.032605	4.845282	3.711007	0.000872	-0.011354	0.001081
B	-0.579463	8.956318	2.655782	-0.000402	0.011497	-0.001645
B	-0.983708	0.054306	1.827988	0.008473	0.013253	-0.014667
B	3.436850	13.747295	4.538802	-0.008904	-0.013194	0.015046
B	5.591279	6.955106	1.355407	-0.008398	0.013255	0.014578
B	-3.138137	6.846495	5.011383	0.008822	-0.013226	-0.014900
Si	0.631772	3.486686	4.508512	0.002400	-0.004668	0.014148
Si	1.821370	10.314915	1.858278	-0.002541	0.004638	-0.014235
Si	-0.333059	10.387486	5.041673	-0.002356	-0.004650	-0.014134
Si	2.786201	3.414115	1.325117	0.002478	0.004642	0.014237
O	0.061445	3.072947	3.041906	0.010255	0.006754	0.010853
O	2.391697	10.728653	3.324884	-0.010627	-0.006845	-0.010869
O	4.546126	9.973747	0.141489	-0.010108	0.006723	-0.010889
O	-2.092984	3.827853	6.225301	0.010520	-0.006883	0.010868
O	2.197450	3.933608	4.519003	-0.004474	0.016069	0.033985
O	0.255692	9.867992	1.847787	0.004281	-0.015883	-0.034851
O	-1.898737	10.834409	5.031182	0.004525	0.016132	-0.033871
O	4.351879	2.967192	1.335608	-0.004341	-0.015912	0.034717
O	-0.212316	4.798696	5.055280	-0.004077	-0.010490	0.005978
O	2.665458	9.002905	1.311510	0.004280	0.010718	-0.006148
O	0.511030	11.699496	4.494905	0.004045	-0.010394	-0.005870

O	1.942113	2.102105	1.871885	-0.004234	0.010606	0.006049
O	0.525580	2.169271	5.472081	-0.023349	-0.000738	0.010042
O	1.927562	11.632329	0.894709	0.022440	0.001135	-0.009470
O	-0.226867	9.070071	4.078104	0.023493	-0.000642	-0.010141
O	2.680009	4.731529	2.288686	-0.022602	0.001112	0.009553
O	0.058846	0.698526	2.444964	0.008122	0.013302	-0.020390
O	2.394296	13.103075	3.921826	-0.008501	-0.013255	0.020699
O	4.548725	7.599326	0.738431	-0.008067	0.013308	0.020314
O	-2.095583	6.202275	5.628359	0.008428	-0.013296	-0.020567
O	-2.459230	13.184059	5.445139	-0.029526	-0.004059	0.034492
O	4.912372	0.617542	0.921651	0.028313	0.004364	-0.033261
O	2.757943	6.283259	4.105046	0.029340	-0.004111	-0.034247
O	-0.304801	7.518342	2.261744	-0.028150	0.004423	0.033065
O	-0.175430	2.374756	0.744070	-0.006235	0.051880	0.004457
O	2.628573	11.426844	5.622720	0.006067	-0.052543	-0.004686
O	4.783002	9.275557	2.439325	0.006237	0.051784	-0.004440
O	-2.329859	4.526044	3.927465	-0.006085	-0.052406	0.004672
O	-1.223866	12.517207	2.155216	-0.027583	0.023806	0.004586
O	3.677009	1.284394	4.211574	0.028200	-0.024155	-0.005072
O	5.831438	5.616407	1.028179	0.027557	0.023772	-0.004575
O	-3.378295	8.185194	5.338611	-0.028161	-0.024134	0.005109
H	-0.637445	12.195109	2.878812	-0.035037	0.008600	0.002560
H	3.090587	1.606491	3.487978	0.035978	-0.008856	-0.003260
H	5.245016	5.294309	0.304583	0.034970	0.008549	-0.002512
H	-2.791874	8.507292	6.062207	-0.035898	-0.008800	0.003249

143 f = 7.016710 THz 44.087291 2PiTHz 234.052256 cm-1 29.018792 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000503	0.022892	0.007126
Li	-1.316675	4.156264	2.365404	0.000113	-0.023302	-0.008435
Li	-3.471104	2.744536	5.548798	-0.000115	-0.023468	0.008460
Li	5.924247	11.057064	0.817991	-0.000375	0.022666	-0.007166
Na	2.049025	6.784862	1.629696	-0.012788	0.027732	-0.012593
Na	0.404117	7.016739	4.737094	0.013500	-0.028821	0.012341

Na	2.558546	13.685662	1.553699	-0.013556	-0.029424	-0.012527
Na	-0.105403	0.115939	4.813091	0.012799	0.027449	0.012485
B	4.155007	8.978944	1.168663	0.015267	0.004806	0.000249
B	-1.701865	4.822656	5.198127	-0.015876	-0.003910	0.000094
B	0.452564	2.078144	2.014732	0.015899	-0.004355	-0.000038
B	2.000578	11.723457	4.352058	-0.015255	0.004540	-0.000208
B	-2.733891	11.746082	5.839177	-0.022964	0.002256	0.020494
B	5.187034	2.055518	0.527613	0.023536	-0.002606	-0.021369
B	3.032605	4.845282	3.711007	-0.023590	-0.002158	0.021334
B	-0.579463	8.956318	2.655782	0.022896	0.002592	-0.020493
B	-0.983708	0.054306	1.827988	0.018683	-0.003585	-0.023821
B	3.436850	13.747295	4.538802	-0.017645	0.003341	0.023090
B	5.591279	6.955106	1.355407	0.017493	0.003596	-0.022871
B	-3.138137	6.846495	5.011383	-0.018930	-0.003212	0.024102
Si	0.631772	3.486686	4.508512	0.011426	-0.001353	0.000806
Si	1.821370	10.314915	1.858278	-0.011023	0.001487	-0.000341
Si	-0.333059	10.387486	5.041673	0.011082	0.001511	0.000356
Si	2.786201	3.414115	1.325117	-0.011339	-0.001390	-0.000892
O	0.061445	3.072947	3.041906	0.024728	0.001257	-0.002305
O	2.391697	10.728653	3.324884	-0.023840	-0.001244	0.002613
O	4.546126	9.973747	0.141489	0.023998	-0.001255	-0.002718
O	-2.092984	3.827853	6.225301	-0.024560	0.001263	0.002103
O	2.197450	3.933608	4.519003	0.009718	-0.007568	0.033394
O	0.255692	9.867992	1.847787	-0.008946	0.007053	-0.032437
O	-1.898737	10.834409	5.031182	0.009043	0.006960	0.032454
O	4.351879	2.967192	1.335608	-0.009553	-0.007597	-0.033602
O	-0.212316	4.798696	5.055280	-0.013791	-0.022127	0.007351
O	2.665458	9.002905	1.311510	0.013699	0.022116	-0.006409
O	0.511030	11.699496	4.494905	-0.013646	0.021980	0.006291
O	1.942113	2.102105	1.871885	0.013892	-0.022358	-0.007513
O	0.525580	2.169271	5.472081	0.048017	-0.013695	-0.021762
O	1.927562	11.632329	0.894709	-0.046723	0.012813	0.020830
O	-0.226867	9.070071	4.078104	0.046726	0.012997	-0.020896
O	2.680009	4.731529	2.288686	-0.047804	-0.013520	0.021599
O	0.058846	0.698526	2.444964	0.005498	-0.002243	-0.005109
O	2.394296	13.103075	3.921826	-0.004062	0.001836	0.003829

O	4.548725	7.599326	0.738431	0.003855	0.002025	-0.003509
O	-2.095583	6.202275	5.628359	-0.005834	-0.001953	0.005591
O	-2.459230	13.184059	5.445139	-0.047769	0.012574	0.055306
O	4.912372	0.617542	0.921651	0.050037	-0.013360	-0.057440
O	2.757943	6.283259	4.105046	-0.050495	-0.012966	0.057814
O	-0.304801	7.518342	2.261744	0.047541	0.012913	-0.055124
O	-0.175430	2.374756	0.744070	0.012152	0.020431	0.009610
O	2.628573	11.426844	5.622720	-0.012326	-0.018669	-0.009024
O	4.783002	9.275557	2.439325	0.012363	-0.017956	0.008939
O	-2.329859	4.526044	3.927465	-0.012049	0.021568	-0.009740
O	-1.223866	12.517207	2.155216	-0.009730	0.005573	-0.007563
O	3.677009	1.284394	4.211574	0.008466	-0.004879	0.009099
O	5.831438	5.616407	1.028179	-0.008446	-0.004549	-0.008988
O	-3.378295	8.185194	5.338611	0.009913	0.006113	0.007533
H	-0.637445	12.195109	2.878812	-0.023306	0.007388	0.004399
H	3.090587	1.606491	3.487978	0.021961	-0.006999	-0.002928
H	5.245016	5.294309	0.304583	-0.021850	-0.006638	0.002950
H	-2.791874	8.507292	6.062207	0.023589	0.007858	-0.004474

144 f = 7.004460 THz 44.010319 2PiTHz 233.643622 cm-1 28.968128 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.009801	0.011318	0.024540
Li	-1.316675	4.156264	2.365404	-0.010340	0.009898	0.023927
Li	-3.471104	2.744536	5.548798	0.009796	0.009925	-0.024058
Li	5.924247	11.057064	0.817991	0.010326	0.011256	-0.024393
Na	2.049025	6.784862	1.629696	-0.011640	0.026137	-0.001646
Na	0.404117	7.016739	4.737094	-0.011250	0.026401	-0.001764
Na	2.558546	13.685662	1.553699	0.011068	0.024967	0.001217
Na	-0.105403	0.115939	4.813091	0.011839	0.027580	0.002191
B	4.155007	8.978944	1.168663	0.012174	-0.009759	-0.006341
B	-1.701865	4.822656	5.198127	0.011289	-0.009562	-0.006275
B	0.452564	2.078144	2.014732	-0.011313	-0.009909	0.006304
B	2.000578	11.723457	4.352058	-0.012153	-0.009388	0.006302
B	-2.733891	11.746082	5.839177	-0.011938	-0.000124	0.016657

B	5.187034	2.055518	0.527613	-0.010677	-0.000357	0.015409
B	3.032605	4.845282	3.711007	0.010675	-0.000269	-0.015422
B	-0.579463	8.956318	2.655782	0.011915	-0.000233	-0.016631
B	-0.983708	0.054306	1.827988	-0.021930	-0.001445	0.016971
B	3.436850	13.747295	4.538802	-0.022986	-0.001087	0.018044
B	5.591279	6.955106	1.355407	0.023033	-0.001287	-0.018302
B	-3.138137	6.846495	5.011383	0.021907	-0.001272	-0.016672
Si	0.631772	3.486686	4.508512	-0.005499	-0.002037	-0.009175
Si	1.821370	10.314915	1.858278	-0.005977	-0.002061	-0.008999
Si	-0.333059	10.387486	5.041673	0.006140	-0.001972	0.009292
Si	2.786201	3.414115	1.325117	0.005312	-0.002087	0.008870
O	0.061445	3.072947	3.041906	-0.013343	-0.000576	-0.007745
O	2.391697	10.728653	3.324884	-0.014202	-0.000365	-0.007586
O	4.546126	9.973747	0.141489	0.014694	-0.000633	0.007689
O	-2.092984	3.827853	6.225301	0.012821	-0.000330	0.007619
O	2.197450	3.933608	4.519003	-0.011218	0.010218	-0.019197
O	0.255692	9.867992	1.847787	-0.011744	0.010964	-0.020364
O	-1.898737	10.834409	5.031182	0.011805	0.010671	0.021136
O	4.351879	2.967192	1.335608	0.011152	0.010594	0.018387
O	-0.212316	4.798696	5.055280	0.002893	0.003427	-0.020410
O	2.665458	9.002905	1.311510	0.003576	0.004440	-0.020905
O	0.511030	11.699496	4.494905	-0.003607	0.004579	0.020893
O	1.942113	2.102105	1.871885	-0.002865	0.003318	0.020406
O	0.525580	2.169271	5.472081	-0.019609	0.013094	0.014605
O	1.927562	11.632329	0.894709	-0.022762	0.013923	0.016052
O	-0.226867	9.070071	4.078104	0.022242	0.013976	-0.015872
O	2.680009	4.731529	2.288686	0.020088	0.013068	-0.014782
O	0.058846	0.698526	2.444964	-0.031442	0.002866	0.031365
O	2.394296	13.103075	3.921826	-0.031988	0.003266	0.031634
O	4.548725	7.599326	0.738431	0.031913	0.002990	-0.031818
O	-2.095583	6.202275	5.628359	0.031540	0.003107	-0.031148
O	-2.459230	13.184059	5.445139	-0.048212	0.008267	0.044634
O	4.912372	0.617542	0.921651	-0.045867	0.007577	0.042162
O	2.757943	6.283259	4.105046	0.045467	0.007557	-0.041497
O	-0.304801	7.518342	2.261744	0.048594	0.008254	-0.045224
O	-0.175430	2.374756	0.744070	0.005018	-0.047868	-0.011771

O	2.628573	11.426844	5.622720	0.004343	-0.048468	-0.012281
O	4.783002	9.275557	2.439325	-0.004436	-0.049138	0.012310
O	-2.329859	4.526044	3.927465	-0.004939	-0.047190	0.011732
O	-1.223866	12.517207	2.155216	0.025075	-0.020936	-0.029173
O	3.677009	1.284394	4.211574	0.025050	-0.020968	-0.028882
O	5.831438	5.616407	1.028179	-0.025568	-0.021293	0.028789
O	-3.378295	8.185194	5.338611	-0.024479	-0.020624	0.029290
H	-0.637445	12.195109	2.878812	0.027370	-0.014878	-0.028472
H	3.090587	1.606491	3.487978	0.027829	-0.015265	-0.028767
H	5.245016	5.294309	0.304583	-0.028519	-0.015259	0.028635
H	-2.791874	8.507292	6.062207	-0.026570	-0.014910	0.028612

145 f = 6.888065 THz 43.278990 2PiTHz 229.761117 cm-1 28.486758
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000820	-0.013522	-0.005703
Li	-1.316675	4.156264	2.365404	-0.000631	0.014383	0.005889
Li	-3.471104	2.744536	5.548798	0.000929	0.013580	-0.005858
Li	5.924247	11.057064	0.817991	-0.000558	-0.014312	0.005705
Na	2.049025	6.784862	1.629696	-0.014687	0.081350	-0.016789
Na	0.404117	7.016739	4.737094	0.014356	-0.077595	0.015468
Na	2.558546	13.685662	1.553699	-0.014741	-0.081148	-0.016705
Na	-0.105403	0.115939	4.813091	0.014305	0.077723	0.015493
B	4.155007	8.978944	1.168663	0.000358	0.011304	-0.003913
B	-1.701865	4.822656	5.198127	-0.000149	-0.009598	0.004199
B	0.452564	2.078144	2.014732	0.000292	-0.011362	-0.003880
B	2.000578	11.723457	4.352058	-0.000221	0.009547	0.004243
B	-2.733891	11.746082	5.839177	0.003940	0.001529	-0.010507
B	5.187034	2.055518	0.527613	-0.004296	-0.003659	0.010425
B	3.032605	4.845282	3.711007	0.003980	-0.001520	-0.010571
B	-0.579463	8.956318	2.655782	-0.004241	0.003645	0.010356
B	-0.983708	0.054306	1.827988	-0.011197	-0.004608	0.007565
B	3.436850	13.747295	4.538802	0.010152	0.003016	-0.006189
B	5.591279	6.955106	1.355407	-0.011064	0.004590	0.007479
B	-3.138137	6.846495	5.011383	0.010273	-0.003025	-0.006265

Si	0.631772	3.486686	4.508512	-0.003191	-0.005128	-0.012924
Si	1.821370	10.314915	1.858278	0.003475	0.005200	0.012820
Si	-0.333059	10.387486	5.041673	-0.003146	0.005114	-0.012862
Si	2.786201	3.414115	1.325117	0.003540	-0.005195	0.012890
O	0.061445	3.072947	3.041906	0.006851	0.008717	-0.019528
O	2.391697	10.728653	3.324884	-0.005993	-0.008576	0.018725
O	4.546126	9.973747	0.141489	0.006943	-0.008725	-0.019474
O	-2.092984	3.827853	6.225301	-0.005852	0.008552	0.018763
O	2.197450	3.933608	4.519003	-0.007453	-0.002236	-0.021378
O	0.255692	9.867992	1.847787	0.007970	0.002834	0.020880
O	-1.898737	10.834409	5.031182	-0.007376	0.002298	-0.021293
O	4.351879	2.967192	1.335608	0.008070	-0.002769	0.020994
O	-0.212316	4.798696	5.055280	-0.005074	-0.017228	-0.002261
O	2.665458	9.002905	1.311510	0.005539	0.018383	0.001497
O	0.511030	11.699496	4.494905	-0.005091	0.017271	-0.002097
O	1.942113	2.102105	1.871885	0.005530	-0.018333	0.001639
O	0.525580	2.169271	5.472081	-0.015359	0.017595	0.012341
O	1.927562	11.632329	0.894709	0.015706	-0.018626	-0.012937
O	-0.226867	9.070071	4.078104	-0.015224	-0.017523	0.012269
O	2.680009	4.731529	2.288686	0.015803	0.018720	-0.013005
O	0.058846	0.698526	2.444964	-0.026316	0.006680	0.025924
O	2.394296	13.103075	3.921826	0.024728	-0.007830	-0.023595
O	4.548725	7.599326	0.738431	-0.026123	-0.006673	0.025737
O	-2.095583	6.202275	5.628359	0.024903	0.007834	-0.023764
O	-2.459230	13.184059	5.445139	0.011479	0.005079	-0.004394
O	4.912372	0.617542	0.921651	-0.013256	-0.007088	0.005865
O	2.757943	6.283259	4.105046	0.011722	-0.005028	-0.004609
O	-0.304801	7.518342	2.261744	-0.012987	0.007123	0.005635
O	-0.175430	2.374756	0.744070	0.004684	-0.031506	-0.010104
O	2.628573	11.426844	5.622720	-0.004303	0.026593	0.009559
O	4.783002	9.275557	2.439325	0.004633	0.031189	-0.010011
O	-2.329859	4.526044	3.927465	-0.004354	-0.026857	0.009636
O	-1.223866	12.517207	2.155216	0.018774	-0.012354	-0.008089
O	3.677009	1.284394	4.211574	-0.018040	0.010026	0.008218
O	5.831438	5.616407	1.028179	0.018634	0.012219	-0.007895
O	-3.378295	8.185194	5.338611	-0.018181	-0.010145	0.008404

H	-0.637445	12.195109	2.878812	0.011906	0.004517	0.005962
H	3.090587	1.606491	3.487978	-0.010667	-0.006843	-0.006256
H	5.245016	5.294309	0.304583	0.011768	-0.004628	0.006147
H	-2.791874	8.507292	6.062207	-0.010800	0.006764	-0.006093

146 f = 6.786627 THz 42.641638 2PiTHz 226.377516 cm-1 28.067245 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.003121	0.009414	0.001533
Li	-1.316675	4.156264	2.365404	0.003146	0.008755	0.001173
Li	-3.471104	2.744536	5.548798	0.003076	-0.009486	0.001476
Li	5.924247	11.057064	0.817991	0.003185	-0.008691	0.001233
Na	2.049025	6.784862	1.629696	-0.006655	0.055135	-0.021590
Na	0.404117	7.016739	4.737094	-0.008050	0.061271	-0.022739
Na	2.558546	13.685662	1.553699	-0.006791	-0.055335	-0.021308
Na	-0.105403	0.115939	4.813091	-0.007916	-0.061009	-0.023048
B	4.155007	8.978944	1.168663	0.002392	0.020565	0.004959
B	-1.701865	4.822656	5.198127	0.002572	0.021346	0.004629
B	0.452564	2.078144	2.014732	0.002385	-0.020526	0.005032
B	2.000578	11.723457	4.352058	0.002586	-0.021400	0.004625
B	-2.733891	11.746082	5.839177	-0.004547	-0.027952	-0.002036
B	5.187034	2.055518	0.527613	-0.004486	-0.027696	-0.002425
B	3.032605	4.845282	3.711007	-0.004565	0.027964	-0.002012
B	-0.579463	8.956318	2.655782	-0.004518	0.027674	-0.002442
B	-0.983708	0.054306	1.827988	-0.011285	-0.018357	0.018240
B	3.436850	13.747295	4.538802	-0.011845	-0.018728	0.018369
B	5.591279	6.955106	1.355407	-0.011283	0.018376	0.018180
B	-3.138137	6.846495	5.011383	-0.011833	0.018711	0.018404
Si	0.631772	3.486686	4.508512	0.004438	0.000975	0.001129
Si	1.821370	10.314915	1.858278	0.004348	0.000554	0.000177
Si	-0.333059	10.387486	5.041673	0.004443	-0.000977	0.001089
Si	2.786201	3.414115	1.325117	0.004332	-0.000549	0.000215
O	0.061445	3.072947	3.041906	0.014018	0.004644	-0.009587
O	2.391697	10.728653	3.324884	0.014938	0.005286	-0.011108
O	4.546126	9.973747	0.141489	0.014110	-0.004618	-0.009649

O	-2.092984	3.827853	6.225301	0.014843	-0.005304	-0.011060
O	2.197450	3.933608	4.519003	0.008141	0.006939	-0.004467
O	0.255692	9.867992	1.847787	0.007702	0.006727	-0.005365
O	-1.898737	10.834409	5.031182	0.008156	-0.006942	-0.004450
O	4.351879	2.967192	1.335608	0.007694	-0.006701	-0.005441
O	-0.212316	4.798696	5.055280	0.006888	0.016050	-0.007213
O	2.665458	9.002905	1.311510	0.006356	0.014497	-0.007301
O	0.511030	11.699496	4.494905	0.006901	-0.016101	-0.007318
O	1.942113	2.102105	1.871885	0.006372	-0.014453	-0.007107
O	0.525580	2.169271	5.472081	0.005475	-0.017401	-0.009731
O	1.927562	11.632329	0.894709	0.004842	-0.016359	-0.009197
O	-0.226867	9.070071	4.078104	0.005336	0.017352	-0.009726
O	2.680009	4.731529	2.288686	0.004862	0.016397	-0.009186
O	0.058846	0.698526	2.444964	-0.017855	-0.012900	0.029039
O	2.394296	13.103075	3.921826	-0.019646	-0.012464	0.030677
O	4.548725	7.599326	0.738431	-0.017865	0.012933	0.029000
O	-2.095583	6.202275	5.628359	-0.019569	0.012444	0.030602
O	-2.459230	13.184059	5.445139	-0.019595	-0.027187	0.016867
O	4.912372	0.617542	0.921651	-0.019205	-0.026570	0.017182
O	2.757943	6.283259	4.105046	-0.019621	0.027186	0.016937
O	-0.304801	7.518342	2.261744	-0.019222	0.026560	0.017153
O	-0.175430	2.374756	0.744070	0.003755	-0.058088	-0.005288
O	2.628573	11.426844	5.622720	0.004171	-0.060015	-0.005995
O	4.783002	9.275557	2.439325	0.003717	0.058076	-0.005347
O	-2.329859	4.526044	3.927465	0.004152	0.059976	-0.005982
O	-1.223866	12.517207	2.155216	0.008823	-0.026950	0.006451
O	3.677009	1.284394	4.211574	0.010089	-0.027782	0.005577
O	5.831438	5.616407	1.028179	0.008806	0.026983	0.006312
O	-3.378295	8.185194	5.338611	0.010126	0.027739	0.005733
H	-0.637445	12.195109	2.878812	0.017002	-0.028603	-0.001278
H	3.090587	1.606491	3.487978	0.017615	-0.028154	-0.000991
H	5.245016	5.294309	0.304583	0.016971	0.028646	-0.001417
H	-2.791874	8.507292	6.062207	0.017735	0.028095	-0.000884

147 f = 6.256865 THz 39.313045 2PiTHz 208.706560 cm-1 25.876325

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.004356	-0.001833	-0.024274
Li	-1.316675	4.156264	2.365404	-0.003476	0.002704	0.023736
Li	-3.471104	2.744536	5.548798	-0.003520	-0.002636	0.023782
Li	5.924247	11.057064	0.817991	0.004366	0.001788	-0.024282
Na	2.049025	6.784862	1.629696	-0.004091	0.004333	0.008262
Na	0.404117	7.016739	4.737094	0.003953	-0.003989	-0.008099
Na	2.558546	13.685662	1.553699	0.003959	0.004010	-0.008171
Na	-0.105403	0.115939	4.813091	-0.004099	-0.004344	0.008270
B	4.155007	8.978944	1.168663	0.000899	0.009536	-0.014753
B	-1.701865	4.822656	5.198127	-0.000884	-0.009108	0.015228
B	0.452564	2.078144	2.014732	-0.000907	0.009077	0.015224
B	2.000578	11.723457	4.352058	0.000896	-0.009494	-0.014693
B	-2.733891	11.746082	5.839177	-0.011377	-0.023290	0.007984
B	5.187034	2.055518	0.527613	0.011663	0.023591	-0.007741
B	3.032605	4.845282	3.711007	0.011699	-0.023565	-0.007765
B	-0.579463	8.956318	2.655782	-0.011396	0.023259	0.007931
B	-0.983708	0.054306	1.827988	-0.013232	0.019386	-0.025623
B	3.436850	13.747295	4.538802	0.012803	-0.019658	0.024772
B	5.591279	6.955106	1.355407	0.012756	0.019665	0.024666
B	-3.138137	6.846495	5.011383	-0.013165	-0.019391	-0.025602
Si	0.631772	3.486686	4.508512	0.005278	0.004907	0.003150
Si	1.821370	10.314915	1.858278	-0.005008	-0.004758	-0.002658
Si	-0.333059	10.387486	5.041673	-0.005012	0.004758	-0.002707
Si	2.786201	3.414115	1.325117	0.005267	-0.004919	0.003164
O	0.061445	3.072947	3.041906	-0.010038	0.006319	0.010102
O	2.391697	10.728653	3.324884	0.009865	-0.006846	-0.009360
O	4.546126	9.973747	0.141489	0.009896	0.006857	-0.009423
O	-2.092984	3.827853	6.225301	-0.010012	-0.006358	0.010096
O	2.197450	3.933608	4.519003	0.014597	-0.034904	-0.025989
O	0.255692	9.867992	1.847787	-0.014150	0.034459	0.026129
O	-1.898737	10.834409	5.031182	-0.014175	-0.034540	0.026193
O	4.351879	2.967192	1.335608	0.014599	0.034948	-0.025966
O	-0.212316	4.798696	5.055280	0.007053	-0.004000	0.029857
O	2.665458	9.002905	1.311510	-0.006741	0.004247	-0.028968

O	0.511030	11.699496	4.494905	-0.006757	-0.004210	-0.028950
O	1.942113	2.102105	1.871885	0.007033	0.003991	0.029864
O	0.525580	2.169271	5.472081	0.028593	-0.001159	-0.009165
O	1.927562	11.632329	0.894709	-0.028289	0.001332	0.009523
O	-0.226867	9.070071	4.078104	-0.028296	-0.001327	0.009462
O	2.680009	4.731529	2.288686	0.028591	0.001169	-0.009178
O	0.058846	0.698526	2.444964	-0.020472	0.006311	0.001167
O	2.394296	13.103075	3.921826	0.020103	-0.007109	-0.001408
O	4.548725	7.599326	0.738431	0.020089	0.007162	-0.001517
O	-2.095583	6.202275	5.628359	-0.020439	-0.006353	0.001205
O	-2.459230	13.184059	5.445139	0.013486	-0.036651	0.008841
O	4.912372	0.617542	0.921651	-0.013845	0.037105	-0.009137
O	2.757943	6.283259	4.105046	-0.013730	-0.037059	-0.009200
O	-0.304801	7.518342	2.261744	0.013398	0.036599	0.008808
O	-0.175430	2.374756	0.744070	0.012058	0.016285	0.011453
O	2.628573	11.426844	5.622720	-0.011569	-0.016404	-0.011082
O	4.783002	9.275557	2.439325	-0.011575	0.016443	-0.011134
O	-2.329859	4.526044	3.927465	0.012079	-0.016299	0.011455
O	-1.223866	12.517207	2.155216	-0.018226	0.008286	-0.078832
O	3.677009	1.284394	4.211574	0.017280	-0.008879	0.076530
O	5.831438	5.616407	1.028179	0.017232	0.008903	0.076361
O	-3.378295	8.185194	5.338611	-0.018180	-0.008311	-0.078756
H	-0.637445	12.195109	2.878812	-0.034196	-0.008723	-0.074757
H	3.090587	1.606491	3.487978	0.032176	0.007766	0.073059
H	5.245016	5.294309	0.304583	0.032107	-0.007751	0.072906
H	-2.791874	8.507292	6.062207	-0.034157	0.008718	-0.074682

148 f = 6.245334 THz 39.240593 2PiTHz 208.321922 cm-1 25.828636

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.028768	0.029837	-0.016275
Li	-1.316675	4.156264	2.365404	0.028911	0.029658	-0.016936
Li	-3.471104	2.744536	5.548798	0.028918	-0.029763	-0.016986
Li	5.924247	11.057064	0.817991	0.028749	-0.029794	-0.016284
Na	2.049025	6.784862	1.629696	-0.005669	0.006535	0.000538

Na	0.404117	7.016739	4.737094	-0.005855	0.006677	0.000544
Na	2.558546	13.685662	1.553699	-0.005783	-0.006565	0.000638
Na	-0.105403	0.115939	4.813091	-0.005692	-0.006638	0.000521
B	4.155007	8.978944	1.168663	-0.000058	0.012779	0.017521
B	-1.701865	4.822656	5.198127	-0.000016	0.013143	0.017037
B	0.452564	2.078144	2.014732	-0.000039	-0.013123	0.017048
B	2.000578	11.723457	4.352058	-0.000086	-0.012840	0.017479
B	-2.733891	11.746082	5.839177	0.010420	0.011441	0.006822
B	5.187034	2.055518	0.527613	0.010094	0.010733	0.007096
B	3.032605	4.845282	3.711007	0.010109	-0.010704	0.007059
B	-0.579463	8.956318	2.655782	0.010473	-0.011405	0.006855
B	-0.983708	0.054306	1.827988	-0.015240	-0.007685	-0.028651
B	3.436850	13.747295	4.538802	-0.015680	-0.007085	-0.029416
B	5.591279	6.955106	1.355407	-0.015554	0.007072	-0.029334
B	-3.138137	6.846495	5.011383	-0.015257	0.007690	-0.028632
Si	0.631772	3.486686	4.508512	0.009537	0.004972	0.015807
Si	1.821370	10.314915	1.858278	0.009681	0.005100	0.015852
Si	-0.333059	10.387486	5.041673	0.009651	-0.005101	0.015903
Si	2.786201	3.414115	1.325117	0.009524	-0.004950	0.015773
O	0.061445	3.072947	3.041906	-0.004027	-0.015494	0.023192
O	2.391697	10.728653	3.324884	-0.004323	-0.015235	0.023412
O	4.546126	9.973747	0.141489	-0.004369	0.015219	0.023471
O	-2.092984	3.827853	6.225301	-0.003959	0.015417	0.023095
O	2.197450	3.933608	4.519003	0.015530	-0.016025	0.005504
O	0.255692	9.867992	1.847787	0.015923	-0.017028	0.004741
O	-1.898737	10.834409	5.031182	0.015928	0.017120	0.004685
O	4.351879	2.967192	1.335608	0.015493	0.015999	0.005574
O	-0.212316	4.798696	5.055280	0.010055	0.007136	0.030306
O	2.665458	9.002905	1.311510	0.010232	0.006905	0.031259
O	0.511030	11.699496	4.494905	0.010230	-0.006988	0.031233
O	1.942113	2.102105	1.871885	0.010014	-0.007055	0.030311
O	0.525580	2.169271	5.472081	0.010764	0.005714	0.010917
O	1.927562	11.632329	0.894709	0.011661	0.005637	0.010573
O	-0.226867	9.070071	4.078104	0.011645	-0.005635	0.010624
O	2.680009	4.731529	2.288686	0.010787	-0.005672	0.010867
O	0.058846	0.698526	2.444964	-0.012866	-0.025362	-0.008218

O	2.394296	13.103075	3.921826	-0.013538	-0.025136	-0.008155
O	4.548725	7.599326	0.738431	-0.013424	0.025087	-0.008107
O	-2.095583	6.202275	5.628359	-0.012924	0.025342	-0.008140
O	-2.459230	13.184059	5.445139	-0.013123	0.018002	-0.010347
O	4.912372	0.617542	0.921651	-0.012630	0.016872	-0.010109
O	2.757943	6.283259	4.105046	-0.012643	-0.016844	-0.010114
O	-0.304801	7.518342	2.261744	-0.012949	-0.017956	-0.010343
O	-0.175430	2.374756	0.744070	0.016887	-0.004794	0.011741
O	2.628573	11.426844	5.622720	0.017240	-0.004368	0.012043
O	4.783002	9.275557	2.439325	0.017262	0.004290	0.012089
O	-2.329859	4.526044	3.927465	0.016921	0.004900	0.011705
O	-1.223866	12.517207	2.155216	-0.033086	-0.018153	-0.076941
O	3.677009	1.284394	4.211574	-0.033569	-0.017906	-0.079313
O	5.831438	5.616407	1.028179	-0.033505	0.017854	-0.079141
O	-3.378295	8.185194	5.338611	-0.033036	0.018179	-0.076947
H	-0.637445	12.195109	2.878812	-0.069717	-0.030645	-0.056373
H	3.090587	1.606491	3.487978	-0.070632	-0.030862	-0.058632
H	5.245016	5.294309	0.304583	-0.070565	0.030847	-0.058481
H	-2.791874	8.507292	6.062207	-0.069651	0.030636	-0.056371

149 f = 5.918349 THz 37.186084 2PiTHz 197.414871 cm-1 24.476333 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.010377	0.020269	-0.012489
Li	-1.316675	4.156264	2.365404	-0.010408	-0.020363	0.012462
Li	-3.471104	2.744536	5.548798	0.010325	-0.020270	-0.012426
Li	5.924247	11.057064	0.817991	-0.010414	0.020324	0.012462
Na	2.049025	6.784862	1.629696	0.010771	0.022516	-0.005519
Na	0.404117	7.016739	4.737094	-0.010757	-0.022715	0.005900
Na	2.558546	13.685662	1.553699	0.010848	-0.022492	-0.005732
Na	-0.105403	0.115939	4.813091	-0.010698	0.022728	0.005727
B	4.155007	8.978944	1.168663	-0.002875	-0.016570	0.008103
B	-1.701865	4.822656	5.198127	0.002857	0.016561	-0.008178
B	0.452564	2.078144	2.014732	-0.002882	0.016568	0.008159
B	2.000578	11.723457	4.352058	0.002865	-0.016563	-0.008195

B	-2.733891	11.746082	5.839177	-0.000586	-0.006565	-0.015503
B	5.187034	2.055518	0.527613	0.000569	0.006558	0.015514
B	3.032605	4.845282	3.711007	-0.000566	0.006553	-0.015531
B	-0.579463	8.956318	2.655782	0.000537	-0.006554	0.015516
B	-0.983708	0.054306	1.827988	0.014100	0.003788	0.010278
B	3.436850	13.747295	4.538802	-0.014016	-0.003822	-0.010264
B	5.591279	6.955106	1.355407	0.014133	-0.003775	0.010259
B	-3.138137	6.846495	5.011383	-0.014026	0.003823	-0.010339
Si	0.631772	3.486686	4.508512	0.000452	0.011518	0.006040
Si	1.821370	10.314915	1.858278	-0.000484	-0.011548	-0.006058
Si	-0.333059	10.387486	5.041673	0.000420	-0.011517	0.006009
Si	2.786201	3.414115	1.325117	-0.000501	0.011518	-0.006072
O	0.061445	3.072947	3.041906	-0.023741	-0.009305	0.023674
O	2.391697	10.728653	3.324884	0.023703	0.009252	-0.023665
O	4.546126	9.973747	0.141489	-0.023739	0.009312	0.023627
O	-2.092984	3.827853	6.225301	0.023654	-0.009245	-0.023660
O	2.197450	3.933608	4.519003	0.014273	-0.034559	-0.045122
O	0.255692	9.867992	1.847787	-0.014338	0.034655	0.045189
O	-1.898737	10.834409	5.031182	0.014243	0.034571	-0.045123
O	4.351879	2.967192	1.335608	-0.014339	-0.034618	0.045102
O	-0.212316	4.798696	5.055280	0.010997	0.024785	-0.004434
O	2.665458	9.002905	1.311510	-0.011048	-0.024855	0.004396
O	0.511030	11.699496	4.494905	0.010987	-0.024815	-0.004518
O	1.942113	2.102105	1.871885	-0.011046	0.024830	0.004428
O	0.525580	2.169271	5.472081	-0.015960	0.029447	0.025598
O	1.927562	11.632329	0.894709	0.015966	-0.029449	-0.025591
O	-0.226867	9.070071	4.078104	-0.016095	-0.029498	0.025630
O	2.680009	4.731529	2.288686	0.015972	0.029412	-0.025603
O	0.058846	0.698526	2.444964	0.016721	0.007517	-0.002823
O	2.394296	13.103075	3.921826	-0.016646	-0.007510	0.002789
O	4.548725	7.599326	0.738431	0.016788	-0.007505	-0.002903
O	-2.095583	6.202275	5.628359	-0.016659	0.007530	0.002745
O	-2.459230	13.184059	5.445139	-0.034179	0.010374	0.017766
O	4.912372	0.617542	0.921651	0.034256	-0.010415	-0.017770
O	2.757943	6.283259	4.105046	-0.034174	-0.010390	0.017693
O	-0.304801	7.518342	2.261744	0.034280	0.010449	-0.017799

O	-0.175430	2.374756	0.744070	-0.006103	0.036567	0.012477
O	2.628573	11.426844	5.622720	0.006041	-0.036467	-0.012467
O	4.783002	9.275557	2.439325	-0.006118	-0.036554	0.012419
O	-2.329859	4.526044	3.927465	0.006065	0.036469	-0.012474
O	-1.223866	12.517207	2.155216	-0.013130	0.017306	0.046928
O	3.677009	1.284394	4.211574	0.013247	-0.017302	-0.046822
O	5.831438	5.616407	1.028179	-0.013104	-0.017311	0.047002
O	-3.378295	8.185194	5.338611	0.013204	0.017311	-0.046944
H	-0.637445	12.195109	2.878812	-0.010471	0.008383	0.041433
H	3.090587	1.606491	3.487978	0.010668	-0.008337	-0.041363
H	5.245016	5.294309	0.304583	-0.010432	-0.008426	0.041514
H	-2.791874	8.507292	6.062207	0.010574	0.008343	-0.041445

150 f = 5.728637 THz 35.994090 2PiTHz 191.086766 cm-1 23.691748
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.002645	-0.024902	0.002755
Li	-1.316675	4.156264	2.365404	0.002780	-0.025074	0.002712
Li	-3.471104	2.744536	5.548798	0.002719	0.025119	0.002779
Li	5.924247	11.057064	0.817991	0.002723	0.024909	0.002684
Na	2.049025	6.784862	1.629696	-0.007594	0.009821	0.011509
Na	0.404117	7.016739	4.737094	-0.007666	0.009674	0.010759
Na	2.558546	13.685662	1.553699	-0.007633	-0.009565	0.010815
Na	-0.105403	0.115939	4.813091	-0.007593	-0.009917	0.011465
B	4.155007	8.978944	1.168663	0.001210	0.020593	-0.005134
B	-1.701865	4.822656	5.198127	0.001238	0.020787	-0.005160
B	0.452564	2.078144	2.014732	0.001243	-0.020809	-0.005157
B	2.000578	11.723457	4.352058	0.001188	-0.020568	-0.005156
B	-2.733891	11.746082	5.839177	-0.002987	-0.018206	0.003284
B	5.187034	2.055518	0.527613	-0.002946	-0.018286	0.003281
B	3.032605	4.845282	3.711007	-0.002930	0.018304	0.003287
B	-0.579463	8.956318	2.655782	-0.002981	0.018177	0.003270
B	-0.983708	0.054306	1.827988	0.017480	-0.033205	-0.023013
B	3.436850	13.747295	4.538802	0.017513	-0.033005	-0.022953
B	5.591279	6.955106	1.355407	0.017511	0.033010	-0.023021

B	-3.138137	6.846495	5.011383	0.017504	0.033202	-0.022973
Si	0.631772	3.486686	4.508512	-0.003905	0.004988	0.006584
Si	1.821370	10.314915	1.858278	-0.003975	0.004994	0.006582
Si	-0.333059	10.387486	5.041673	-0.003922	-0.004998	0.006615
Si	2.786201	3.414115	1.325117	-0.003926	-0.004991	0.006575
O	0.061445	3.072947	3.041906	0.001980	-0.037373	0.015774
O	2.391697	10.728653	3.324884	0.001870	-0.037106	0.015713
O	4.546126	9.973747	0.141489	0.001939	0.037136	0.015748
O	-2.092984	3.827853	6.225301	0.001951	0.037353	0.015767
O	2.197450	3.933608	4.519003	-0.015401	0.049498	0.033347
O	0.255692	9.867992	1.847787	-0.015406	0.049208	0.033147
O	-1.898737	10.834409	5.031182	-0.015377	-0.049300	0.033264
O	4.351879	2.967192	1.335608	-0.015397	-0.049414	0.033271
O	-0.212316	4.798696	5.055280	-0.007190	0.010809	-0.017483
O	2.665458	9.002905	1.311510	-0.007199	0.010786	-0.017356
O	0.511030	11.699496	4.494905	-0.007216	-0.010746	-0.017325
O	1.942113	2.102105	1.871885	-0.007183	-0.010827	-0.017491
O	0.525580	2.169271	5.472081	-0.013690	0.010413	0.011788
O	1.927562	11.632329	0.894709	-0.013817	0.010422	0.011786
O	-0.226867	9.070071	4.078104	-0.013689	-0.010362	0.011740
O	2.680009	4.731529	2.288686	-0.013741	-0.010457	0.011820
O	0.058846	0.698526	2.444964	0.021614	-0.033865	-0.029841
O	2.394296	13.103075	3.921826	0.021542	-0.033553	-0.029734
O	4.548725	7.599326	0.738431	0.021564	0.033608	-0.029781
O	-2.095583	6.202275	5.628359	0.021604	0.033821	-0.029793
O	-2.459230	13.184059	5.445139	0.027177	-0.037432	-0.036048
O	4.912372	0.617542	0.921651	0.027208	-0.037552	-0.036159
O	2.757943	6.283259	4.105046	0.027292	0.037601	-0.036204
O	-0.304801	7.518342	2.261744	0.027150	0.037372	-0.036047
O	-0.175430	2.374756	0.744070	-0.009846	0.004674	0.005576
O	2.628573	11.426844	5.622720	-0.009858	0.004791	0.005523
O	4.783002	9.275557	2.439325	-0.009871	-0.004837	0.005587
O	-2.329859	4.526044	3.927465	-0.009827	-0.004678	0.005553
O	-1.223866	12.517207	2.155216	0.001114	-0.021939	0.004655
O	3.677009	1.284394	4.211574	0.001432	-0.021783	0.004703
O	5.831438	5.616407	1.028179	0.001400	0.021804	0.004549

O	-3.378295	8.185194	5.338611	0.001129	0.021913	0.004770
H	-0.637445	12.195109	2.878812	0.010873	-0.019704	-0.001111
H	3.090587	1.606491	3.487978	0.011333	-0.019544	-0.001165
H	5.245016	5.294309	0.304583	0.011267	0.019596	-0.001309
H	-2.791874	8.507292	6.062207	0.010930	0.019661	-0.001019

151 f = 5.489746 THz 34.493094 2PiTHz 183.118226 cm-1 22.703775
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.007771	-0.042483	0.003038
Li	-1.316675	4.156264	2.365404	0.008153	-0.041431	0.002867
Li	-3.471104	2.744536	5.548798	-0.008113	-0.041389	-0.002833
Li	5.924247	11.057064	0.817991	-0.007715	-0.042443	-0.002968
Na	2.049025	6.784862	1.629696	-0.006630	-0.005432	-0.017839
Na	0.404117	7.016739	4.737094	-0.007457	-0.005244	-0.015336
Na	2.558546	13.685662	1.553699	0.007427	-0.005223	0.015342
Na	-0.105403	0.115939	4.813091	0.006571	-0.005408	0.017804
B	4.155007	8.978944	1.168663	0.013014	-0.002221	-0.010613
B	-1.701865	4.822656	5.198127	0.012943	-0.002725	-0.010391
B	0.452564	2.078144	2.014732	-0.012927	-0.002786	0.010419
B	2.000578	11.723457	4.352058	-0.012978	-0.002146	0.010494
B	-2.733891	11.746082	5.839177	-0.016621	0.010718	0.004512
B	5.187034	2.055518	0.527613	-0.016435	0.011417	0.004530
B	3.032605	4.845282	3.711007	0.016471	0.011477	-0.004538
B	-0.579463	8.956318	2.655782	0.016566	0.010645	-0.004497
B	-0.983708	0.054306	1.827988	-0.009851	-0.003871	-0.027042
B	3.436850	13.747295	4.538802	-0.009473	-0.003587	-0.025769
B	5.591279	6.955106	1.355407	0.009557	-0.003653	0.025732
B	-3.138137	6.846495	5.011383	0.009717	-0.003848	0.027131
Si	0.631772	3.486686	4.508512	0.030577	0.007198	0.011198
Si	1.821370	10.314915	1.858278	0.030929	0.007079	0.011793
Si	-0.333059	10.387486	5.041673	-0.030910	0.007065	-0.011821
Si	2.786201	3.414115	1.325117	-0.030532	0.007152	-0.011181
O	0.061445	3.072947	3.041906	0.016904	-0.007682	0.022399
O	2.391697	10.728653	3.324884	0.018000	-0.006477	0.022270

O	4.546126	9.973747	0.141489	-0.017808	-0.006563	-0.022372
O	-2.092984	3.827853	6.225301	-0.016829	-0.007675	-0.022385
O	2.197450	3.933608	4.519003	0.030573	0.009493	0.012041
O	0.255692	9.867992	1.847787	0.031057	0.008999	0.012915
O	-1.898737	10.834409	5.031182	-0.031043	0.009013	-0.012778
O	4.351879	2.967192	1.335608	-0.030535	0.009408	-0.011994
O	-0.212316	4.798696	5.055280	0.015860	-0.006421	0.017154
O	2.665458	9.002905	1.311510	0.016069	-0.006709	0.017895
O	0.511030	11.699496	4.494905	-0.016064	-0.006775	-0.018124
O	1.942113	2.102105	1.871885	-0.015838	-0.006473	-0.017153
O	0.525580	2.169271	5.472081	0.026116	0.000953	-0.001825
O	1.927562	11.632329	0.894709	0.026207	0.000059	-0.002073
O	-0.226867	9.070071	4.078104	-0.026441	-0.000036	0.002124
O	2.680009	4.731529	2.288686	-0.026048	0.000926	0.001823
O	0.058846	0.698526	2.444964	-0.020864	-0.004875	-0.006640
O	2.394296	13.103075	3.921826	-0.021075	-0.003673	-0.005314
O	4.548725	7.599326	0.738431	0.021116	-0.003795	0.005266
O	-2.095583	6.202275	5.628359	0.020765	-0.004842	0.006700
O	-2.459230	13.184059	5.445139	-0.020148	0.010691	-0.005663
O	4.912372	0.617542	0.921651	-0.020517	0.011312	-0.006413
O	2.757943	6.283259	4.105046	0.020510	0.011367	0.006359
O	-0.304801	7.518342	2.261744	0.020179	0.010667	0.005647
O	-0.175430	2.374756	0.744070	-0.022671	0.024589	0.023048
O	2.628573	11.426844	5.622720	-0.023035	0.024550	0.023169
O	4.783002	9.275557	2.439325	0.022978	0.024437	-0.023237
O	-2.329859	4.526044	3.927465	0.022706	0.024670	-0.023034
O	-1.223866	12.517207	2.155216	0.010965	-0.016720	-0.068810
O	3.677009	1.284394	4.211574	0.012556	-0.016459	-0.066812
O	5.831438	5.616407	1.028179	-0.012310	-0.016509	0.066808
O	-3.378295	8.185194	5.338611	-0.011317	-0.016765	0.069057
H	-0.637445	12.195109	2.878812	0.000667	-0.013473	-0.059591
H	3.090587	1.606491	3.487978	0.003009	-0.013032	-0.058081
H	5.245016	5.294309	0.304583	-0.002685	-0.013132	0.058039
H	-2.791874	8.507292	6.062207	-0.000990	-0.013470	0.059799

152 f = 5.423534 THz 34.077071 2PiTHz 180.909624 cm-1 22.429943
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.005269	-0.019024	-0.000221
Li	-1.316675	4.156264	2.365404	0.005595	0.018878	0.000261
Li	-3.471104	2.744536	5.548798	0.005760	-0.019620	0.000175
Li	5.924247	11.057064	0.817991	-0.005574	0.019491	-0.000064
Na	2.049025	6.784862	1.629696	0.007382	-0.005778	-0.018521
Na	0.404117	7.016739	4.737094	-0.007718	0.005656	0.018346
Na	2.558546	13.685662	1.553699	-0.008087	-0.005709	0.019715
Na	-0.105403	0.115939	4.813091	0.007849	0.005810	-0.019867
B	4.155007	8.978944	1.168663	-0.000695	0.023044	0.017231
B	-1.701865	4.822656	5.198127	0.000817	-0.023003	-0.017358
B	0.452564	2.078144	2.014732	0.000719	0.023341	-0.017168
B	2.000578	11.723457	4.352058	-0.000765	-0.023429	0.017163
B	-2.733891	11.746082	5.839177	0.014008	-0.018995	-0.003202
B	5.187034	2.055518	0.527613	-0.014183	0.019008	0.003371
B	3.032605	4.845282	3.711007	-0.014036	-0.019440	0.003310
B	-0.579463	8.956318	2.655782	0.014081	0.019504	-0.003240
B	-0.983708	0.054306	1.827988	0.014996	0.023072	-0.002362
B	3.436850	13.747295	4.538802	-0.015100	-0.023194	0.002176
B	5.591279	6.955106	1.355407	-0.014702	0.023063	0.003065
B	-3.138137	6.846495	5.011383	0.014876	-0.022934	-0.003228
Si	0.631772	3.486686	4.508512	-0.001877	-0.001405	-0.005786
Si	1.821370	10.314915	1.858278	0.002100	0.001529	0.005969
Si	-0.333059	10.387486	5.041673	0.002128	-0.001463	0.006287
Si	2.786201	3.414115	1.325117	-0.002211	0.001357	-0.006222
O	0.061445	3.072947	3.041906	0.020373	0.030931	-0.022355
O	2.391697	10.728653	3.324884	-0.019901	-0.030967	0.022490
O	4.546126	9.973747	0.141489	-0.019389	0.030237	0.022354
O	-2.092984	3.827853	6.225301	0.019678	-0.030227	-0.022410
O	2.197450	3.933608	4.519003	0.003409	-0.026194	0.008944
O	0.255692	9.867992	1.847787	-0.003241	0.026530	-0.008344
O	-1.898737	10.834409	5.031182	-0.003118	-0.026175	-0.007931
O	4.351879	2.967192	1.335608	0.003011	0.025988	0.008416
O	-0.212316	4.798696	5.055280	-0.001223	0.004378	-0.026019

O	2.665458	9.002905	1.311510	0.001309	-0.004211	0.025823
O	0.511030	11.699496	4.494905	0.001311	0.004300	0.026195
O	1.942113	2.102105	1.871885	-0.001410	-0.004589	-0.026581
O	0.525580	2.169271	5.472081	-0.039834	0.008224	0.004360
O	1.927562	11.632329	0.894709	0.039587	-0.008005	-0.004125
O	-0.226867	9.070071	4.078104	0.039606	0.008527	-0.004261
O	2.680009	4.731529	2.288686	-0.040068	-0.008801	0.004492
O	0.058846	0.698526	2.444964	0.002594	0.034853	0.003015
O	2.394296	13.103075	3.921826	-0.002813	-0.034878	-0.003080
O	4.548725	7.599326	0.738431	-0.002769	0.034166	-0.002186
O	-2.095583	6.202275	5.628359	0.002897	-0.034135	0.002026
O	-2.459230	13.184059	5.445139	0.008035	-0.020239	-0.019349
O	4.912372	0.617542	0.921651	-0.008137	0.020152	0.019188
O	2.757943	6.283259	4.105046	-0.008245	-0.020511	0.018621
O	-0.304801	7.518342	2.261744	0.008526	0.020728	-0.018937
O	-0.175430	2.374756	0.744070	-0.010553	0.016857	-0.014155
O	2.628573	11.426844	5.622720	0.010355	-0.016715	0.014275
O	4.783002	9.275557	2.439325	0.010340	0.016886	0.014272
O	-2.329859	4.526044	3.927465	-0.010284	-0.016888	-0.014369
O	-1.223866	12.517207	2.155216	0.068263	0.010470	-0.021892
O	3.677009	1.284394	4.211574	-0.068187	-0.010627	0.021608
O	5.831438	5.616407	1.028179	-0.067216	0.010445	0.023102
O	-3.378295	8.185194	5.338611	0.067362	-0.010389	-0.023043
H	-0.637445	12.195109	2.878812	0.076147	0.018717	-0.024720
H	3.090587	1.606491	3.487978	-0.075975	-0.018856	0.024379
H	5.245016	5.294309	0.304583	-0.074535	0.018601	0.025556
H	-2.791874	8.507292	6.062207	0.074784	-0.018549	-0.025567

153 f = 5.395905 THz 33.903473 2PiTHz 179.988020 cm-1 22.315678 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.010092	0.022440	-0.004986
Li	-1.316675	4.156264	2.365404	-0.009248	-0.024362	0.004657
Li	-3.471104	2.744536	5.548798	0.009127	-0.023809	-0.004594
Li	5.924247	11.057064	0.817991	-0.009896	0.021959	0.004993

Na	2.049025	6.784862	1.629696	-0.016519	0.001581	0.053167
Na	0.404117	7.016739	4.737094	0.016703	-0.001746	-0.052045
Na	2.558546	13.685662	1.553699	-0.016504	-0.001520	0.051571
Na	-0.105403	0.115939	4.813091	0.016276	0.001391	-0.052640
B	4.155007	8.978944	1.168663	-0.001103	-0.013422	0.003247
B	-1.701865	4.822656	5.198127	0.001519	0.013382	-0.003874
B	0.452564	2.078144	2.014732	-0.001506	0.012763	0.004314
B	2.000578	11.723457	4.352058	0.001141	-0.012850	-0.003764
B	-2.733891	11.746082	5.839177	0.001782	0.018607	0.000680
B	5.187034	2.055518	0.527613	-0.002635	-0.018344	-0.000359
B	3.032605	4.845282	3.711007	0.003028	-0.017853	0.000259
B	-0.579463	8.956318	2.655782	-0.002186	0.018110	-0.000579
B	-0.983708	0.054306	1.827988	0.006980	0.004975	0.032833
B	3.436850	13.747295	4.538802	-0.007444	-0.005008	-0.033356
B	5.591279	6.955106	1.355407	0.007793	-0.005606	0.033327
B	-3.138137	6.846495	5.011383	-0.007387	0.005564	-0.032783
Si	0.631772	3.486686	4.508512	0.008071	-0.002597	0.014069
Si	1.821370	10.314915	1.858278	-0.006341	0.002809	-0.013163
Si	-0.333059	10.387486	5.041673	0.006294	0.002817	0.012985
Si	2.786201	3.414115	1.325117	-0.007978	-0.002632	-0.013921
O	0.061445	3.072947	3.041906	0.023932	0.027237	-0.001998
O	2.391697	10.728653	3.324884	-0.022226	-0.027110	0.002993
O	4.546126	9.973747	0.141489	0.022849	-0.027894	-0.003623
O	-2.092984	3.827853	6.225301	-0.024402	0.028059	0.002581
O	2.197450	3.933608	4.519003	0.010732	-0.009741	0.019010
O	0.255692	9.867992	1.847787	-0.009148	0.010610	-0.017611
O	-1.898737	10.834409	5.031182	0.009234	0.011254	0.017926
O	4.351879	2.967192	1.335608	-0.010774	-0.010400	-0.019247
O	-0.212316	4.798696	5.055280	0.004530	-0.007132	0.019542
O	2.665458	9.002905	1.311510	-0.003882	0.006436	-0.018171
O	0.511030	11.699496	4.494905	0.003844	0.006246	0.017333
O	1.942113	2.102105	1.871885	-0.004464	-0.007015	-0.018878
O	0.525580	2.169271	5.472081	0.005563	-0.021948	-0.006305
O	1.927562	11.632329	0.894709	-0.003905	0.021311	0.006046
O	-0.226867	9.070071	4.078104	0.002746	0.021013	-0.005894
O	2.680009	4.731529	2.288686	-0.004494	-0.021731	0.006184

O	0.058846	0.698526	2.444964	-0.007159	0.026512	0.035047
O	2.394296	13.103075	3.921826	0.006252	-0.026402	-0.034868
O	4.548725	7.599326	0.738431	-0.006181	-0.027298	0.034908
O	-2.095583	6.202275	5.628359	0.007086	0.027428	-0.035129
O	-2.459230	13.184059	5.445139	-0.009688	0.016504	-0.017848
O	4.912372	0.617542	0.921651	0.008449	-0.015947	0.018470
O	2.757943	6.283259	4.105046	-0.008235	-0.015448	-0.018988
O	-0.304801	7.518342	2.261744	0.009458	0.016000	0.018341
O	-0.175430	2.374756	0.744070	-0.006528	-0.004946	0.003614
O	2.628573	11.426844	5.622720	0.005300	0.005937	-0.002271
O	4.783002	9.275557	2.439325	-0.005600	0.005515	0.001858
O	-2.329859	4.526044	3.927465	0.006825	-0.004507	-0.003239
O	-1.223866	12.517207	2.155216	0.032146	0.004957	0.049693
O	3.677009	1.284394	4.211574	-0.031062	-0.005583	-0.051876
O	5.831438	5.616407	1.028179	0.032759	-0.005895	0.051481
O	-3.378295	8.185194	5.338611	-0.033989	0.005205	-0.049134
H	-0.637445	12.195109	2.878812	0.049577	0.008028	0.038022
H	3.090587	1.606491	3.487978	-0.048218	-0.008573	-0.040370
H	5.245016	5.294309	0.304583	0.050179	-0.009134	0.039868
H	-2.791874	8.507292	6.062207	-0.051596	0.008523	-0.037430

154 f = 5.275632 THz 33.147772 2PiTHz 175.976129 cm-1 21.818267 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.035181	-0.006242	-0.013440
Li	-1.316675	4.156264	2.365404	-0.035028	-0.006250	-0.013446
Li	-3.471104	2.744536	5.548798	-0.035065	0.006137	-0.013402
Li	5.924247	11.057064	0.817991	-0.035152	0.006173	-0.013497
Na	2.049025	6.784862	1.629696	0.019944	0.009102	0.007943
Na	0.404117	7.016739	4.737094	0.020302	0.009054	0.007201
Na	2.558546	13.685662	1.553699	0.020333	-0.009022	0.007421
Na	-0.105403	0.115939	4.813091	0.019967	-0.009125	0.007858
B	4.155007	8.978944	1.168663	-0.009681	0.000487	0.013971
B	-1.701865	4.822656	5.198127	-0.009596	0.000454	0.013716
B	0.452564	2.078144	2.014732	-0.009650	-0.000434	0.013758

B	2.000578	11.723457	4.352058	-0.009706	-0.000502	0.013957
B	-2.733891	11.746082	5.839177	0.005638	-0.013058	-0.008926
B	5.187034	2.055518	0.527613	0.005504	-0.012899	-0.008892
B	3.032605	4.845282	3.711007	0.005574	0.012933	-0.008909
B	-0.579463	8.956318	2.655782	0.005652	0.013079	-0.008923
B	-0.983708	0.054306	1.827988	0.015681	-0.011083	-0.000538
B	3.436850	13.747295	4.538802	0.015506	-0.011191	-0.000477
B	5.591279	6.955106	1.355407	0.015490	0.011158	-0.000373
B	-3.138137	6.846495	5.011383	0.015725	0.011090	-0.000487
Si	0.631772	3.486686	4.508512	-0.014723	-0.012137	-0.003780
Si	1.821370	10.314915	1.858278	-0.014777	-0.012122	-0.003710
Si	-0.333059	10.387486	5.041673	-0.014788	0.012129	-0.003697
Si	2.786201	3.414115	1.325117	-0.014843	0.012173	-0.003829
O	0.061445	3.072947	3.041906	-0.055694	-0.017192	0.013381
O	2.391697	10.728653	3.324884	-0.056026	-0.017326	0.013586
O	4.546126	9.973747	0.141489	-0.055995	0.017276	0.013562
O	-2.092984	3.827853	6.225301	-0.055763	0.017207	0.013306
O	2.197450	3.933608	4.519003	-0.019145	0.004761	-0.044787
O	0.255692	9.867992	1.847787	-0.019234	0.004880	-0.045005
O	-1.898737	10.834409	5.031182	-0.019261	-0.004927	-0.044936
O	4.351879	2.967192	1.335608	-0.019272	-0.004729	-0.044848
O	-0.212316	4.798696	5.055280	-0.008566	-0.027736	0.040425
O	2.665458	9.002905	1.311510	-0.008620	-0.027845	0.040838
O	0.511030	11.699496	4.494905	-0.008645	0.027852	0.040832
O	1.942113	2.102105	1.871885	-0.008639	0.027723	0.040343
O	0.525580	2.169271	5.472081	0.042868	-0.029304	-0.019197
O	1.927562	11.632329	0.894709	0.043249	-0.029398	-0.019251
O	-0.226867	9.070071	4.078104	0.043281	0.029456	-0.019277
O	2.680009	4.731529	2.288686	0.042763	0.029289	-0.019178
O	0.058846	0.698526	2.444964	0.018426	-0.014250	-0.003961
O	2.394296	13.103075	3.921826	0.018365	-0.014427	-0.003954
O	4.548725	7.599326	0.738431	0.018379	0.014402	-0.003888
O	-2.095583	6.202275	5.628359	0.018501	0.014258	-0.003963
O	-2.459230	13.184059	5.445139	0.009582	-0.009827	0.004862
O	4.912372	0.617542	0.921651	0.009524	-0.009697	0.005011
O	2.757943	6.283259	4.105046	0.009600	0.009740	0.005002

O	-0.304801	7.518342	2.261744	0.009558	0.009809	0.004969
O	-0.175430	2.374756	0.744070	-0.000396	-0.002005	0.009839
O	2.628573	11.426844	5.622720	-0.000272	-0.002102	0.009960
O	4.783002	9.275557	2.439325	-0.000252	0.002151	0.009967
O	-2.329859	4.526044	3.927465	-0.000298	0.002097	0.009747
O	-1.223866	12.517207	2.155216	0.017504	-0.011402	-0.002777
O	3.677009	1.284394	4.211574	0.016930	-0.011395	-0.002489
O	5.831438	5.616407	1.028179	0.016895	0.011353	-0.002341
O	-3.378295	8.185194	5.338611	0.017496	0.011370	-0.002619
H	-0.637445	12.195109	2.878812	0.011763	-0.008345	0.002456
H	3.090587	1.606491	3.487978	0.011193	-0.008430	0.002708
H	5.245016	5.294309	0.304583	0.011185	0.008434	0.002812
H	-2.791874	8.507292	6.062207	0.011793	0.008304	0.002590

155 f = 5.062724 THz 31.810031 2PiTHz 168.874279 cm-1 20.937750
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.006431	0.004778	-0.004164
Li	-1.316675	4.156264	2.365404	0.007490	0.005295	-0.005266
Li	-3.471104	2.744536	5.548798	-0.007442	0.005082	0.005199
Li	5.924247	11.057064	0.817991	-0.006468	0.004722	0.004086
Na	2.049025	6.784862	1.629696	0.014275	-0.023789	0.033415
Na	0.404117	7.016739	4.737094	0.014111	-0.024161	0.034215
Na	2.558546	13.685662	1.553699	-0.014098	-0.024350	-0.033632
Na	-0.105403	0.115939	4.813091	-0.014122	-0.023623	-0.033888
B	4.155007	8.978944	1.168663	-0.012670	0.003616	0.001617
B	-1.701865	4.822656	5.198127	-0.012486	0.003211	0.001341
B	0.452564	2.078144	2.014732	0.012407	0.003265	-0.001256
B	2.000578	11.723457	4.352058	0.012646	0.003631	-0.001656
B	-2.733891	11.746082	5.839177	0.003227	-0.005329	-0.005346
B	5.187034	2.055518	0.527613	0.002801	-0.004721	-0.004843
B	3.032605	4.845282	3.711007	-0.002857	-0.004747	0.004903
B	-0.579463	8.956318	2.655782	-0.003312	-0.005362	0.005393
B	-0.983708	0.054306	1.827988	0.003465	0.012422	0.020728
B	3.436850	13.747295	4.538802	0.003966	0.012704	0.021853

B	5.591279	6.955106	1.355407	-0.003697	0.012772	-0.021962
B	-3.138137	6.846495	5.011383	-0.003520	0.012403	-0.020789
Si	0.631772	3.486686	4.508512	0.006234	-0.004677	0.009656
Si	1.821370	10.314915	1.858278	0.005726	-0.004944	0.009553
Si	-0.333059	10.387486	5.041673	-0.005826	-0.004805	-0.009583
Si	2.786201	3.414115	1.325117	-0.006289	-0.004783	-0.009571
O	0.061445	3.072947	3.041906	0.039583	0.030390	-0.014244
O	2.391697	10.728653	3.324884	0.039954	0.031338	-0.015099
O	4.546126	9.973747	0.141489	-0.040075	0.031391	0.015065
O	-2.092984	3.827853	6.225301	-0.039578	0.030235	0.014283
O	2.197450	3.933608	4.519003	-0.003796	0.030140	0.042215
O	0.255692	9.867992	1.847787	-0.004296	0.029728	0.042649
O	-1.898737	10.834409	5.031182	0.004195	0.029828	-0.042687
O	4.351879	2.967192	1.335608	0.003770	0.030105	-0.042042
O	-0.212316	4.798696	5.055280	-0.013116	-0.021416	0.023181
O	2.665458	9.002905	1.311510	-0.013443	-0.021619	0.023210
O	0.511030	11.699496	4.494905	0.013398	-0.021510	-0.023277
O	1.942113	2.102105	1.871885	0.013053	-0.021507	-0.023072
O	0.525580	2.169271	5.472081	0.019231	-0.028909	-0.016552
O	1.927562	11.632329	0.894709	0.018749	-0.029598	-0.017019
O	-0.226867	9.070071	4.078104	-0.018895	-0.029514	0.017057
O	2.680009	4.731529	2.288686	-0.019317	-0.029016	0.016629
O	0.058846	0.698526	2.444964	-0.001912	0.019172	0.024050
O	2.394296	13.103075	3.921826	-0.001723	0.020105	0.024957
O	4.548725	7.599326	0.738431	0.001897	0.020106	-0.025020
O	-2.095583	6.202275	5.628359	0.001714	0.019078	-0.023927
O	-2.459230	13.184059	5.445139	-0.010054	0.009590	0.032709
O	4.912372	0.617542	0.921651	-0.010786	0.010155	0.032449
O	2.757943	6.283259	4.105046	0.010749	0.010144	-0.032503
O	-0.304801	7.518342	2.261744	0.010070	0.009599	-0.032584
O	-0.175430	2.374756	0.744070	0.003319	-0.011558	-0.000145
O	2.628573	11.426844	5.622720	0.003837	-0.012292	-0.001032
O	4.783002	9.275557	2.439325	-0.003922	-0.012323	0.001000
O	-2.329859	4.526044	3.927465	-0.003354	-0.011584	0.000194
O	-1.223866	12.517207	2.155216	0.034077	0.005002	0.006740
O	3.677009	1.284394	4.211574	0.034934	0.005529	0.009067

O	5.831438	5.616407	1.028179	-0.034241	0.005726	-0.009465
O	-3.378295	8.185194	5.338611	-0.033981	0.005051	-0.006956
H	-0.637445	12.195109	2.878812	0.049322	-0.002208	-0.008016
H	3.090587	1.606491	3.487978	0.051053	-0.001391	-0.006199
H	5.245016	5.294309	0.304583	-0.050321	-0.001314	0.005828
H	-2.791874	8.507292	6.062207	-0.049247	-0.002174	0.007822

156 f = 5.002737 THz 31.433126 2PiTHz 166.873349 cm-1 20.689666 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.029864	-0.008631	-0.044207
Li	-1.316675	4.156264	2.365404	-0.029843	0.009376	0.043922
Li	-3.471104	2.744536	5.548798	0.029764	0.008858	-0.044210
Li	5.924247	11.057064	0.817991	-0.029892	-0.009143	0.043938
Na	2.049025	6.784862	1.629696	-0.002734	-0.010407	-0.007809
Na	0.404117	7.016739	4.737094	0.003418	0.009788	0.008528
Na	2.558546	13.685662	1.553699	-0.003096	0.009740	-0.008297
Na	-0.105403	0.115939	4.813091	0.003034	-0.010517	0.007980
B	4.155007	8.978944	1.168663	0.016093	-0.003171	-0.025692
B	-1.701865	4.822656	5.198127	-0.016702	0.003047	0.025878
B	0.452564	2.078144	2.014732	0.016418	0.003278	-0.025782
B	2.000578	11.723457	4.352058	-0.016361	-0.002967	0.025785
B	-2.733891	11.746082	5.839177	-0.021119	0.002614	0.021430
B	5.187034	2.055518	0.527613	0.020935	-0.002662	-0.021439
B	3.032605	4.845282	3.711007	-0.021260	-0.002711	0.021615
B	-0.579463	8.956318	2.655782	0.020792	0.002554	-0.021227
B	-0.983708	0.054306	1.827988	0.008461	0.009429	0.003810
B	3.436850	13.747295	4.538802	-0.007898	-0.009173	-0.003615
B	5.591279	6.955106	1.355407	0.008356	-0.009080	0.003313
B	-3.138137	6.846495	5.011383	-0.007984	0.009511	-0.004116
Si	0.631772	3.486686	4.508512	-0.030536	-0.000407	-0.015645
Si	1.821370	10.314915	1.858278	0.030233	0.000332	0.015902
Si	-0.333059	10.387486	5.041673	-0.030579	0.000274	-0.015785
Si	2.786201	3.414115	1.325117	0.030181	-0.000447	0.015744
O	0.061445	3.072947	3.041906	-0.002741	0.011262	-0.032380

O	2.391697	10.728653	3.324884	0.003494	-0.010059	0.031845
O	4.546126	9.973747	0.141489	-0.003608	-0.010463	-0.031909
O	-2.092984	3.827853	6.225301	0.002575	0.010824	0.032300
O	2.197450	3.933608	4.519003	-0.034190	0.006323	0.007273
O	0.255692	9.867992	1.847787	0.033673	-0.005518	-0.005872
O	-1.898737	10.834409	5.031182	-0.033969	-0.005576	0.006285
O	4.351879	2.967192	1.335608	0.033887	0.006274	-0.006924
O	-0.212316	4.798696	5.055280	-0.023919	0.003168	-0.010915
O	2.665458	9.002905	1.311510	0.023249	-0.003606	0.011384
O	0.511030	11.699496	4.494905	-0.023537	-0.003693	-0.011409
O	1.942113	2.102105	1.871885	0.023622	0.003129	0.010942
O	0.525580	2.169271	5.472081	-0.023341	-0.000838	-0.013568
O	1.927562	11.632329	0.894709	0.023164	0.000282	0.013331
O	-0.226867	9.070071	4.078104	-0.023739	0.000135	-0.013098
O	2.680009	4.731529	2.288686	0.022810	-0.000935	0.013753
O	0.058846	0.698526	2.444964	0.019656	0.007888	-0.013920
O	2.394296	13.103075	3.921826	-0.019934	-0.006999	0.014813
O	4.548725	7.599326	0.738431	0.019706	-0.007376	-0.014532
O	-2.095583	6.202275	5.628359	-0.019881	0.007486	0.014210
O	-2.459230	13.184059	5.445139	-0.016485	0.000184	0.011553
O	4.912372	0.617542	0.921651	0.016291	-0.000068	-0.010788
O	2.757943	6.283259	4.105046	-0.016286	0.000070	0.010851
O	-0.304801	7.518342	2.261744	0.016501	0.000331	-0.011515
O	-0.175430	2.374756	0.744070	0.030771	-0.022019	-0.042314
O	2.628573	11.426844	5.622720	-0.030887	0.021766	0.042177
O	4.783002	9.275557	2.439325	0.030571	0.021647	-0.042162
O	-2.329859	4.526044	3.927465	-0.031079	-0.022126	0.042316
O	-1.223866	12.517207	2.155216	-0.009956	0.021367	0.042945
O	3.677009	1.284394	4.211574	0.012650	-0.021715	-0.043959
O	5.831438	5.616407	1.028179	-0.010763	-0.021196	0.042815
O	-3.378295	8.185194	5.338611	0.011913	0.021888	-0.044124
H	-0.637445	12.195109	2.878812	0.006190	0.027973	0.034385
H	3.090587	1.606491	3.487978	-0.003051	-0.028150	-0.035653
H	5.245016	5.294309	0.304583	0.005073	-0.027997	0.034577
H	-2.791874	8.507292	6.062207	-0.004091	0.028129	-0.035501

157 f = 4.963919 THz 31.189222 2PiTHz 165.578502 cm-1 20.529125
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.000839	0.024884	-0.011678
Li	-1.316675	4.156264	2.365404	-0.000036	0.024143	-0.012466
Li	-3.471104	2.744536	5.548798	-0.000672	-0.024515	-0.011456
Li	5.924247	11.057064	0.817991	-0.000194	-0.024664	-0.012609
Na	2.049025	6.784862	1.629696	0.014539	0.001254	0.011138
Na	0.404117	7.016739	4.737094	0.014941	0.000587	0.009128
Na	2.558546	13.685662	1.553699	0.015051	-0.000698	0.009535
Na	-0.105403	0.115939	4.813091	0.014576	-0.000803	0.011055
B	4.155007	8.978944	1.168663	-0.012132	-0.010638	0.003786
B	-1.701865	4.822656	5.198127	-0.011573	-0.010414	0.002989
B	0.452564	2.078144	2.014732	-0.012059	0.010308	0.003605
B	2.000578	11.723457	4.352058	-0.011790	0.010747	0.003295
B	-2.733891	11.746082	5.839177	-0.014771	0.004316	0.008517
B	5.187034	2.055518	0.527613	-0.015342	0.004397	0.008958
B	3.032605	4.845282	3.711007	-0.014776	-0.004319	0.008442
B	-0.579463	8.956318	2.655782	-0.015280	-0.004375	0.008886
B	-0.983708	0.054306	1.827988	0.019004	-0.002059	-0.012713
B	3.436850	13.747295	4.538802	0.019230	-0.001653	-0.012425
B	5.591279	6.955106	1.355407	0.018754	0.001695	-0.012340
B	-3.138137	6.846495	5.011383	0.019404	0.001837	-0.012635
Si	0.631772	3.486686	4.508512	-0.014281	0.002382	0.004587
Si	1.821370	10.314915	1.858278	-0.015082	0.002448	0.004369
Si	-0.333059	10.387486	5.041673	-0.014335	-0.002411	0.004710
Si	2.786201	3.414115	1.325117	-0.015061	-0.002352	0.004255
O	0.061445	3.072947	3.041906	-0.003533	0.020462	-0.004303
O	2.391697	10.728653	3.324884	-0.004014	0.021077	-0.004886
O	4.546126	9.973747	0.141489	-0.003654	-0.021040	-0.004349
O	-2.092984	3.827853	6.225301	-0.003514	-0.020804	-0.005117
O	2.197450	3.933608	4.519003	-0.011273	-0.000548	0.017797
O	0.255692	9.867992	1.847787	-0.012092	-0.000617	0.017628
O	-1.898737	10.834409	5.031182	-0.011362	0.000473	0.017817
O	4.351879	2.967192	1.335608	-0.012186	0.000268	0.018088

O	-0.212316	4.798696	5.055280	-0.012072	0.003685	-0.002048
O	2.665458	9.002905	1.311510	-0.012706	0.003673	-0.001726
O	0.511030	11.699496	4.494905	-0.012237	-0.003382	-0.001308
O	1.942113	2.102105	1.871885	-0.012741	-0.003722	-0.002280
O	0.525580	2.169271	5.472081	-0.026457	0.006919	0.010027
O	1.927562	11.632329	0.894709	-0.026711	0.006782	0.009681
O	-0.226867	9.070071	4.078104	-0.026079	-0.006601	0.009789
O	2.680009	4.731529	2.288686	-0.026981	-0.006791	0.009668
O	0.058846	0.698526	2.444964	-0.011686	0.019127	0.013599
O	2.394296	13.103075	3.921826	-0.011286	0.019641	0.013543
O	4.548725	7.599326	0.738431	-0.011939	-0.019564	0.013984
O	-2.095583	6.202275	5.628359	-0.011096	-0.019379	0.013315
O	-2.459230	13.184059	5.445139	-0.001290	-0.003623	0.003694
O	4.912372	0.617542	0.921651	-0.001750	-0.003701	0.003787
O	2.757943	6.283259	4.105046	-0.001299	0.003678	0.003650
O	-0.304801	7.518342	2.261744	-0.001950	0.003462	0.004123
O	-0.175430	2.374756	0.744070	-0.014143	0.005797	-0.000232
O	2.628573	11.426844	5.622720	-0.013345	0.005432	-0.001043
O	4.783002	9.275557	2.439325	-0.014029	-0.005746	-0.000198
O	-2.329859	4.526044	3.927465	-0.013339	-0.005247	-0.001248
O	-1.223866	12.517207	2.155216	0.083602	-0.021583	-0.052492
O	3.677009	1.284394	4.211574	0.083573	-0.020895	-0.051207
O	5.831438	5.616407	1.028179	0.083463	0.021208	-0.052013
O	-3.378295	8.185194	5.338611	0.083831	0.021147	-0.051682
H	-0.637445	12.195109	2.878812	0.088256	-0.005790	-0.048502
H	3.090587	1.606491	3.487978	0.088777	-0.005071	-0.047586
H	5.245016	5.294309	0.304583	0.088327	0.005644	-0.048277
H	-2.791874	8.507292	6.062207	0.088887	0.005247	-0.047929

158 f = 4.877448 THz 30.645907 2PiTHz 162.694136 cm-1 20.171509 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.010232	-0.018345	0.010458
Li	-1.316675	4.156264	2.365404	-0.010903	0.018691	-0.010485
Li	-3.471104	2.744536	5.548798	-0.010693	-0.018623	-0.010729

Li	5.924247	11.057064	0.817991	0.010479	0.018426	0.010154
Na	2.049025	6.784862	1.629696	0.006779	-0.017124	-0.083721
Na	0.404117	7.016739	4.737094	-0.007096	0.015938	0.080809
Na	2.558546	13.685662	1.553699	-0.007015	-0.015975	0.081304
Na	-0.105403	0.115939	4.813091	0.006901	0.017112	-0.083292
B	4.155007	8.978944	1.168663	0.007132	0.013309	-0.012662
B	-1.701865	4.822656	5.198127	-0.007610	-0.013714	0.013431
B	0.452564	2.078144	2.014732	-0.007597	0.013677	0.013269
B	2.000578	11.723457	4.352058	0.007155	-0.013320	-0.012844
B	-2.733891	11.746082	5.839177	-0.002901	0.003984	0.001234
B	5.187034	2.055518	0.527613	0.002900	-0.004277	-0.001098
B	3.032605	4.845282	3.711007	0.002797	0.004300	-0.000940
B	-0.579463	8.956318	2.655782	-0.003018	-0.003935	0.001415
B	-0.983708	0.054306	1.827988	-0.008293	0.009509	0.015220
B	3.436850	13.747295	4.538802	0.009118	-0.009997	-0.016124
B	5.591279	6.955106	1.355407	0.009088	0.009994	-0.015872
B	-3.138137	6.846495	5.011383	-0.008350	-0.009556	0.015504
Si	0.631772	3.486686	4.508512	-0.002709	0.002033	0.005622
Si	1.821370	10.314915	1.858278	0.002126	-0.001893	-0.005222
Si	-0.333059	10.387486	5.041673	0.002339	0.001913	-0.005029
Si	2.786201	3.414115	1.325117	-0.002516	-0.002036	0.005801
O	0.061445	3.072947	3.041906	-0.018887	0.017647	0.005976
O	2.391697	10.728653	3.324884	0.017981	-0.017481	-0.005490
O	4.546126	9.973747	0.141489	0.018165	0.017444	-0.005289
O	-2.092984	3.827853	6.225301	-0.018696	-0.017728	0.006145
O	2.197450	3.933608	4.519003	-0.002049	-0.002268	-0.013398
O	0.255692	9.867992	1.847787	0.001265	0.003111	0.013905
O	-1.898737	10.834409	5.031182	0.001475	-0.003160	0.014004
O	4.351879	2.967192	1.335608	-0.001868	0.002175	-0.013276
O	-0.212316	4.798696	5.055280	-0.003628	-0.010271	0.034507
O	2.665458	9.002905	1.311510	0.003040	0.010047	-0.033648
O	0.511030	11.699496	4.494905	0.003133	-0.009970	-0.033458
O	1.942113	2.102105	1.871885	-0.003554	0.010327	0.034686
O	0.525580	2.169271	5.472081	0.020240	-0.010997	-0.007334
O	1.927562	11.632329	0.894709	-0.020375	0.011081	0.007603
O	-0.226867	9.070071	4.078104	-0.020154	-0.010947	0.007679

O	2.680009	4.731529	2.288686	0.020442	0.011119	-0.007280
O	0.058846	0.698526	2.444964	-0.009697	0.014016	0.016046
O	2.394296	13.103075	3.921826	0.009648	-0.013795	-0.016219
O	4.548725	7.599326	0.738431	0.009618	0.013742	-0.016002
O	-2.095583	6.202275	5.628359	-0.009736	-0.014107	0.016266
O	-2.459230	13.184059	5.445139	0.002425	-0.003408	-0.009205
O	4.912372	0.617542	0.921651	-0.001714	0.002772	0.008355
O	2.757943	6.283259	4.105046	-0.001853	-0.002809	0.008709
O	-0.304801	7.518342	2.261744	0.002304	0.003404	-0.008862
O	-0.175430	2.374756	0.744070	0.003010	0.001097	0.006684
O	2.628573	11.426844	5.622720	-0.003130	-0.000666	-0.006468
O	4.783002	9.275557	2.439325	-0.003323	0.000570	-0.006156
O	-2.329859	4.526044	3.927465	0.002843	-0.001187	0.006954
O	-1.223866	12.517207	2.155216	-0.010691	0.012437	0.027128
O	3.677009	1.284394	4.211574	0.012834	-0.013201	-0.028599
O	5.831438	5.616407	1.028179	0.013008	0.013217	-0.028323
O	-3.378295	8.185194	5.338611	-0.010580	-0.012477	0.027485
H	-0.637445	12.195109	2.878812	-0.000950	0.004766	0.017007
H	3.090587	1.606491	3.487978	0.002997	-0.005268	-0.018288
H	5.245016	5.294309	0.304583	0.003382	0.005262	-0.018157
H	-2.791874	8.507292	6.062207	-0.000600	-0.004829	0.017198

159 f = 4.752630 THz 29.861657 2PiTHz 158.530681 cm-1 19.655306 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.021948	0.009099	0.035988
Li	-1.316675	4.156264	2.365404	-0.021978	0.008445	0.036022
Li	-3.471104	2.744536	5.548798	0.022201	0.008588	-0.035811
Li	5.924247	11.057064	0.817991	0.021706	0.008895	-0.036241
Na	2.049025	6.784862	1.629696	0.001314	-0.027987	-0.034004
Na	0.404117	7.016739	4.737094	0.001417	-0.027117	-0.033587
Na	2.558546	13.685662	1.553699	-0.001424	-0.027251	0.033290
Na	-0.105403	0.115939	4.813091	-0.001225	-0.027900	0.034417
B	4.155007	8.978944	1.168663	-0.011268	-0.000312	0.023380
B	-1.701865	4.822656	5.198127	-0.010776	0.000057	0.022879

B	0.452564	2.078144	2.014732	0.010840	-0.000049	-0.023008
B	2.000578	11.723457	4.352058	0.011165	-0.000180	-0.023277
B	-2.733891	11.746082	5.839177	0.014713	0.007285	-0.025179
B	5.187034	2.055518	0.527613	0.014484	0.006907	-0.025129
B	3.032605	4.845282	3.711007	-0.014552	0.006761	0.025182
B	-0.579463	8.956318	2.655782	-0.014705	0.007418	0.025126
B	-0.983708	0.054306	1.827988	0.007409	0.007277	-0.028976
B	3.436850	13.747295	4.538802	0.007464	0.007318	-0.029513
B	5.591279	6.955106	1.355407	-0.007412	0.007277	0.029807
B	-3.138137	6.846495	5.011383	-0.007425	0.007316	0.028661
Si	0.631772	3.486686	4.508512	-0.019020	0.000858	-0.015663
Si	1.821370	10.314915	1.858278	-0.019399	0.000845	-0.015925
Si	-0.333059	10.387486	5.041673	0.019309	0.000995	0.015885
Si	2.786201	3.414115	1.325117	0.019057	0.000693	0.015678
O	0.061445	3.072947	3.041906	0.004570	0.009860	-0.029276
O	2.391697	10.728653	3.324884	0.003885	0.009238	-0.029264
O	4.546126	9.973747	0.141489	-0.004267	0.009076	0.029236
O	-2.092984	3.827853	6.225301	-0.004182	0.009936	0.029240
O	2.197450	3.933608	4.519003	-0.025737	0.018434	0.017072
O	0.255692	9.867992	1.847787	-0.026292	0.019050	0.016511
O	-1.898737	10.834409	5.031182	0.026197	0.019148	-0.016914
O	4.351879	2.967192	1.335608	0.025792	0.018330	-0.016629
O	-0.212316	4.798696	5.055280	-0.019544	-0.004624	-0.006937
O	2.665458	9.002905	1.311510	-0.020030	-0.004806	-0.006859
O	0.511030	11.699496	4.494905	0.019972	-0.004510	0.007229
O	1.942113	2.102105	1.871885	0.019559	-0.004947	0.006509
O	0.525580	2.169271	5.472081	-0.011325	-0.001444	-0.020315
O	1.927562	11.632329	0.894709	-0.010950	-0.001355	-0.020420
O	-0.226867	9.070071	4.078104	0.011237	-0.001013	0.020228
O	2.680009	4.731529	2.288686	0.010934	-0.001817	0.020510
O	0.058846	0.698526	2.444964	0.004476	0.001830	-0.019169
O	2.394296	13.103075	3.921826	0.005328	0.001234	-0.020341
O	4.548725	7.599326	0.738431	-0.005285	0.001083	0.020540
O	-2.095583	6.202275	5.628359	-0.004574	0.001907	0.019010
O	-2.459230	13.184059	5.445139	0.005658	0.011562	-0.024434
O	4.912372	0.617542	0.921651	0.005915	0.010944	-0.024623

O	2.757943	6.283259	4.105046	-0.005901	0.010930	0.024328
O	-0.304801	7.518342	2.261744	-0.005697	0.011596	0.024741
O	-0.175430	2.374756	0.744070	0.023203	-0.012748	-0.034687
O	2.628573	11.426844	5.622720	0.023587	-0.012683	-0.034903
O	4.783002	9.275557	2.439325	-0.023579	-0.012564	0.034899
O	-2.329859	4.526044	3.927465	-0.023260	-0.012863	0.034651
O	-1.223866	12.517207	2.155216	0.004671	0.002029	-0.052328
O	3.677009	1.284394	4.211574	0.004131	0.002179	-0.052695
O	5.831438	5.616407	1.028179	-0.003891	0.002134	0.053122
O	-3.378295	8.185194	5.338611	-0.004683	0.002121	0.051799
H	-0.637445	12.195109	2.878812	-0.015874	-0.007885	-0.042363
H	3.090587	1.606491	3.487978	-0.016445	-0.007838	-0.042733
H	5.245016	5.294309	0.304583	0.016948	-0.007871	0.042969
H	-2.791874	8.507292	6.062207	0.015653	-0.007861	0.042011

160 f = 4.389385 THz 27.579319 2PiTHz 146.414116 cm-1 18.153043 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.008681	-0.002139	-0.001633
Li	-1.316675	4.156264	2.365404	-0.008628	0.002077	0.002095
Li	-3.471104	2.744536	5.548798	0.009092	0.002143	-0.001848
Li	5.924247	11.057064	0.817991	-0.008636	-0.002208	0.001501
Na	2.049025	6.784862	1.629696	0.009624	0.022741	0.041413
Na	0.404117	7.016739	4.737094	-0.009371	-0.022437	-0.040424
Na	2.558546	13.685662	1.553699	0.009370	-0.023585	0.041803
Na	-0.105403	0.115939	4.813091	-0.008598	0.023173	-0.040680
B	4.155007	8.978944	1.168663	-0.005983	-0.010607	-0.011339
B	-1.701865	4.822656	5.198127	0.006098	0.010804	0.011247
B	0.452564	2.078144	2.014732	-0.005935	0.010432	-0.011644
B	2.000578	11.723457	4.352058	0.006146	-0.010722	0.011049
B	-2.733891	11.746082	5.839177	0.011170	-0.019030	0.010606
B	5.187034	2.055518	0.527613	-0.011192	0.019354	-0.010846
B	3.032605	4.845282	3.711007	0.010988	0.019010	0.010944
B	-0.579463	8.956318	2.655782	-0.011200	-0.019101	-0.010690
B	-0.983708	0.054306	1.827988	-0.034768	0.022557	-0.007169

B	3.436850	13.747295	4.538802	0.034653	-0.022508	0.006658
B	5.591279	6.955106	1.355407	-0.034477	-0.022572	-0.006367
B	-3.138137	6.846495	5.011383	0.034309	0.022502	0.006998
Si	0.631772	3.486686	4.508512	0.009699	0.014145	-0.007608
Si	1.821370	10.314915	1.858278	-0.009849	-0.014329	0.007204
Si	-0.333059	10.387486	5.041673	0.009836	-0.013710	-0.007507
Si	2.786201	3.414115	1.325117	-0.009685	0.013985	0.007463
O	0.061445	3.072947	3.041906	0.008432	0.017568	-0.008933
O	2.391697	10.728653	3.324884	-0.008418	-0.018130	0.008575
O	4.546126	9.973747	0.141489	0.008091	-0.017697	-0.008789
O	-2.092984	3.827853	6.225301	-0.007928	0.017983	0.008767
O	2.197450	3.933608	4.519003	0.008616	0.018825	0.008184
O	0.255692	9.867992	1.847787	-0.008689	-0.019293	-0.008351
O	-1.898737	10.834409	5.031182	0.008736	-0.018538	0.007586
O	4.351879	2.967192	1.335608	-0.008466	0.019147	-0.007786
O	-0.212316	4.798696	5.055280	0.006508	0.003648	0.009681
O	2.665458	9.002905	1.311510	-0.006493	-0.003606	-0.010367
O	0.511030	11.699496	4.494905	0.006667	-0.003105	0.010146
O	1.942113	2.102105	1.871885	-0.006409	0.003095	-0.010571
O	0.525580	2.169271	5.472081	-0.000154	0.013642	-0.012501
O	1.927562	11.632329	0.894709	-0.000290	-0.013567	0.012370
O	-0.226867	9.070071	4.078104	0.000350	-0.012936	-0.012604
O	2.680009	4.731529	2.288686	-0.000530	0.013069	0.012779
O	0.058846	0.698526	2.444964	-0.021970	0.009226	-0.013008
O	2.394296	13.103075	3.921826	0.022371	-0.009708	0.012130
O	4.548725	7.599326	0.738431	-0.021682	-0.009438	-0.012446
O	-2.095583	6.202275	5.628359	0.021951	0.009629	0.012586
O	-2.459230	13.184059	5.445139	0.024668	-0.025285	0.010077
O	4.912372	0.617542	0.921651	-0.024940	0.025683	-0.010229
O	2.757943	6.283259	4.105046	0.024557	0.025369	0.010178
O	-0.304801	7.518342	2.261744	-0.024938	-0.025575	-0.009317
O	-0.175430	2.374756	0.744070	-0.008844	0.013274	-0.008521
O	2.628573	11.426844	5.622720	0.008971	-0.013391	0.007995
O	4.783002	9.275557	2.439325	-0.008934	-0.013187	-0.008246
O	-2.329859	4.526044	3.927465	0.008753	0.013309	0.008331
O	-1.223866	12.517207	2.155216	-0.070350	0.027369	0.001112

O	3.677009	1.284394	4.211574	0.069550	-0.027276	-0.001777
O	5.831438	5.616407	1.028179	-0.069626	-0.027382	0.002136
O	-3.378295	8.185194	5.338611	0.069198	0.027227	-0.001246
H	-0.637445	12.195109	2.878812	-0.081218	0.014653	0.002261
H	3.090587	1.606491	3.487978	0.080085	-0.014690	-0.002740
H	5.245016	5.294309	0.304583	-0.079873	-0.014698	0.002857
H	-2.791874	8.507292	6.062207	0.079770	0.014506	-0.002170

161 f = 4.336884 THz 27.249444 2PiTHz 144.662866 cm-1 17.935916 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.002226	0.013804	-0.006897
Li	-1.316675	4.156264	2.365404	0.002054	-0.013865	0.006036
Li	-3.471104	2.744536	5.548798	-0.002165	-0.013644	-0.005894
Li	5.924247	11.057064	0.817991	0.001843	0.013864	0.006733
Na	2.049025	6.784862	1.629696	0.016911	-0.013551	-0.070225
Na	0.404117	7.016739	4.737094	-0.018416	0.012789	0.068836
Na	2.558546	13.685662	1.553699	0.017125	0.012945	-0.070106
Na	-0.105403	0.115939	4.813091	-0.017529	-0.012486	0.068518
B	4.155007	8.978944	1.168663	-0.001528	-0.001039	0.011510
B	-1.701865	4.822656	5.198127	0.001726	0.001059	-0.011408
B	0.452564	2.078144	2.014732	-0.001793	0.001209	0.011811
B	2.000578	11.723457	4.352058	0.001419	-0.000697	-0.011071
B	-2.733891	11.746082	5.839177	0.001207	-0.004780	-0.004252
B	5.187034	2.055518	0.527613	-0.001226	0.004171	0.004416
B	3.032605	4.845282	3.711007	0.001497	0.004386	-0.004412
B	-0.579463	8.956318	2.655782	-0.000876	-0.004422	0.004129
B	-0.983708	0.054306	1.827988	-0.018041	0.014189	0.034161
B	3.436850	13.747295	4.538802	0.018039	-0.014164	-0.033258
B	5.591279	6.955106	1.355407	-0.017832	-0.014133	0.033419
B	-3.138137	6.846495	5.011383	0.017922	0.014282	-0.034340
Si	0.631772	3.486686	4.508512	0.012716	0.003001	0.007079
Si	1.821370	10.314915	1.858278	-0.012188	-0.002791	-0.006604
Si	-0.333059	10.387486	5.041673	0.012326	-0.002863	0.006808
Si	2.786201	3.414115	1.325117	-0.012521	0.002497	-0.006748

O	0.061445	3.072947	3.041906	0.020158	0.016317	0.001706
O	2.391697	10.728653	3.324884	-0.019859	-0.015128	-0.001413
O	4.546126	9.973747	0.141489	0.019595	-0.015595	0.001644
O	-2.092984	3.827853	6.225301	-0.019936	0.015946	-0.001373
O	2.197450	3.933608	4.519003	0.008785	0.012822	0.014609
O	0.255692	9.867992	1.847787	-0.008238	-0.012658	-0.014529
O	-1.898737	10.834409	5.031182	0.008221	-0.013200	0.014322
O	4.351879	2.967192	1.335608	-0.008716	0.012013	-0.014126
O	-0.212316	4.798696	5.055280	0.001038	-0.008726	0.011551
O	2.665458	9.002905	1.311510	-0.000658	0.008560	-0.010322
O	0.511030	11.699496	4.494905	0.000624	0.008907	0.011236
O	1.942113	2.102105	1.871885	-0.001078	-0.008966	-0.010983
O	0.525580	2.169271	5.472081	0.015513	-0.005245	-0.001180
O	1.927562	11.632329	0.894709	-0.014947	0.005074	0.001187
O	-0.226867	9.070071	4.078104	0.015742	0.005402	-0.001432
O	2.680009	4.731529	2.288686	-0.015082	-0.005600	0.001261
O	0.058846	0.698526	2.444964	-0.020901	0.015333	0.034837
O	2.394296	13.103075	3.921826	0.019988	-0.014352	-0.033359
O	4.548725	7.599326	0.738431	-0.020163	-0.014737	0.033793
O	-2.095583	6.202275	5.628359	0.020387	0.015123	-0.034529
O	-2.459230	13.184059	5.445139	0.010809	-0.008478	-0.018707
O	4.912372	0.617542	0.921651	-0.010342	0.007714	0.018661
O	2.757943	6.283259	4.105046	0.010769	0.008047	-0.019400
O	-0.304801	7.518342	2.261744	-0.010354	-0.008136	0.018466
O	-0.175430	2.374756	0.744070	-0.002543	-0.003447	0.010121
O	2.628573	11.426844	5.622720	0.002247	0.003602	-0.009474
O	4.783002	9.275557	2.439325	-0.002037	0.003532	0.009712
O	-2.329859	4.526044	3.927465	0.002715	-0.003617	-0.009799
O	-1.223866	12.517207	2.155216	-0.025890	0.015387	0.036005
O	3.677009	1.284394	4.211574	0.026663	-0.015334	-0.034600
O	5.831438	5.616407	1.028179	-0.026173	-0.015336	0.034967
O	-3.378295	8.185194	5.338611	0.025745	0.015427	-0.036065
H	-0.637445	12.195109	2.878812	-0.025656	0.015031	0.035937
H	3.090587	1.606491	3.487978	0.026758	-0.014727	-0.034632
H	5.245016	5.294309	0.304583	-0.026136	-0.014642	0.034855
H	-2.791874	8.507292	6.062207	0.025257	0.015134	-0.035849

162 f = 4.320726 THz 27.147923 2PiTHz 144.123906 cm-1 17.869093
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.013958	-0.007112	0.013876
Li	-1.316675	4.156264	2.365404	-0.011534	0.007884	-0.013084
Li	-3.471104	2.744536	5.548798	-0.011603	-0.007897	-0.013645
Li	5.924247	11.057064	0.817991	0.013883	0.007239	0.013530
Na	2.049025	6.784862	1.629696	-0.029684	0.049398	0.023136
Na	0.404117	7.016739	4.737094	0.038259	-0.043599	-0.010677
Na	2.558546	13.685662	1.553699	0.038311	0.043172	-0.011254
Na	-0.105403	0.115939	4.813091	-0.030568	-0.049332	0.023050
B	4.155007	8.978944	1.168663	0.001287	0.010305	-0.003621
B	-1.701865	4.822656	5.198127	-0.000489	-0.007869	0.000056
B	0.452564	2.078144	2.014732	-0.000160	0.007972	-0.000051
B	2.000578	11.723457	4.352058	0.001649	-0.010575	-0.003749
B	-2.733891	11.746082	5.839177	-0.003948	0.008002	0.005186
B	5.187034	2.055518	0.527613	0.001923	-0.005487	-0.004845
B	3.032605	4.845282	3.711007	0.001777	0.006144	-0.004750
B	-0.579463	8.956318	2.655782	-0.004333	-0.008232	0.005196
B	-0.983708	0.054306	1.827988	0.017542	0.003276	0.016977
B	3.436850	13.747295	4.538802	-0.018127	-0.002762	-0.016917
B	5.591279	6.955106	1.355407	-0.018973	0.002297	-0.016346
B	-3.138137	6.846495	5.011383	0.017951	-0.002652	0.016954
Si	0.631772	3.486686	4.508512	-0.002962	-0.025452	-0.006661
Si	1.821370	10.314915	1.858278	0.001709	0.022956	0.004352
Si	-0.333059	10.387486	5.041673	0.002187	-0.023203	0.004360
Si	2.786201	3.414115	1.325117	-0.003055	0.025811	-0.006684
O	0.061445	3.072947	3.041906	-0.025064	-0.000475	-0.004657
O	2.391697	10.728653	3.324884	0.025562	-0.003975	0.002358
O	4.546126	9.973747	0.141489	0.025884	0.003308	0.002332
O	-2.092984	3.827853	6.225301	-0.025524	0.000645	-0.004589
O	2.197450	3.933608	4.519003	-0.004144	-0.018526	-0.035829
O	0.255692	9.867992	1.847787	0.003894	0.013304	0.034647
O	-1.898737	10.834409	5.031182	0.004445	-0.013325	0.034691

O	4.351879	2.967192	1.335608	-0.003965	0.019730	-0.036431
O	-0.212316	4.798696	5.055280	0.001416	-0.031471	0.014963
O	2.665458	9.002905	1.311510	-0.001108	0.032021	-0.021548
O	0.511030	11.699496	4.494905	-0.000684	-0.032006	-0.021127
O	1.942113	2.102105	1.871885	0.001808	0.031432	0.014860
O	0.525580	2.169271	5.472081	0.016187	-0.036623	-0.014970
O	1.927562	11.632329	0.894709	-0.020753	0.036238	0.015449
O	-0.226867	9.070071	4.078104	-0.020673	-0.036469	0.015371
O	2.680009	4.731529	2.288686	0.015680	0.036766	-0.014743
O	0.058846	0.698526	2.444964	0.022741	0.005141	0.002180
O	2.394296	13.103075	3.921826	-0.018993	-0.008582	-0.006053
O	4.548725	7.599326	0.738431	-0.019933	0.008037	-0.005451
O	-2.095583	6.202275	5.628359	0.022670	-0.005069	0.002376
O	-2.459230	13.184059	5.445139	-0.002669	0.000347	-0.026081
O	4.912372	0.617542	0.921651	-0.001166	0.002945	0.030505
O	2.757943	6.283259	4.105046	-0.000698	-0.001954	0.030140
O	-0.304801	7.518342	2.261744	-0.003128	-0.000556	-0.026073
O	-0.175430	2.374756	0.744070	0.001577	-0.005172	-0.004491
O	2.628573	11.426844	5.622720	-0.002499	0.003800	0.001990
O	4.783002	9.275557	2.439325	-0.002966	-0.004058	0.002185
O	-2.329859	4.526044	3.927465	0.001308	0.005384	-0.004432
O	-1.223866	12.517207	2.155216	0.031144	0.002166	0.019652
O	3.677009	1.284394	4.211574	-0.034333	-0.001738	-0.020622
O	5.831438	5.616407	1.028179	-0.035728	0.001151	-0.019682
O	-3.378295	8.185194	5.338611	0.032191	-0.001550	0.019888
H	-0.637445	12.195109	2.878812	0.050836	-0.000634	0.004120
H	3.090587	1.606491	3.487978	-0.053581	0.001013	-0.005420
H	5.245016	5.294309	0.304583	-0.055165	-0.001629	-0.004304
H	-2.791874	8.507292	6.062207	0.052063	0.000816	0.004455

163 f = 4.300128 THz 27.018499 2PiTHz 143.436814 cm-1 17.783905 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.010287	-0.004366	-0.000218
Li	-1.316675	4.156264	2.365404	-0.012952	-0.003456	-0.002713

Li	-3.471104	2.744536	5.548798	-0.012332	0.003677	-0.002452
Li	5.924247	11.057064	0.817991	-0.010901	0.004173	-0.000642
Na	2.049025	6.784862	1.629696	-0.041006	-0.024196	-0.057530
Na	0.404117	7.016739	4.737094	-0.034476	-0.034680	-0.065329
Na	2.558546	13.685662	1.553699	-0.035105	0.034237	-0.063331
Na	-0.105403	0.115939	4.813091	-0.040499	0.024630	-0.059617
B	4.155007	8.978944	1.168663	-0.006167	-0.011775	0.018087
B	-1.701865	4.822656	5.198127	-0.005341	-0.012918	0.018776
B	0.452564	2.078144	2.014732	-0.005830	0.013118	0.018157
B	2.000578	11.723457	4.352058	-0.005552	0.011577	0.018660
B	-2.733891	11.746082	5.839177	0.011498	-0.010611	-0.001443
B	5.187034	2.055518	0.527613	0.011741	-0.012143	-0.002827
B	3.032605	4.845282	3.711007	0.012169	0.012024	-0.002230
B	-0.579463	8.956318	2.655782	0.010972	0.010785	-0.002032
B	-0.983708	0.054306	1.827988	0.005219	-0.002087	-0.000691
B	3.436850	13.747295	4.538802	0.001561	-0.002005	-0.002356
B	5.591279	6.955106	1.355407	0.000942	0.002105	-0.003371
B	-3.138137	6.846495	5.011383	0.005685	0.002004	0.000415
Si	0.631772	3.486686	4.508512	0.005281	0.010816	0.010776
Si	1.821370	10.314915	1.858278	0.005471	0.016004	0.012331
Si	-0.333059	10.387486	5.041673	0.005506	-0.015992	0.011842
Si	2.786201	3.414115	1.325117	0.005327	-0.010806	0.011262
O	0.061445	3.072947	3.041906	-0.004011	0.021010	0.010784
O	2.391697	10.728653	3.324884	0.001071	0.021478	0.011724
O	4.546126	9.973747	0.141489	0.000599	-0.021751	0.011285
O	-2.092984	3.827853	6.225301	-0.003564	-0.020776	0.011251
O	2.197450	3.933608	4.519003	-0.000644	0.027607	0.004210
O	0.255692	9.867992	1.847787	-0.000298	0.031599	0.011296
O	-1.898737	10.834409	5.031182	0.000036	-0.030717	0.010866
O	4.351879	2.967192	1.335608	-0.000851	-0.028336	0.004580
O	-0.212316	4.798696	5.055280	-0.002983	-0.005045	0.033350
O	2.665458	9.002905	1.311510	-0.004141	0.001140	0.030365
O	0.511030	11.699496	4.494905	-0.003480	-0.001323	0.030481
O	1.942113	2.102105	1.871885	-0.003507	0.005241	0.033268
O	0.525580	2.169271	5.472081	0.025059	-0.001087	-0.004281
O	1.927562	11.632329	0.894709	0.022442	0.005922	-0.001230

O	-0.226867	9.070071	4.078104	0.021600	-0.006163	-0.001633
O	2.680009	4.731529	2.288686	0.025866	0.001323	-0.003870
O	0.058846	0.698526	2.444964	-0.014777	0.016293	0.017307
O	2.394296	13.103075	3.921826	-0.019241	0.015779	0.018265
O	4.548725	7.599326	0.738431	-0.019995	-0.015788	0.017472
O	-2.095583	6.202275	5.628359	-0.014222	-0.016318	0.018205
O	-2.459230	13.184059	5.445139	0.019234	-0.014456	-0.024059
O	4.912372	0.617542	0.921651	0.019412	-0.014692	-0.019869
O	2.757943	6.283259	4.105046	0.019603	0.014452	-0.018576
O	-0.304801	7.518342	2.261744	0.018994	0.014790	-0.025419
O	-0.175430	2.374756	0.744070	0.006646	0.006236	0.011211
O	2.628573	11.426844	5.622720	0.006587	0.007013	0.012477
O	4.783002	9.275557	2.439325	0.006055	-0.007165	0.011892
O	-2.329859	4.526044	3.927465	0.007048	-0.006096	0.011860
O	-1.223866	12.517207	2.155216	0.017995	-0.001817	0.003415
O	3.677009	1.284394	4.211574	0.011630	-0.001519	0.001369
O	5.831438	5.616407	1.028179	0.010553	0.001499	0.000636
O	-3.378295	8.185194	5.338611	0.018820	0.001810	0.004366
H	-0.637445	12.195109	2.878812	0.016974	-0.003511	0.003152
H	3.090587	1.606491	3.487978	0.007210	-0.002657	0.003880
H	5.245016	5.294309	0.304583	0.005939	0.002812	0.003156
H	-2.791874	8.507292	6.062207	0.017968	0.003296	0.004135

164 f = 4.205728 THz 26.425369 2PiTHz 140.287983 cm-1 17.393499

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.024261	-0.006258	-0.013289
Li	-1.316675	4.156264	2.365404	0.024206	0.006125	0.014259
Li	-3.471104	2.744536	5.548798	-0.024428	0.006225	-0.014269
Li	5.924247	11.057064	0.817991	0.024004	-0.006279	0.013158
Na	2.049025	6.784862	1.629696	0.015734	0.026889	0.012151
Na	0.404117	7.016739	4.737094	-0.016083	-0.027218	-0.012169
Na	2.558546	13.685662	1.553699	0.015409	-0.026685	0.011320
Na	-0.105403	0.115939	4.813091	-0.016273	0.027584	-0.013049
B	4.155007	8.978944	1.168663	0.027736	0.001281	0.009248

B	-1.701865	4.822656	5.198127	-0.028453	-0.002013	-0.008676
B	0.452564	2.078144	2.014732	0.028320	-0.001797	0.009019
B	2.000578	11.723457	4.352058	-0.027893	0.001565	-0.008959
B	-2.733891	11.746082	5.839177	-0.017186	-0.023214	-0.019332
B	5.187034	2.055518	0.527613	0.017910	0.023478	0.019178
B	3.032605	4.845282	3.711007	-0.017682	0.023668	-0.019227
B	-0.579463	8.956318	2.655782	0.017380	-0.023033	0.019228
B	-0.983708	0.054306	1.827988	0.018014	0.010516	0.011962
B	3.436850	13.747295	4.538802	-0.017898	-0.010623	-0.012797
B	5.591279	6.955106	1.355407	0.017922	-0.010657	0.012818
B	-3.138137	6.846495	5.011383	-0.017988	0.010566	-0.012048
Si	0.631772	3.486686	4.508512	-0.003935	0.012166	0.012249
Si	1.821370	10.314915	1.858278	0.003599	-0.011795	-0.012203
Si	-0.333059	10.387486	5.041673	-0.003532	-0.012052	0.012329
Si	2.786201	3.414115	1.325117	0.004030	0.011825	-0.012043
O	0.061445	3.072947	3.041906	0.010545	-0.016662	0.016533
O	2.391697	10.728653	3.324884	-0.010797	0.015996	-0.016260
O	4.546126	9.973747	0.141489	0.010748	0.015459	0.016340
O	-2.092984	3.827853	6.225301	-0.010523	-0.017106	-0.016341
O	2.197450	3.933608	4.519003	-0.016292	0.050539	0.012256
O	0.255692	9.867992	1.847787	0.015536	-0.048984	-0.011871
O	-1.898737	10.834409	5.031182	-0.015552	-0.049471	0.011912
O	4.351879	2.967192	1.335608	0.016280	0.049908	-0.012036
O	-0.212316	4.798696	5.055280	-0.028881	0.003031	-0.008503
O	2.665458	9.002905	1.311510	0.028054	-0.003032	0.008448
O	0.511030	11.699496	4.494905	-0.028156	-0.002978	-0.007891
O	1.942113	2.102105	1.871885	0.028788	0.002987	0.009072
O	0.525580	2.169271	5.472081	0.030720	0.009398	0.013746
O	1.927562	11.632329	0.894709	-0.029915	-0.009161	-0.013843
O	-0.226867	9.070071	4.078104	0.030342	-0.009212	0.013708
O	2.680009	4.731529	2.288686	-0.030293	0.009228	-0.013782
O	0.058846	0.698526	2.444964	0.040133	-0.008267	-0.006439
O	2.394296	13.103075	3.921826	-0.039614	0.007626	0.005613
O	4.548725	7.599326	0.738431	0.039207	0.007204	-0.005211
O	-2.095583	6.202275	5.628359	-0.040559	-0.008584	0.006805
O	-2.459230	13.184059	5.445139	-0.001373	-0.032019	-0.041891

O	4.912372	0.617542	0.921651	0.001601	0.032493	0.041447
O	2.757943	6.283259	4.105046	-0.001212	0.032771	-0.041978
O	-0.304801	7.518342	2.261744	0.001680	-0.031787	0.041501
O	-0.175430	2.374756	0.744070	0.020903	0.011073	0.016311
O	2.628573	11.426844	5.622720	-0.020040	-0.011069	-0.016387
O	4.783002	9.275557	2.439325	0.020146	-0.011176	0.016520
O	-2.329859	4.526044	3.927465	-0.020779	0.010932	-0.016093
O	-1.223866	12.517207	2.155216	0.015441	0.008529	0.006692
O	3.677009	1.284394	4.211574	-0.015996	-0.008601	-0.007958
O	5.831438	5.616407	1.028179	0.016301	-0.008635	0.008044
O	-3.378295	8.185194	5.338611	-0.015229	0.008576	-0.006762
H	-0.637445	12.195109	2.878812	0.013387	0.007711	0.010052
H	3.090587	1.606491	3.487978	-0.014327	-0.008403	-0.011378
H	5.245016	5.294309	0.304583	0.014603	-0.008432	0.011481
H	-2.791874	8.507292	6.062207	-0.013311	0.007761	-0.010024

165 f = 4.174178 THz 26.227133 2PiTHz 139.235583 cm-1 17.263018 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.023173	-0.003836	0.018763
Li	-1.316675	4.156264	2.365404	0.022802	-0.004550	0.018771
Li	-3.471104	2.744536	5.548798	-0.022764	-0.004413	-0.018637
Li	5.924247	11.057064	0.817991	-0.023255	-0.003949	-0.018901
Na	2.049025	6.784862	1.629696	0.020268	0.013336	0.016772
Na	0.404117	7.016739	4.737094	0.021191	0.014857	0.018587
Na	2.558546	13.685662	1.553699	-0.021649	0.014310	-0.018267
Na	-0.105403	0.115939	4.813091	-0.019745	0.013850	-0.016983
B	4.155007	8.978944	1.168663	-0.023626	-0.017433	-0.007942
B	-1.701865	4.822656	5.198127	-0.022981	-0.017672	-0.007980
B	0.452564	2.078144	2.014732	0.022960	-0.017751	0.007961
B	2.000578	11.723457	4.352058	0.023629	-0.017346	0.007951
B	-2.733891	11.746082	5.839177	0.017197	0.014300	0.015629
B	5.187034	2.055518	0.527613	0.016751	0.013718	0.015435
B	3.032605	4.845282	3.711007	-0.016790	0.013679	-0.015406
B	-0.579463	8.956318	2.655782	-0.017174	0.014342	-0.015669

B	-0.983708	0.054306	1.827988	0.007673	-0.003966	-0.003193
B	3.436850	13.747295	4.538802	0.008802	-0.003633	-0.003290
B	5.591279	6.955106	1.355407	-0.008648	-0.003698	0.003510
B	-3.138137	6.846495	5.011383	-0.007800	-0.003904	0.002975
Si	0.631772	3.486686	4.508512	-0.006618	0.001597	0.008054
Si	1.821370	10.314915	1.858278	-0.006876	0.001794	0.008174
Si	-0.333059	10.387486	5.041673	0.006852	0.002054	-0.008227
Si	2.786201	3.414115	1.325117	0.006608	0.001338	-0.008015
O	0.061445	3.072947	3.041906	-0.004871	-0.044445	0.021171
O	2.391697	10.728653	3.324884	-0.004930	-0.044427	0.021293
O	4.546126	9.973747	0.141489	0.004704	-0.044447	-0.021340
O	-2.092984	3.827853	6.225301	0.005054	-0.044421	-0.021130
O	2.197450	3.933608	4.519003	-0.018201	0.037190	0.007296
O	0.255692	9.867992	1.847787	-0.018649	0.038028	0.007176
O	-1.898737	10.834409	5.031182	0.018623	0.038239	-0.007513
O	4.351879	2.967192	1.335608	0.018183	0.036947	-0.006970
O	-0.212316	4.798696	5.055280	-0.024276	0.001088	-0.020508
O	2.665458	9.002905	1.311510	-0.024893	0.001101	-0.020557
O	0.511030	11.699496	4.494905	0.024918	0.001403	0.020699
O	1.942113	2.102105	1.871885	0.024223	0.000792	0.020357
O	0.525580	2.169271	5.472081	0.028246	0.001547	0.012390
O	1.927562	11.632329	0.894709	0.028752	0.001548	0.012426
O	-0.226867	9.070071	4.078104	-0.028620	0.001915	-0.012558
O	2.680009	4.731529	2.288686	-0.028392	0.001185	-0.012269
O	0.058846	0.698526	2.444964	0.040968	-0.035775	-0.022905
O	2.394296	13.103075	3.921826	0.042221	-0.035540	-0.023196
O	4.548725	7.599326	0.738431	-0.042021	-0.035622	0.023260
O	-2.095583	6.202275	5.628359	-0.041155	-0.035703	0.022838
O	-2.459230	13.184059	5.445139	-0.004010	0.026137	0.030320
O	4.912372	0.617542	0.921651	-0.004396	0.025390	0.029446
O	2.757943	6.283259	4.105046	0.004426	0.025452	-0.029775
O	-0.304801	7.518342	2.261744	0.004008	0.026089	-0.030008
O	-0.175430	2.374756	0.744070	0.021157	-0.001218	0.013989
O	2.628573	11.426844	5.622720	0.021649	-0.000719	0.014093
O	4.783002	9.275557	2.439325	-0.021626	-0.000676	-0.014136
O	-2.329859	4.526044	3.927465	-0.021204	-0.001282	-0.013954

O	-1.223866	12.517207	2.155216	-0.015648	-0.002384	-0.013640
O	3.677009	1.284394	4.211574	-0.013916	-0.002243	-0.014009
O	5.831438	5.616407	1.028179	0.014155	-0.002313	0.014286
O	-3.378295	8.185194	5.338611	0.015446	-0.002322	0.013385
H	-0.637445	12.195109	2.878812	-0.010900	-0.019398	-0.026996
H	3.090587	1.606491	3.487978	-0.008902	-0.019296	-0.027528
H	5.245016	5.294309	0.304583	0.009345	-0.019312	0.027632
H	-2.791874	8.507292	6.062207	0.010505	-0.019406	0.026913

166 f = 3.956591 THz 24.859995 2PiTHz 131.977670 cm-1 16.363152 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.003696	0.036552	-0.016360
Li	-1.316675	4.156264	2.365404	-0.002354	-0.035213	0.015859
Li	-3.471104	2.744536	5.548798	-0.003414	0.036667	0.016526
Li	5.924247	11.057064	0.817991	0.002465	-0.035488	-0.015846
Na	2.049025	6.784862	1.629696	0.017848	0.001445	-0.037205
Na	0.404117	7.016739	4.737094	-0.018628	-0.003695	0.038740
Na	2.558546	13.685662	1.553699	-0.017278	0.001262	0.037628
Na	-0.105403	0.115939	4.813091	0.018440	-0.003927	-0.038235
B	4.155007	8.978944	1.168663	-0.008196	-0.011349	0.004447
B	-1.701865	4.822656	5.198127	0.010092	0.009971	-0.003991
B	0.452564	2.078144	2.014732	0.008240	-0.011301	-0.004764
B	2.000578	11.723457	4.352058	-0.009911	0.009546	0.003811
B	-2.733891	11.746082	5.839177	-0.007049	0.012019	-0.000240
B	5.187034	2.055518	0.527613	0.005188	-0.011030	-0.000994
B	3.032605	4.845282	3.711007	0.006881	0.011991	0.000529
B	-0.579463	8.956318	2.655782	-0.005449	-0.011291	0.001056
B	-0.983708	0.054306	1.827988	0.025768	-0.025036	-0.030204
B	3.436850	13.747295	4.538802	-0.033640	0.026601	0.031346
B	5.591279	6.955106	1.355407	-0.025586	-0.025111	0.030030
B	-3.138137	6.846495	5.011383	0.033615	0.026785	-0.031186
Si	0.631772	3.486686	4.508512	0.006257	-0.009006	0.000907
Si	1.821370	10.314915	1.858278	-0.005438	0.008101	-0.002020
Si	-0.333059	10.387486	5.041673	-0.006357	-0.008777	-0.001029

Si	2.786201	3.414115	1.325117	0.005339	0.008626	0.002008
O	0.061445	3.072947	3.041906	-0.005075	-0.035138	0.013215
O	2.391697	10.728653	3.324884	0.005821	0.034432	-0.014415
O	4.546126	9.973747	0.141489	0.004967	-0.034945	-0.013343
O	-2.092984	3.827853	6.225301	-0.005971	0.035310	0.014529
O	2.197450	3.933608	4.519003	-0.002364	0.016908	-0.001465
O	0.255692	9.867992	1.847787	0.002140	-0.014078	0.003847
O	-1.898737	10.834409	5.031182	0.002370	0.017424	0.001403
O	4.351879	2.967192	1.335608	-0.002206	-0.013492	-0.003936
O	-0.212316	4.798696	5.055280	0.005312	-0.011822	-0.000159
O	2.665458	9.002905	1.311510	-0.004477	0.009603	-0.000254
O	0.511030	11.699496	4.494905	-0.005192	-0.011806	-0.000157
O	1.942113	2.102105	1.871885	0.004463	0.009890	-0.000207
O	0.525580	2.169271	5.472081	0.012783	-0.009288	-0.000468
O	1.927562	11.632329	0.894709	-0.012773	0.008088	-0.001343
O	-0.226867	9.070071	4.078104	-0.013315	-0.009208	0.000539
O	2.680009	4.731529	2.288686	0.012530	0.008400	0.001616
O	0.058846	0.698526	2.444964	0.031332	-0.028492	-0.033477
O	2.394296	13.103075	3.921826	-0.036367	0.027199	0.032973
O	4.548725	7.599326	0.738431	-0.030918	-0.028404	0.033039
O	-2.095583	6.202275	5.628359	0.037038	0.027864	-0.033491
O	-2.459230	13.184059	5.445139	-0.019105	0.015614	0.008663
O	4.912372	0.617542	0.921651	0.013078	-0.012875	-0.008330
O	2.757943	6.283259	4.105046	0.018705	0.015428	-0.007925
O	-0.304801	7.518342	2.261744	-0.013347	-0.013176	0.008699
O	-0.175430	2.374756	0.744070	0.001467	0.003006	0.004379
O	2.628573	11.426844	5.622720	-0.002691	-0.004582	-0.005116
O	4.783002	9.275557	2.439325	-0.001671	0.002874	-0.004571
O	-2.329859	4.526044	3.927465	0.002618	-0.004358	0.005107
O	-1.223866	12.517207	2.155216	0.033901	-0.028232	-0.039847
O	3.677009	1.284394	4.211574	-0.048946	0.030997	0.041858
O	5.831438	5.616407	1.028179	-0.033538	-0.028210	0.039486
O	-3.378295	8.185194	5.338611	0.048651	0.031112	-0.041584
H	-0.637445	12.195109	2.878812	0.029218	-0.027233	-0.035994
H	3.090587	1.606491	3.487978	-0.046333	0.026860	0.038021
H	5.245016	5.294309	0.304583	-0.028666	-0.027287	0.035521

H -2.791874 8.507292 6.062207 0.046215 0.026934 -0.037852

167 f = 3.943184 THz 24.775757 2PiTHz 131.530464 cm-1 16.307705

meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.006667	0.004956	-0.001887
Li	-1.316675	4.156264	2.365404	0.007171	0.010390	-0.004543
Li	-3.471104	2.744536	5.548798	-0.006789	0.004436	0.001820
Li	5.924247	11.057064	0.817991	-0.007163	0.010915	0.004578
Na	2.049025	6.784862	1.629696	-0.007618	-0.014841	0.009218
Na	0.404117	7.016739	4.737094	-0.003760	-0.014464	0.002903
Na	2.558546	13.685662	1.553699	0.007046	-0.014728	-0.009386
Na	-0.105403	0.115939	4.813091	0.004362	-0.014470	-0.002977
B	4.155007	8.978944	1.168663	0.011069	-0.008417	0.003889
B	-1.701865	4.822656	5.198127	0.009561	-0.010777	0.004579
B	0.452564	2.078144	2.014732	-0.011134	-0.008959	-0.003775
B	2.000578	11.723457	4.352058	-0.009577	-0.010131	-0.004627
B	-2.733891	11.746082	5.839177	-0.008970	0.004431	-0.008405
B	5.187034	2.055518	0.527613	-0.009986	0.005879	-0.008250
B	3.032605	4.845282	3.711007	0.009002	0.004032	0.008261
B	-0.579463	8.956318	2.655782	0.009946	0.006322	0.008369
B	-0.983708	0.054306	1.827988	-0.050042	0.011584	0.009646
B	3.436850	13.747295	4.538802	-0.044742	0.007683	0.004251
B	5.591279	6.955106	1.355407	0.049671	0.011955	-0.009383
B	-3.138137	6.846495	5.011383	0.045165	0.007295	-0.004520
Si	0.631772	3.486686	4.508512	0.004721	-0.002686	-0.006370
Si	1.821370	10.314915	1.858278	0.005626	-0.003682	-0.006181
Si	-0.333059	10.387486	5.041673	-0.004680	-0.002282	0.006423
Si	2.786201	3.414115	1.325117	-0.005713	-0.004179	0.006154
O	0.061445	3.072947	3.041906	0.005364	0.001069	-0.008100
O	2.391697	10.728653	3.324884	0.004567	-0.004086	-0.005982
O	4.546126	9.973747	0.141489	-0.005450	0.001679	0.008262
O	-2.092984	3.827853	6.225301	-0.004503	-0.004890	0.005813
O	2.197450	3.933608	4.519003	-0.001414	0.019098	0.014768
O	0.255692	9.867992	1.847787	-0.001814	0.021949	0.014430

O	-1.898737	10.834409	5.031182	0.001418	0.019391	-0.014819
O	4.351879	2.967192	1.335608	0.001735	0.021478	-0.014319
O	-0.212316	4.798696	5.055280	0.003890	-0.011639	-0.000502
O	2.665458	9.002905	1.311510	0.004675	-0.012993	-0.000552
O	0.511030	11.699496	4.494905	-0.003898	-0.011237	0.000496
O	1.942113	2.102105	1.871885	-0.004750	-0.013413	0.000655
O	0.525580	2.169271	5.472081	0.001565	-0.005403	-0.011688
O	1.927562	11.632329	0.894709	0.003452	-0.006443	-0.011690
O	-0.226867	9.070071	4.078104	-0.001404	-0.005065	0.011802
O	2.680009	4.731529	2.288686	-0.003590	-0.006831	0.011550
O	0.058846	0.698526	2.444964	-0.035694	-0.003827	0.002406
O	2.394296	13.103075	3.921826	-0.029973	-0.007877	-0.003143
O	4.548725	7.599326	0.738431	0.035587	-0.003283	-0.002402
O	-2.095583	6.202275	5.628359	0.029925	-0.008608	0.003288
O	-2.459230	13.184059	5.445139	-0.032393	0.014106	-0.001894
O	4.912372	0.617542	0.921651	-0.035211	0.016077	-0.000422
O	2.757943	6.283259	4.105046	0.032669	0.013829	0.001688
O	-0.304801	7.518342	2.261744	0.035031	0.016454	0.000498
O	-0.175430	2.374756	0.744070	-0.006185	-0.009765	-0.004213
O	2.628573	11.426844	5.622720	-0.005846	-0.008641	-0.003555
O	4.783002	9.275557	2.439325	0.006156	-0.009298	0.004334
O	-2.329859	4.526044	3.927465	0.005836	-0.009167	0.003463
O	-1.223866	12.517207	2.155216	-0.094507	0.019371	0.016170
O	3.677009	1.284394	4.211574	-0.086693	0.014644	0.008784
O	5.831438	5.616407	1.028179	0.093704	0.019565	-0.015610
O	-3.378295	8.185194	5.338611	0.087777	0.014457	-0.009357
H	-0.637445	12.195109	2.878812	-0.107736	-0.000245	0.016493
H	3.090587	1.606491	3.487978	-0.100526	-0.004508	0.009762
H	5.245016	5.294309	0.304583	0.106921	-0.000053	-0.015929
H	-2.791874	8.507292	6.062207	0.101635	-0.004745	-0.010324

168 f = 3.858239 THz 24.242033 2PiTHz 128.697009 cm-1 15.956401 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.008511	0.022994	-0.006404

Li	-1.316675	4.156264	2.365404	0.007729	-0.023188	0.006371
Li	-3.471104	2.744536	5.548798	-0.007729	-0.022839	-0.006221
Li	5.924247	11.057064	0.817991	0.008516	0.022748	0.006265
Na	2.049025	6.784862	1.629696	-0.050476	0.001488	0.006360
Na	0.404117	7.016739	4.737094	0.052178	-0.001050	-0.006093
Na	2.558546	13.685662	1.553699	-0.052367	-0.000992	0.006550
Na	-0.105403	0.115939	4.813091	0.050539	0.001394	-0.006594
B	4.155007	8.978944	1.168663	0.004020	0.029518	0.006145
B	-1.701865	4.822656	5.198127	-0.003420	-0.028975	-0.005814
B	0.452564	2.078144	2.014732	0.003556	-0.029090	0.005730
B	2.000578	11.723457	4.352058	-0.004083	0.029593	-0.006097
B	-2.733891	11.746082	5.839177	-0.001495	0.014562	-0.011819
B	5.187034	2.055518	0.527613	0.001163	-0.015011	0.011336
B	3.032605	4.845282	3.711007	-0.001080	-0.014915	-0.011371
B	-0.579463	8.956318	2.655782	0.001505	0.014483	0.011760
B	-0.983708	0.054306	1.827988	-0.019028	-0.016928	0.014715
B	3.436850	13.747295	4.538802	0.019293	0.016720	-0.015368
B	5.591279	6.955106	1.355407	-0.019620	0.016490	0.015644
B	-3.138137	6.846495	5.011383	0.019277	-0.016724	-0.014949
Si	0.631772	3.486686	4.508512	0.001333	-0.018765	0.004113
Si	1.821370	10.314915	1.858278	-0.001317	0.018810	-0.004361
Si	-0.333059	10.387486	5.041673	0.001314	0.018661	0.004321
Si	2.786201	3.414115	1.325117	-0.001235	-0.018632	-0.004143
O	0.061445	3.072947	3.041906	-0.005708	-0.041617	0.013263
O	2.391697	10.728653	3.324884	0.005474	0.042344	-0.013668
O	4.546126	9.973747	0.141489	-0.005373	0.042001	0.013525
O	-2.092984	3.827853	6.225301	0.005666	-0.041243	-0.013167
O	2.197450	3.933608	4.519003	-0.001689	-0.008826	-0.004927
O	0.255692	9.867992	1.847787	0.002107	0.007593	0.004395
O	-1.898737	10.834409	5.031182	-0.002051	0.007633	-0.004399
O	4.351879	2.967192	1.335608	0.001718	-0.008882	0.004802
O	-0.212316	4.798696	5.055280	-0.002980	-0.016188	-0.007241
O	2.665458	9.002905	1.311510	0.003653	0.016533	0.007619
O	0.511030	11.699496	4.494905	-0.003672	0.016388	-0.007601
O	1.942113	2.102105	1.871885	0.003079	-0.016045	0.007208
O	0.525580	2.169271	5.472081	0.012789	-0.013056	0.010607

O	1.927562	11.632329	0.894709	-0.013680	0.013142	-0.010898
O	-0.226867	9.070071	4.078104	0.013676	0.013019	0.010834
O	2.680009	4.731529	2.288686	-0.012619	-0.012918	-0.010647
O	0.058846	0.698526	2.444964	0.009415	-0.036907	-0.009766
O	2.394296	13.103075	3.921826	-0.009906	0.037513	0.009605
O	4.548725	7.599326	0.738431	0.009540	0.037278	-0.009270
O	-2.095583	6.202275	5.628359	-0.009012	-0.036601	0.009405
O	-2.459230	13.184059	5.445139	0.013199	0.007455	-0.016932
O	4.912372	0.617542	0.921651	-0.012896	-0.008264	0.015869
O	2.757943	6.283259	4.105046	0.013013	-0.008184	-0.015884
O	-0.304801	7.518342	2.261744	-0.013289	0.007367	0.016880
O	-0.175430	2.374756	0.744070	0.003597	-0.021608	0.008520
O	2.628573	11.426844	5.622720	-0.004002	0.021684	-0.009103
O	4.783002	9.275557	2.439325	0.004036	0.021750	0.009060
O	-2.329859	4.526044	3.927465	-0.003538	-0.021601	-0.008509
O	-1.223866	12.517207	2.155216	-0.049993	-0.006887	0.031825
O	3.677009	1.284394	4.211574	0.051453	0.006510	-0.032364
O	5.831438	5.616407	1.028179	-0.052051	0.006213	0.032793
O	-3.378295	8.185194	5.338611	0.050204	-0.006683	-0.032081
H	-0.637445	12.195109	2.878812	-0.052707	-0.010087	0.032637
H	3.090587	1.606491	3.487978	0.054209	0.010391	-0.032855
H	5.245016	5.294309	0.304583	-0.054832	0.010134	0.033289
H	-2.791874	8.507292	6.062207	0.052878	-0.009850	-0.032879

169 f = 3.689422 THz 23.181325 2PiTHz 123.065884 cm-1 15.258230 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.011246	-0.004469	-0.011928
Li	-1.316675	4.156264	2.365404	-0.012280	-0.004542	-0.012900
Li	-3.471104	2.744536	5.548798	-0.012204	0.004559	-0.012857
Li	5.924247	11.057064	0.817991	-0.011293	0.004478	-0.011964
Na	2.049025	6.784862	1.629696	-0.015903	0.012506	0.064391
Na	0.404117	7.016739	4.737094	-0.018779	0.012023	0.065267
Na	2.558546	13.685662	1.553699	-0.018709	-0.011866	0.065106
Na	-0.105403	0.115939	4.813091	-0.016029	-0.012632	0.064349

B	4.155007	8.978944	1.168663	-0.005133	-0.008266	0.004787
B	-1.701865	4.822656	5.198127	-0.005578	-0.008826	0.004739
B	0.452564	2.078144	2.014732	-0.005666	0.008861	0.004706
B	2.000578	11.723457	4.352058	-0.005084	0.008252	0.004788
B	-2.733891	11.746082	5.839177	0.013037	-0.004726	-0.019853
B	5.187034	2.055518	0.527613	0.013167	-0.005177	-0.020809
B	3.032605	4.845282	3.711007	0.013221	0.005113	-0.020727
B	-0.579463	8.956318	2.655782	0.013026	0.004764	-0.019908
B	-0.983708	0.054306	1.827988	-0.005344	0.006479	-0.003705
B	3.436850	13.747295	4.538802	-0.005363	0.006451	-0.003482
B	5.591279	6.955106	1.355407	-0.005349	-0.006433	-0.003526
B	-3.138137	6.846495	5.011383	-0.005301	-0.006489	-0.003670
Si	0.631772	3.486686	4.508512	0.005038	0.020489	-0.009633
Si	1.821370	10.314915	1.858278	0.005240	0.020185	-0.009028
Si	-0.333059	10.387486	5.041673	0.005247	-0.020168	-0.009044
Si	2.786201	3.414115	1.325117	0.005031	-0.020512	-0.009599
O	0.061445	3.072947	3.041906	0.006587	0.032282	-0.013513
O	2.391697	10.728653	3.324884	0.007330	0.031353	-0.012952
O	4.546126	9.973747	0.141489	0.007312	-0.031399	-0.012976
O	-2.092984	3.827853	6.225301	0.006595	-0.032172	-0.013441
O	2.197450	3.933608	4.519003	0.003188	0.025448	-0.011248
O	0.255692	9.867992	1.847787	0.003555	0.024695	-0.010200
O	-1.898737	10.834409	5.031182	0.003588	-0.024598	-0.010197
O	4.351879	2.967192	1.335608	0.003151	-0.025566	-0.011250
O	-0.212316	4.798696	5.055280	-0.001303	0.009110	0.012430
O	2.665458	9.002905	1.311510	-0.000922	0.009514	0.011782
O	0.511030	11.699496	4.494905	-0.000874	-0.009518	0.011789
O	1.942113	2.102105	1.871885	-0.001386	-0.009110	0.012387
O	0.525580	2.169271	5.472081	0.024130	0.010156	-0.021666
O	1.927562	11.632329	0.894709	0.023258	0.010377	-0.020505
O	-0.226867	9.070071	4.078104	0.023221	-0.010348	-0.020547
O	2.680009	4.731529	2.288686	0.024234	-0.010203	-0.021596
O	0.058846	0.698526	2.444964	-0.029647	0.020157	0.023116
O	2.394296	13.103075	3.921826	-0.029003	0.019447	0.022800
O	4.548725	7.599326	0.738431	-0.029072	-0.019479	0.022833
O	-2.095583	6.202275	5.628359	-0.029498	-0.020076	0.023070

O	-2.459230	13.184059	5.445139	0.017760	-0.010927	-0.037322
O	4.912372	0.617542	0.921651	0.018360	-0.011551	-0.038486
O	2.757943	6.283259	4.105046	0.018372	0.011464	-0.038368
O	-0.304801	7.518342	2.261744	0.017814	0.010992	-0.037442
O	-0.175430	2.374756	0.744070	0.009647	-0.001490	-0.005148
O	2.628573	11.426844	5.622720	0.009725	-0.001604	-0.004754
O	4.783002	9.275557	2.439325	0.009697	0.001600	-0.004771
O	-2.329859	4.526044	3.927465	0.009708	0.001461	-0.005081
O	-1.223866	12.517207	2.155216	-0.008900	0.006176	-0.005543
O	3.677009	1.284394	4.211574	-0.009504	0.006134	-0.005733
O	5.831438	5.616407	1.028179	-0.009487	-0.006115	-0.005795
O	-3.378295	8.185194	5.338611	-0.008918	-0.006194	-0.005499
H	-0.637445	12.195109	2.878812	-0.025450	0.007538	0.007412
H	3.090587	1.606491	3.487978	-0.026105	0.007141	0.007097
H	5.245016	5.294309	0.304583	-0.026088	-0.007118	0.007026
H	-2.791874	8.507292	6.062207	-0.025488	-0.007554	0.007476

170 f = 3.439624 THz 21.611796 2PiTHz 114.733506 cm-1 14.225147 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.015032	0.000935	-0.021335
Li	-1.316675	4.156264	2.365404	0.014656	-0.001282	0.020622
Li	-3.471104	2.744536	5.548798	0.014183	0.001397	0.020952
Li	5.924247	11.057064	0.817991	-0.015521	-0.000803	-0.021005
Na	2.049025	6.784862	1.629696	-0.078211	-0.022176	-0.021425
Na	0.404117	7.016739	4.737094	0.080331	0.022118	0.019924
Na	2.558546	13.685662	1.553699	0.081804	-0.022675	0.022185
Na	-0.105403	0.115939	4.813091	-0.076865	0.021624	-0.019241
B	4.155007	8.978944	1.168663	-0.008599	-0.013219	-0.001709
B	-1.701865	4.822656	5.198127	0.007582	0.012744	0.001763
B	0.452564	2.078144	2.014732	0.007980	-0.012933	0.002274
B	2.000578	11.723457	4.352058	-0.008211	0.013048	-0.001188
B	-2.733891	11.746082	5.839177	0.006813	-0.006561	-0.018165
B	5.187034	2.055518	0.527613	-0.006018	0.006516	0.017831
B	3.032605	4.845282	3.711007	-0.006324	-0.006383	0.017288

B	-0.579463	8.956318	2.655782	0.006534	0.006747	-0.018728
B	-0.983708	0.054306	1.827988	-0.000772	-0.002959	0.001755
B	3.436850	13.747295	4.538802	0.000326	0.003366	-0.000935
B	5.591279	6.955106	1.355407	0.000057	-0.003204	-0.001894
B	-3.138137	6.846495	5.011383	-0.001116	0.003075	0.000824
Si	0.631772	3.486686	4.508512	0.000320	-0.006342	0.012632
Si	1.821370	10.314915	1.858278	-0.000290	0.007964	-0.012452
Si	-0.333059	10.387486	5.041673	-0.000385	-0.008002	-0.012720
Si	2.786201	3.414115	1.325117	0.000252	0.006268	0.012369
O	0.061445	3.072947	3.041906	0.008502	-0.020726	0.013075
O	2.391697	10.728653	3.324884	-0.007811	0.022421	-0.013098
O	4.546126	9.973747	0.141489	-0.008032	-0.022543	-0.013416
O	-2.092984	3.827853	6.225301	0.008302	0.020577	0.012766
O	2.197450	3.933608	4.519003	0.003859	-0.016343	0.019352
O	0.255692	9.867992	1.847787	-0.004137	0.018875	-0.018999
O	-1.898737	10.834409	5.031182	-0.004069	-0.018404	-0.019077
O	4.351879	2.967192	1.335608	0.003943	0.016740	0.019279
O	-0.212316	4.798696	5.055280	0.005940	0.007916	-0.009087
O	2.665458	9.002905	1.311510	-0.006707	-0.006870	0.009743
O	0.511030	11.699496	4.494905	-0.006363	0.006726	0.009933
O	1.942113	2.102105	1.871885	0.006295	-0.008076	-0.008877
O	0.525580	2.169271	5.472081	-0.019288	0.002007	0.021557
O	1.927562	11.632329	0.894709	0.020768	-0.000831	-0.021880
O	-0.226867	9.070071	4.078104	0.020114	0.000830	-0.022288
O	2.680009	4.731529	2.288686	-0.019922	-0.002046	0.021158
O	0.058846	0.698526	2.444964	0.010249	-0.015900	-0.006516
O	2.394296	13.103075	3.921826	-0.012211	0.016949	0.008906
O	4.548725	7.599326	0.738431	-0.012666	-0.017024	0.008111
O	-2.095583	6.202275	5.628359	0.009758	0.015813	-0.007303
O	-2.459230	13.184059	5.445139	0.014672	-0.011407	-0.025023
O	4.912372	0.617542	0.921651	-0.013268	0.010765	0.023250
O	2.757943	6.283259	4.105046	-0.013557	-0.010562	0.022313
O	-0.304801	7.518342	2.261744	0.014461	0.011679	-0.026008
O	-0.175430	2.374756	0.744070	-0.002393	-0.002041	0.008922
O	2.628573	11.426844	5.622720	0.002879	0.002130	-0.008177
O	4.783002	9.275557	2.439325	0.002641	-0.002150	-0.008812

O	-2.329859	4.526044	3.927465	-0.002651	0.001999	0.008305
O	-1.223866	12.517207	2.155216	-0.013870	-0.003307	-0.005961
O	3.677009	1.284394	4.211574	0.011948	0.003986	0.006923
O	5.831438	5.616407	1.028179	0.012001	-0.003777	0.006006
O	-3.378295	8.185194	5.338611	-0.013923	0.003479	-0.006888
H	-0.637445	12.195109	2.878812	-0.012882	-0.013944	-0.011810
H	3.090587	1.606491	3.487978	0.009683	0.014144	0.013519
H	5.245016	5.294309	0.304583	0.009635	-0.014014	0.012713
H	-2.791874	8.507292	6.062207	-0.013074	0.014053	-0.012605

171 f = 3.410721 THz 21.430195 2PiTHz 113.769416 cm-1 14.105615 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.013644	0.006091	-0.009364
Li	-1.316675	4.156264	2.365404	0.013343	0.005145	-0.010031
Li	-3.471104	2.744536	5.548798	-0.013975	0.005216	0.009268
Li	5.924247	11.057064	0.817991	-0.012982	0.006020	0.010121
Na	2.049025	6.784862	1.629696	-0.042174	-0.020209	-0.068528
Na	0.404117	7.016739	4.737094	-0.045740	-0.021889	-0.071026
Na	2.558546	13.685662	1.553699	0.043425	-0.021006	0.070383
Na	-0.105403	0.115939	4.813091	0.044194	-0.021077	0.069292
B	4.155007	8.978944	1.168663	-0.011404	-0.003210	-0.014561
B	-1.701865	4.822656	5.198127	-0.012041	-0.004872	-0.014791
B	0.452564	2.078144	2.014732	0.011742	-0.004411	0.014728
B	2.000578	11.723457	4.352058	0.011745	-0.003662	0.014616
B	-2.733891	11.746082	5.839177	0.008700	0.006307	0.015377
B	5.187034	2.055518	0.527613	0.009135	0.005200	0.014985
B	3.032605	4.845282	3.711007	-0.008873	0.005521	-0.015707
B	-0.579463	8.956318	2.655782	-0.008921	0.005990	-0.014661
B	-0.983708	0.054306	1.827988	0.008637	0.005857	0.028667
B	3.436850	13.747295	4.538802	0.008710	0.006563	0.028300
B	5.591279	6.955106	1.355407	-0.008827	0.006597	-0.028167
B	-3.138137	6.846495	5.011383	-0.008484	0.005813	-0.028794
Si	0.631772	3.486686	4.508512	0.002147	-0.001463	0.007301
Si	1.821370	10.314915	1.858278	0.002195	-0.000825	0.007617

Si	-0.333059	10.387486	5.041673	-0.002132	-0.000541	-0.007149
Si	2.786201	3.414115	1.325117	-0.002165	-0.001708	-0.007782
O	0.061445	3.072947	3.041906	0.007173	-0.001274	0.007540
O	2.391697	10.728653	3.324884	0.007524	-0.000601	0.007693
O	4.546126	9.973747	0.141489	-0.007184	0.000209	-0.007203
O	-2.092984	3.827853	6.225301	-0.007506	-0.002064	-0.008034
O	2.197450	3.933608	4.519003	-0.002997	0.014749	0.003327
O	0.255692	9.867992	1.847787	-0.002626	0.014403	0.004032
O	-1.898737	10.834409	5.031182	0.002854	0.015199	-0.003311
O	4.351879	2.967192	1.335608	0.002812	0.013996	-0.004098
O	-0.212316	4.798696	5.055280	-0.011110	-0.005273	-0.005334
O	2.665458	9.002905	1.311510	-0.010533	-0.004055	-0.005447
O	0.511030	11.699496	4.494905	0.010812	-0.004307	0.005078
O	1.942113	2.102105	1.871885	0.010875	-0.004971	0.005713
O	0.525580	2.169271	5.472081	0.019500	-0.001111	0.010337
O	1.927562	11.632329	0.894709	0.018230	-0.000177	0.010940
O	-0.226867	9.070071	4.078104	-0.018966	-0.000269	-0.010083
O	2.680009	4.731529	2.288686	-0.018704	-0.000973	-0.011213
O	0.058846	0.698526	2.444964	0.012676	-0.000268	0.024775
O	2.394296	13.103075	3.921826	0.012679	0.000387	0.024545
O	4.548725	7.599326	0.738431	-0.012204	0.001008	-0.024864
O	-2.095583	6.202275	5.628359	-0.013072	-0.000873	-0.024476
O	-2.459230	13.184059	5.445139	0.007334	0.008831	0.027971
O	4.912372	0.617542	0.921651	0.007758	0.007810	0.027704
O	2.757943	6.283259	4.105046	-0.007158	0.008319	-0.028656
O	-0.304801	7.518342	2.261744	-0.007914	0.008294	-0.026976
O	-0.175430	2.374756	0.744070	0.007985	-0.000613	0.017422
O	2.628573	11.426844	5.622720	0.007657	0.000307	0.017462
O	4.783002	9.275557	2.439325	-0.007709	0.000364	-0.017149
O	-2.329859	4.526044	3.927465	-0.007888	-0.000662	-0.017746
O	-1.223866	12.517207	2.155216	-0.000877	0.007430	0.027963
O	3.677009	1.284394	4.211574	-0.000423	0.007800	0.026638
O	5.831438	5.616407	1.028179	-0.000230	0.007835	-0.026789
O	-3.378295	8.185194	5.338611	0.001572	0.007387	-0.027809
H	-0.637445	12.195109	2.878812	0.001994	0.005018	0.024753
H	3.090587	1.606491	3.487978	0.002236	0.005123	0.023433

H	5.245016	5.294309	0.304583	-0.002883	0.005565	-0.023786
H	-2.791874	8.507292	6.062207	-0.001290	0.004561	-0.024405

172 f = 3.290897 THz 20.677313 2PiTHz 109.772492 cm-1 13.610059 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.031621	-0.016912	-0.011914
Li	-1.316675	4.156264	2.365404	0.032023	0.017224	0.011672
Li	-3.471104	2.744536	5.548798	0.031949	-0.017156	0.011702
Li	5.924247	11.057064	0.817991	-0.031717	0.016980	-0.011885
Na	2.049025	6.784862	1.629696	0.048261	0.009064	0.004239
Na	0.404117	7.016739	4.737094	-0.051556	-0.009055	-0.002653
Na	2.558546	13.685662	1.553699	-0.051127	0.008869	-0.002307
Na	-0.105403	0.115939	4.813091	0.048438	-0.009219	0.004525
B	4.155007	8.978944	1.168663	-0.017126	-0.005284	-0.003313
B	-1.701865	4.822656	5.198127	0.017357	0.005235	0.002820
B	0.452564	2.078144	2.014732	0.017436	-0.005269	0.002863
B	2.000578	11.723457	4.352058	-0.017064	0.005240	-0.003251
B	-2.733891	11.746082	5.839177	-0.003322	-0.011200	-0.023177
B	5.187034	2.055518	0.527613	0.003356	0.011317	0.023168
B	3.032605	4.845282	3.711007	0.003293	-0.011266	0.023125
B	-0.579463	8.956318	2.655782	-0.003353	0.011272	-0.023254
B	-0.983708	0.054306	1.827988	-0.003701	0.007249	0.021648
B	3.436850	13.747295	4.538802	0.004044	-0.007160	-0.021586
B	5.591279	6.955106	1.355407	0.004121	0.007232	-0.021773
B	-3.138137	6.846495	5.011383	-0.003705	-0.007187	0.021507
Si	0.631772	3.486686	4.508512	0.013394	-0.018894	0.012193
Si	1.821370	10.314915	1.858278	-0.013228	0.018237	-0.012539
Si	-0.333059	10.387486	5.041673	-0.013244	-0.018237	-0.012564
Si	2.786201	3.414115	1.325117	0.013400	0.018883	0.012176
O	0.061445	3.072947	3.041906	0.010397	-0.021032	0.013516
O	2.391697	10.728653	3.324884	-0.010471	0.020620	-0.013826
O	4.546126	9.973747	0.141489	-0.010531	-0.020635	-0.013847
O	-2.092984	3.827853	6.225301	0.010343	0.021030	0.013516
O	2.197450	3.933608	4.519003	0.019132	-0.038554	0.009844

O	0.255692	9.867992	1.847787	-0.018936	0.037837	-0.010431
O	-1.898737	10.834409	5.031182	-0.018895	-0.037652	-0.010487
O	4.351879	2.967192	1.335608	0.019184	0.038686	0.009786
O	-0.212316	4.798696	5.055280	0.017380	-0.009651	-0.002870
O	2.665458	9.002905	1.311510	-0.017182	0.009021	0.002368
O	0.511030	11.699496	4.494905	-0.017110	-0.009069	0.002403
O	1.942113	2.102105	1.871885	0.017466	0.009595	-0.002835
O	0.525580	2.169271	5.472081	-0.004389	-0.007699	0.023293
O	1.927562	11.632329	0.894709	0.004503	0.007128	-0.023467
O	-0.226867	9.070071	4.078104	0.004388	-0.007131	-0.023506
O	2.680009	4.731529	2.288686	-0.004487	0.007680	0.023274
O	0.058846	0.698526	2.444964	0.030975	-0.015745	-0.010005
O	2.394296	13.103075	3.921826	-0.029989	0.015468	0.009486
O	4.548725	7.599326	0.738431	-0.030015	-0.015498	0.009376
O	-2.095583	6.202275	5.628359	0.030920	0.015736	-0.010108
O	-2.459230	13.184059	5.445139	0.015675	-0.024629	-0.045346
O	4.912372	0.617542	0.921651	-0.016053	0.025102	0.046326
O	2.757943	6.283259	4.105046	-0.016074	-0.025017	0.046199
O	-0.304801	7.518342	2.261744	0.015746	0.024750	-0.045544
O	-0.175430	2.374756	0.744070	0.010404	-0.002336	0.007598
O	2.628573	11.426844	5.622720	-0.010248	0.002197	-0.007928
O	4.783002	9.275557	2.439325	-0.010294	-0.002222	-0.008006
O	-2.329859	4.526044	3.927465	0.010336	0.002325	0.007545
O	-1.223866	12.517207	2.155216	-0.022433	0.009806	0.017589
O	3.677009	1.284394	4.211574	0.023300	-0.009863	-0.017746
O	5.831438	5.616407	1.028179	0.023551	0.009958	-0.017921
O	-3.378295	8.185194	5.338611	-0.022278	-0.009714	0.017430
H	-0.637445	12.195109	2.878812	-0.021694	-0.005895	0.009761
H	3.090587	1.606491	3.487978	0.023039	0.006108	-0.010158
H	5.245016	5.294309	0.304583	0.023314	-0.006092	-0.010312
H	-2.791874	8.507292	6.062207	-0.021541	0.005911	0.009640

173 f = 2.964905 THz 18.629045 2PiTHz 98.898567 cm-1 12.261864 meV

X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.002779	0.013749	0.004172
Li	-1.316675	4.156264	2.365404	0.001320	-0.015375	-0.000625
Li	-3.471104	2.744536	5.548798	-0.001329	-0.015340	0.000600
Li	5.924247	11.057064	0.817991	0.002852	0.013716	-0.004129
Na	2.049025	6.784862	1.629696	0.065752	0.012469	0.026644
Na	0.404117	7.016739	4.737094	-0.095629	-0.011613	-0.007223
Na	2.558546	13.685662	1.553699	0.095467	-0.011538	0.007254
Na	-0.105403	0.115939	4.813091	-0.065970	0.012541	-0.026695
B	4.155007	8.978944	1.168663	0.001176	0.022726	-0.000390
B	-1.701865	4.822656	5.198127	-0.003712	-0.023533	0.002513
B	0.452564	2.078144	2.014732	0.003730	-0.023536	-0.002588
B	2.000578	11.723457	4.352058	-0.001116	0.022723	0.000424
B	-2.733891	11.746082	5.839177	-0.001035	0.021008	0.001424
B	5.187034	2.055518	0.527613	0.003156	-0.019805	-0.002935
B	3.032605	4.845282	3.711007	-0.003164	-0.019792	0.002885
B	-0.579463	8.956318	2.655782	0.001069	0.021000	-0.001349
B	-0.983708	0.054306	1.827988	0.001065	-0.016537	-0.000727
B	3.436850	13.747295	4.538802	0.002512	0.015931	-0.003385
B	5.591279	6.955106	1.355407	-0.002476	0.015925	0.003453
B	-3.138137	6.846495	5.011383	-0.001031	-0.016523	0.000664
Si	0.631772	3.486686	4.508512	-0.001362	-0.020768	-0.001202
Si	1.821370	10.314915	1.858278	0.000391	0.021295	0.000353
Si	-0.333059	10.387486	5.041673	-0.000335	0.021345	-0.000304
Si	2.786201	3.414115	1.325117	0.001368	-0.020727	0.001138
O	0.061445	3.072947	3.041906	0.002137	-0.021241	-0.002538
O	2.391697	10.728653	3.324884	-0.001229	0.019784	0.001470
O	4.546126	9.973747	0.141489	0.001263	0.019829	-0.001414
O	-2.092984	3.827853	6.225301	-0.002160	-0.021185	0.002492
O	2.197450	3.933608	4.519003	-0.002622	-0.018773	0.002060
O	0.255692	9.867992	1.847787	0.001298	0.019102	-0.001608
O	-1.898737	10.834409	5.031182	-0.001241	0.019171	0.001642
O	4.351879	2.967192	1.335608	0.002620	-0.018750	-0.002142
O	-0.212316	4.798696	5.055280	-0.004348	-0.023525	0.000395
O	2.665458	9.002905	1.311510	0.001825	0.022276	-0.000304
O	0.511030	11.699496	4.494905	-0.001768	0.022320	0.000326
O	1.942113	2.102105	1.871885	0.004353	-0.023473	-0.000466

O	0.525580	2.169271	5.472081	0.000567	-0.020821	-0.001658
O	1.927562	11.632329	0.894709	-0.000019	0.021679	0.000985
O	-0.226867	9.070071	4.078104	0.000048	0.021711	-0.000917
O	2.680009	4.731529	2.288686	-0.000556	-0.020786	0.001602
O	0.058846	0.698526	2.444964	-0.000088	-0.018779	-0.001330
O	2.394296	13.103075	3.921826	0.002890	0.017731	-0.002360
O	4.548725	7.599326	0.738431	-0.002784	0.017759	0.002366
O	-2.095583	6.202275	5.628359	0.000172	-0.018743	0.001219
O	-2.459230	13.184059	5.445139	0.001656	0.018771	-0.000879
O	4.912372	0.617542	0.921651	0.002090	-0.018487	-0.002911
O	2.757943	6.283259	4.105046	-0.002102	-0.018489	0.002904
O	-0.304801	7.518342	2.261744	-0.001662	0.018727	0.001015
O	-0.175430	2.374756	0.744070	0.003193	-0.021476	-0.002574
O	2.628573	11.426844	5.622720	-0.000940	0.022289	0.000851
O	4.783002	9.275557	2.439325	0.000982	0.022298	-0.000804
O	-2.329859	4.526044	3.927465	-0.003202	-0.021468	0.002519
O	-1.223866	12.517207	2.155216	-0.013330	-0.010827	0.010749
O	3.677009	1.284394	4.211574	0.013952	0.010449	-0.016114
O	5.831438	5.616407	1.028179	-0.013910	0.010443	0.016180
O	-3.378295	8.185194	5.338611	0.013391	-0.010817	-0.010774
H	-0.637445	12.195109	2.878812	-0.007444	-0.012447	0.005624
H	3.090587	1.606491	3.487978	0.005338	0.009808	-0.010052
H	5.245016	5.294309	0.304583	-0.005244	0.009808	0.010080
H	-2.791874	8.507292	6.062207	0.007544	-0.012460	-0.005669

174 f = 2.861942 THz 17.982112 2PiTHz 95.464108 cm-1 11.836045 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.003109	-0.006560	0.008180
Li	-1.316675	4.156264	2.365404	-0.003872	-0.001663	0.009034
Li	-3.471104	2.744536	5.548798	0.003412	-0.001474	-0.008995
Li	5.924247	11.057064	0.817991	0.002662	-0.006359	-0.008117
Na	2.049025	6.784862	1.629696	-0.100119	-0.001364	0.044218
Na	0.404117	7.016739	4.737094	-0.070419	0.003086	0.050548
Na	2.558546	13.685662	1.553699	0.073895	0.002930	-0.051543

Na	-0.105403	0.115939	4.813091	0.103822	-0.001519	-0.045153
B	4.155007	8.978944	1.168663	-0.008175	-0.006336	0.005168
B	-1.701865	4.822656	5.198127	-0.007265	0.001458	0.004680
B	0.452564	2.078144	2.014732	0.006817	0.001446	-0.004390
B	2.000578	11.723457	4.352058	0.007742	-0.006378	-0.004880
B	-2.733891	11.746082	5.839177	0.006471	0.000245	-0.003588
B	5.187034	2.055518	0.527613	0.005700	0.007126	-0.002830
B	3.032605	4.845282	3.711007	-0.005813	0.007092	0.002718
B	-0.579463	8.956318	2.655782	-0.006592	0.000219	0.003492
B	-0.983708	0.054306	1.827988	0.009603	0.001625	-0.009142
B	3.436850	13.747295	4.538802	0.009576	-0.003794	-0.008647
B	5.591279	6.955106	1.355407	-0.010089	-0.003840	0.008697
B	-3.138137	6.846495	5.011383	-0.010130	0.001562	0.009187
Si	0.631772	3.486686	4.508512	-0.002399	0.005373	-0.001714
Si	1.821370	10.314915	1.858278	-0.002669	-0.001763	-0.001944
Si	-0.333059	10.387486	5.041673	0.002336	-0.002432	0.002103
Si	2.786201	3.414115	1.325117	0.002066	0.004679	0.001860
O	0.061445	3.072947	3.041906	0.002661	0.000149	-0.002139
O	2.391697	10.728653	3.324884	0.003385	-0.006666	-0.002859
O	4.546126	9.973747	0.141489	-0.003377	-0.007139	0.002946
O	-2.092984	3.827853	6.225301	-0.002653	-0.000367	0.002211
O	2.197450	3.933608	4.519003	-0.003422	0.005249	0.001271
O	0.255692	9.867992	1.847787	-0.004096	-0.001081	0.002046
O	-1.898737	10.834409	5.031182	0.003727	-0.001862	-0.001616
O	4.351879	2.967192	1.335608	0.003050	0.004444	-0.000843
O	-0.212316	4.798696	5.055280	-0.007004	0.000534	0.000158
O	2.665458	9.002905	1.311510	-0.008145	-0.007347	0.000318
O	0.511030	11.699496	4.494905	0.007752	-0.007987	-0.000029
O	1.942113	2.102105	1.871885	0.006598	-0.000108	0.000139
O	0.525580	2.169271	5.472081	0.002467	0.006475	-0.000884
O	1.927562	11.632329	0.894709	0.002611	-0.000832	-0.001389
O	-0.226867	9.070071	4.078104	-0.002763	-0.001428	0.001420
O	2.680009	4.731529	2.288686	-0.002603	0.005852	0.000900
O	0.058846	0.698526	2.444964	0.007142	0.000742	-0.007551
O	2.394296	13.103075	3.921826	0.006623	-0.005277	-0.007141
O	4.548725	7.599326	0.738431	-0.007751	-0.005573	0.007759

O	-2.095583	6.202275	5.628359	-0.008301	0.000414	0.008183
O	-2.459230	13.184059	5.445139	0.010902	-0.002191	-0.009444
O	4.912372	0.617542	0.921651	0.010739	0.004051	-0.009259
O	2.757943	6.283259	4.105046	-0.010509	0.004362	0.008299
O	-0.304801	7.518342	2.261744	-0.010690	-0.001888	0.008535
O	-0.175430	2.374756	0.744070	0.005840	0.005988	-0.003039
O	2.628573	11.426844	5.622720	0.006581	-0.001404	-0.003589
O	4.783002	9.275557	2.439325	-0.006797	-0.001492	0.003805
O	-2.329859	4.526044	3.927465	-0.006053	0.005880	0.003248
O	-1.223866	12.517207	2.155216	0.002236	0.001575	-0.014508
O	3.677009	1.284394	4.211574	-0.002135	-0.001982	-0.009934
O	5.831438	5.616407	1.028179	0.000843	-0.002177	0.010084
O	-3.378295	8.185194	5.338611	-0.003527	0.001363	0.014654
H	-0.637445	12.195109	2.878812	-0.007098	-0.004803	-0.010617
H	3.090587	1.606491	3.487978	-0.008841	-0.008608	-0.008097
H	5.245016	5.294309	0.304583	0.006915	-0.008467	0.008576
H	-2.791874	8.507292	6.062207	0.005150	-0.004702	0.011121

175 f = 2.849369 THz 17.903111 2PiTHz 95.044705 cm-1 11.784046 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.010919	-0.004747	0.001389
Li	-1.316675	4.156264	2.365404	-0.010123	-0.004397	0.000880
Li	-3.471104	2.744536	5.548798	-0.010263	0.004414	0.001279
Li	5.924247	11.057064	0.817991	-0.011067	0.005102	0.001747
Na	2.049025	6.784862	1.629696	0.089051	0.003893	-0.023061
Na	0.404117	7.016739	4.737094	0.081955	0.002763	-0.024437
Na	2.558546	13.685662	1.553699	0.079112	-0.002910	-0.022190
Na	-0.105403	0.115939	4.813091	0.084592	-0.003830	-0.021148
B	4.155007	8.978944	1.168663	-0.010346	0.000989	0.006783
B	-1.701865	4.822656	5.198127	-0.009796	0.000396	0.006802
B	0.452564	2.078144	2.014732	-0.010098	-0.000505	0.006994
B	2.000578	11.723457	4.352058	-0.010658	-0.000652	0.007022
B	-2.733891	11.746082	5.839177	-0.003099	0.000611	-0.002281
B	5.187034	2.055518	0.527613	-0.002354	0.000505	-0.002334

B	3.032605	4.845282	3.711007	-0.002107	-0.000869	-0.002443
B	-0.579463	8.956318	2.655782	-0.002838	-0.000556	-0.002472
B	-0.983708	0.054306	1.827988	-0.012330	0.001397	0.001656
B	3.436850	13.747295	4.538802	-0.012394	0.001204	0.001125
B	5.591279	6.955106	1.355407	-0.012052	-0.001002	0.000734
B	-3.138137	6.846495	5.011383	-0.011885	-0.001484	0.001215
Si	0.631772	3.486686	4.508512	-0.007188	0.015760	0.003659
Si	1.821370	10.314915	1.858278	-0.008023	0.016115	0.003795
Si	-0.333059	10.387486	5.041673	-0.008118	-0.015966	0.003694
Si	2.786201	3.414115	1.325117	-0.007292	-0.016028	0.003582
O	0.061445	3.072947	3.041906	0.000440	0.011628	0.002012
O	2.391697	10.728653	3.324884	-0.000076	0.011560	0.002141
O	4.546126	9.973747	0.141489	0.000067	-0.011212	0.002003
O	-2.092984	3.827853	6.225301	0.000533	-0.011635	0.001935
O	2.197450	3.933608	4.519003	-0.008079	0.018379	0.009925
O	0.255692	9.867992	1.847787	-0.008909	0.018907	0.010202
O	-1.898737	10.834409	5.031182	-0.009058	-0.018766	0.010290
O	4.351879	2.967192	1.335608	-0.008227	-0.018646	0.009959
O	-0.212316	4.798696	5.055280	-0.008835	0.014655	0.007137
O	2.665458	9.002905	1.311510	-0.009450	0.015373	0.006891
O	0.511030	11.699496	4.494905	-0.009764	-0.014983	0.006914
O	1.942113	2.102105	1.871885	-0.009129	-0.014722	0.007117
O	0.525580	2.169271	5.472081	-0.002689	0.014068	0.000568
O	1.927562	11.632329	0.894709	-0.003694	0.014349	0.000706
O	-0.226867	9.070071	4.078104	-0.003596	-0.014240	0.000615
O	2.680009	4.731529	2.288686	-0.002576	-0.014388	0.000539
O	0.058846	0.698526	2.444964	-0.026492	0.007307	0.014829
O	2.394296	13.103075	3.921826	-0.027182	0.007307	0.014904
O	4.548725	7.599326	0.738431	-0.026942	-0.007020	0.014557
O	-2.095583	6.202275	5.628359	-0.026127	-0.007342	0.014450
O	-2.459230	13.184059	5.445139	0.004872	-0.007295	-0.021812
O	4.912372	0.617542	0.921651	0.005316	-0.007195	-0.021665
O	2.757943	6.283259	4.105046	0.005770	0.006964	-0.022043
O	-0.304801	7.518342	2.261744	0.005305	0.007434	-0.022266
O	-0.175430	2.374756	0.744070	-0.004638	0.002163	0.005118
O	2.628573	11.426844	5.622720	-0.005449	0.002310	0.005258

O	4.783002	9.275557	2.439325	-0.005182	-0.002190	0.005074
O	-2.329859	4.526044	3.927465	-0.004379	-0.002476	0.004990
O	-1.223866	12.517207	2.155216	-0.030570	0.005052	0.004371
O	3.677009	1.284394	4.211574	-0.030334	0.004658	0.003487
O	5.831438	5.616407	1.028179	-0.030590	-0.004563	0.003091
O	-3.378295	8.185194	5.338611	-0.030369	-0.005108	0.003647
H	-0.637445	12.195109	2.878812	-0.045721	-0.002474	0.012490
H	3.090587	1.606491	3.487978	-0.045311	-0.002854	0.011466
H	5.245016	5.294309	0.304583	-0.045852	0.003247	0.011137
H	-2.791874	8.507292	6.062207	-0.045920	0.002680	0.011941

176 f = 2.092848 THz 13.149753 2PiTHz 69.809898 cm-1 8.655327
meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.014867	-0.004621	-0.011349
Li	-1.316675	4.156264	2.365404	0.014910	0.004579	0.011126
Li	-3.471104	2.744536	5.548798	0.014938	-0.004660	0.011117
Li	5.924247	11.057064	0.817991	-0.014855	0.004584	-0.011366
Na	2.049025	6.784862	1.629696	-0.007759	-0.010815	0.017287
Na	0.404117	7.016739	4.737094	0.007251	0.010927	-0.016821
Na	2.558546	13.685662	1.553699	0.007294	-0.010896	-0.016871
Na	-0.105403	0.115939	4.813091	-0.007831	0.010855	0.017201
B	4.155007	8.978944	1.168663	-0.015827	0.006324	-0.027873
B	-1.701865	4.822656	5.198127	0.015886	-0.006372	0.027628
B	0.452564	2.078144	2.014732	0.015872	0.006300	0.027610
B	2.000578	11.723457	4.352058	-0.015817	-0.006312	-0.027869
B	-2.733891	11.746082	5.839177	-0.026061	0.003338	-0.017094
B	5.187034	2.055518	0.527613	0.026105	-0.003368	0.016847
B	3.032605	4.845282	3.711007	0.026114	0.003284	0.016859
B	-0.579463	8.956318	2.655782	-0.026072	-0.003355	-0.017104
B	-0.983708	0.054306	1.827988	0.023044	-0.000376	0.014627
B	3.436850	13.747295	4.538802	-0.022977	0.000346	-0.014837
B	5.591279	6.955106	1.355407	-0.023066	-0.000388	-0.014804
B	-3.138137	6.846495	5.011383	0.023046	0.000294	0.014655
Si	0.631772	3.486686	4.508512	0.023656	0.011528	0.023271

Si	1.821370	10.314915	1.858278	-0.023590	-0.011594	-0.023528
Si	-0.333059	10.387486	5.041673	-0.023587	0.011602	-0.023541
Si	2.786201	3.414115	1.325117	0.023658	-0.011597	0.023281
O	0.061445	3.072947	3.041906	0.025421	0.019219	0.019994
O	2.391697	10.728653	3.324884	-0.025375	-0.019230	-0.020264
O	4.546126	9.973747	0.141489	-0.025366	0.019219	-0.020285
O	-2.092984	3.827853	6.225301	0.025435	-0.019288	0.020004
O	2.197450	3.933608	4.519003	0.021106	0.016967	0.025357
O	0.255692	9.867992	1.847787	-0.021014	-0.017122	-0.025646
O	-1.898737	10.834409	5.031182	-0.021024	0.017085	-0.025634
O	4.351879	2.967192	1.335608	0.021101	-0.017073	0.025377
O	-0.212316	4.798696	5.055280	0.019282	0.006581	0.032301
O	2.665458	9.002905	1.311510	-0.019204	-0.006636	-0.032539
O	0.511030	11.699496	4.494905	-0.019204	0.006657	-0.032539
O	1.942113	2.102105	1.871885	0.019264	-0.006640	0.032284
O	0.525580	2.169271	5.472081	0.027746	0.006280	0.016719
O	1.927562	11.632329	0.894709	-0.027729	-0.006335	-0.016967
O	-0.226867	9.070071	4.078104	-0.027731	0.006338	-0.016980
O	2.680009	4.731529	2.288686	0.027772	-0.006342	0.016722
O	0.058846	0.698526	2.444964	0.002375	0.014767	0.035137
O	2.394296	13.103075	3.921826	-0.002299	-0.014784	-0.035355
O	4.548725	7.599326	0.738431	-0.002348	0.014788	-0.035343
O	-2.095583	6.202275	5.628359	0.002393	-0.014835	0.035152
O	-2.459230	13.184059	5.445139	-0.030899	0.008663	-0.001331
O	4.912372	0.617542	0.921651	0.030917	-0.008686	0.001164
O	2.757943	6.283259	4.105046	0.030924	0.008597	0.001194
O	-0.304801	7.518342	2.261744	-0.030950	-0.008710	-0.001322
O	-0.175430	2.374756	0.744070	0.024206	0.002351	0.022850
O	2.628573	11.426844	5.622720	-0.024131	-0.002395	-0.023146
O	4.783002	9.275557	2.439325	-0.024137	0.002405	-0.023151
O	-2.329859	4.526044	3.927465	0.024213	-0.002441	0.022878
O	-1.223866	12.517207	2.155216	0.039777	-0.003453	0.006188
O	3.677009	1.284394	4.211574	-0.039590	0.003393	-0.006425
O	5.831438	5.616407	1.028179	-0.039816	-0.003460	-0.006369
O	-3.378295	8.185194	5.338611	0.039759	0.003370	0.006213
H	-0.637445	12.195109	2.878812	0.042941	0.001917	0.008461

H	3.090587	1.606491	3.487978	-0.042709	-0.001893	-0.008692
H	5.245016	5.294309	0.304583	-0.042963	0.001876	-0.008641
H	-2.791874	8.507292	6.062207	0.042910	-0.001978	0.008488

177 f = 1.446213 THz 9.086822 2PiTHz 48.240459 cm-1 5.981057 meV

	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.029481	-0.004617	0.023976
Li	-1.316675	4.156264	2.365404	0.029609	0.004611	-0.023850
Li	-3.471104	2.744536	5.548798	0.029604	-0.004614	-0.023867
Li	5.924247	11.057064	0.817991	-0.029481	0.004585	0.023977
Na	2.049025	6.784862	1.629696	-0.015429	-0.011959	-0.009973
Na	0.404117	7.016739	4.737094	0.015025	0.011972	0.010151
Na	2.558546	13.685662	1.553699	0.014986	-0.011915	0.010104
Na	-0.105403	0.115939	4.813091	-0.015413	0.012016	-0.010006
B	4.155007	8.978944	1.168663	-0.027479	-0.000329	0.025206
B	-1.701865	4.822656	5.198127	0.027601	0.000292	-0.025113
B	0.452564	2.078144	2.014732	0.027607	-0.000295	-0.025110
B	2.000578	11.723457	4.352058	-0.027485	0.000287	0.025204
B	-2.733891	11.746082	5.839177	-0.026530	-0.002550	0.024187
B	5.187034	2.055518	0.527613	0.026628	0.002532	-0.024057
B	3.032605	4.845282	3.711007	0.026619	-0.002521	-0.024074
B	-0.579463	8.956318	2.655782	-0.026535	0.002514	0.024191
B	-0.983708	0.054306	1.827988	0.011074	0.008928	-0.009192
B	3.436850	13.747295	4.538802	-0.010961	-0.008961	0.009284
B	5.591279	6.955106	1.355407	-0.010950	0.008915	0.009299
B	-3.138137	6.846495	5.011383	0.011072	-0.008942	-0.009188
Si	0.631772	3.486686	4.508512	0.028249	0.001413	-0.024605
Si	1.821370	10.314915	1.858278	-0.028137	-0.001477	0.024719
Si	-0.333059	10.387486	5.041673	-0.028135	0.001446	0.024720
Si	2.786201	3.414115	1.325117	0.028258	-0.001403	-0.024610
O	0.061445	3.072947	3.041906	0.029818	0.002866	-0.026145
O	2.391697	10.728653	3.324884	-0.029734	-0.002939	0.026274
O	4.546126	9.973747	0.141489	-0.029715	0.002878	0.026262
O	-2.092984	3.827853	6.225301	0.029843	-0.002900	-0.026169

O	2.197450	3.933608	4.519003	0.030228	-0.006093	-0.024226
O	0.255692	9.867992	1.847787	-0.030112	0.006011	0.024309
O	-1.898737	10.834409	5.031182	-0.030113	-0.006057	0.024315
O	4.351879	2.967192	1.335608	0.030236	0.006094	-0.024202
O	-0.212316	4.798696	5.055280	0.028298	0.002942	-0.025690
O	2.665458	9.002905	1.311510	-0.028177	-0.002991	0.025765
O	0.511030	11.699496	4.494905	-0.028183	0.002965	0.025775
O	1.942113	2.102105	1.871885	0.028301	-0.002920	-0.025670
O	0.525580	2.169271	5.472081	0.024793	0.002060	-0.023780
O	1.927562	11.632329	0.894709	-0.024708	-0.002112	0.023910
O	-0.226867	9.070071	4.078104	-0.024714	0.002086	0.023907
O	2.680009	4.731529	2.288686	0.024788	-0.002041	-0.023801
O	0.058846	0.698526	2.444964	0.021832	0.002054	-0.020538
O	2.394296	13.103075	3.921826	-0.021648	-0.002111	0.020572
O	4.548725	7.599326	0.738431	-0.021646	0.002059	0.020590
O	-2.095583	6.202275	5.628359	0.021807	-0.002077	-0.020513
O	-2.459230	13.184059	5.445139	-0.019973	-0.005832	0.019246
O	4.912372	0.617542	0.921651	0.020038	0.005837	-0.019071
O	2.757943	6.283259	4.105046	0.020039	-0.005829	-0.019085
O	-0.304801	7.518342	2.261744	-0.019979	0.005790	0.019275
O	-0.175430	2.374756	0.744070	0.027870	-0.000973	-0.025361
O	2.628573	11.426844	5.622720	-0.027755	0.000957	0.025459
O	4.783002	9.275557	2.439325	-0.027759	-0.000987	0.025460
O	-2.329859	4.526044	3.927465	0.027855	0.000984	-0.025365
O	-1.223866	12.517207	2.155216	-0.016577	0.018787	0.015765
O	3.677009	1.284394	4.211574	0.016746	-0.018825	-0.015653
O	5.831438	5.616407	1.028179	0.016793	0.018792	-0.015661
O	-3.378295	8.185194	5.338611	-0.016565	-0.018797	0.015764
H	-0.637445	12.195109	2.878812	-0.019958	0.013493	0.016008
H	3.090587	1.606491	3.487978	0.020197	-0.013504	-0.015938
H	5.245016	5.294309	0.304583	0.020243	0.013468	-0.015944
H	-2.791874	8.507292	6.062207	-0.019938	-0.013505	0.016003

178 f/i= 0.017959 THz 0.112841 2PiTHz 0.599052 cm-1 0.074273 meV
 X Y Z dx dy dz

Li	3.769818	9.645336	4.001386	-0.000351	0.000561	-0.033675
Li	-1.316675	4.156264	2.365404	-0.000351	0.000496	-0.033813
Li	-3.471104	2.744536	5.548798	-0.000358	0.000572	-0.033812
Li	5.924247	11.057064	0.817991	-0.000356	0.000502	-0.033679
Na	2.049025	6.784862	1.629696	-0.000267	0.000498	-0.033637
Na	0.404117	7.016739	4.737094	-0.000264	0.000466	-0.033682
Na	2.558546	13.685662	1.553699	-0.000270	0.000605	-0.033685
Na	-0.105403	0.115939	4.813091	-0.000269	0.000568	-0.033632
B	4.155007	8.978944	1.168663	-0.000350	0.000443	-0.033630
B	-1.701865	4.822656	5.198127	-0.000350	0.000481	-0.033891
B	0.452564	2.078144	2.014732	-0.000346	0.000583	-0.033881
B	2.000578	11.723457	4.352058	-0.000347	0.000616	-0.033628
B	-2.733891	11.746082	5.839177	-0.000306	0.000602	-0.033650
B	5.187034	2.055518	0.527613	-0.000351	0.000607	-0.033857
B	3.032605	4.845282	3.711007	-0.000356	0.000464	-0.033865
B	-0.579463	8.956318	2.655782	-0.000302	0.000468	-0.033656
B	-0.983708	0.054306	1.827988	-0.000374	0.000626	-0.033853
B	3.436850	13.747295	4.538802	-0.000322	0.000625	-0.033647
B	5.591279	6.955106	1.355407	-0.000311	0.000439	-0.033656
B	-3.138137	6.846495	5.011383	-0.000380	0.000437	-0.033852
Si	0.631772	3.486686	4.508512	-0.000362	0.000525	-0.033859
Si	1.821370	10.314915	1.858278	-0.000330	0.000555	-0.033638
Si	-0.333059	10.387486	5.041673	-0.000334	0.000512	-0.033640
Si	2.786201	3.414115	1.325117	-0.000362	0.000544	-0.033863
O	0.061445	3.072947	3.041906	-0.000369	0.000539	-0.033849
O	2.391697	10.728653	3.324884	-0.000362	0.000614	-0.033635
O	4.546126	9.973747	0.141489	-0.000365	0.000443	-0.033639
O	-2.092984	3.827853	6.225301	-0.000363	0.000519	-0.033860
O	2.197450	3.933608	4.519003	-0.000357	0.000491	-0.033832
O	0.255692	9.867992	1.847787	-0.000331	0.000521	-0.033630
O	-1.898737	10.834409	5.031182	-0.000330	0.000561	-0.033633
O	4.351879	2.967192	1.335608	-0.000357	0.000583	-0.033831
O	-0.212316	4.798696	5.055280	-0.000360	0.000519	-0.033876
O	2.665458	9.002905	1.311510	-0.000336	0.000518	-0.033570
O	0.511030	11.699496	4.494905	-0.000334	0.000547	-0.033570
O	1.942113	2.102105	1.871885	-0.000356	0.000551	-0.033866

O	0.525580	2.169271	5.472081	-0.000375	0.000552	-0.033846
O	1.927562	11.632329	0.894709	-0.000300	0.000557	-0.033658
O	-0.226867	9.070071	4.078104	-0.000305	0.000510	-0.033661
O	2.680009	4.731529	2.288686	-0.000387	0.000518	-0.033853
O	0.058846	0.698526	2.444964	-0.000328	0.000585	-0.033911
O	2.394296	13.103075	3.921826	-0.000357	0.000642	-0.033616
O	4.548725	7.599326	0.738431	-0.000362	0.000411	-0.033612
O	-2.095583	6.202275	5.628359	-0.000335	0.000474	-0.033913
O	-2.459230	13.184059	5.445139	-0.000292	0.000622	-0.033664
O	4.912372	0.617542	0.921651	-0.000345	0.000619	-0.033879
O	2.757943	6.283259	4.105046	-0.000347	0.000453	-0.033889
O	-0.304801	7.518342	2.261744	-0.000273	0.000453	-0.033686
O	-0.175430	2.374756	0.744070	-0.000350	0.000644	-0.033873
O	2.628573	11.426844	5.622720	-0.000307	0.000650	-0.033649
O	4.783002	9.275557	2.439325	-0.000307	0.000408	-0.033651
O	-2.329859	4.526044	3.927465	-0.000356	0.000426	-0.033884
O	-1.223866	12.517207	2.155216	-0.000478	0.000662	-0.033785
O	3.677009	1.284394	4.211574	-0.000304	0.000624	-0.033694
O	5.831438	5.616407	1.028179	-0.000285	0.000441	-0.033704
O	-3.378295	8.185194	5.338611	-0.000487	0.000397	-0.033774
H	-0.637445	12.195109	2.878812	-0.000535	0.000660	-0.033745
H	3.090587	1.606491	3.487978	-0.000309	0.000612	-0.033688
H	5.245016	5.294309	0.304583	-0.000300	0.000449	-0.033688
H	-2.791874	8.507292	6.062207	-0.000547	0.000398	-0.033732

179 f/i=	0.032483 THz	0.204100 2PiTHz	1.083531 cm-1	0.134341 meV		
	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	0.000063	-0.033808	-0.000678
Li	-1.316675	4.156264	2.365404	0.000026	-0.033809	-0.000699
Li	-3.471104	2.744536	5.548798	0.000226	-0.033804	-0.000391
Li	5.924247	11.057064	0.817991	0.000249	-0.033815	-0.000372
Na	2.049025	6.784862	1.629696	0.000243	-0.033637	-0.000709
Na	0.404117	7.016739	4.737094	0.000199	-0.033763	-0.000725
Na	2.558546	13.685662	1.553699	0.000051	-0.033631	-0.000369
Na	-0.105403	0.115939	4.813091	0.000088	-0.033764	-0.000347

B	4.155007	8.978944	1.168663	0.000230	-0.033617	-0.000539
B	-1.701865	4.822656	5.198127	0.000208	-0.033617	-0.000565
B	0.452564	2.078144	2.014732	0.000051	-0.033605	-0.000529
B	2.000578	11.723457	4.352058	0.000079	-0.033620	-0.000497
B	-2.733891	11.746082	5.839177	0.000100	-0.033874	-0.000504
B	5.187034	2.055518	0.527613	0.000071	-0.033880	-0.000536
B	3.032605	4.845282	3.711007	0.000189	-0.033873	-0.000562
B	-0.579463	8.956318	2.655782	0.000218	-0.033878	-0.000541
B	-0.983708	0.054306	1.827988	0.000320	-0.033780	-0.000494
B	3.436850	13.747295	4.538802	0.000324	-0.033784	-0.000483
B	5.591279	6.955106	1.355407	-0.000028	-0.033785	-0.000578
B	-3.138137	6.846495	5.011383	-0.000038	-0.033782	-0.000586
Si	0.631772	3.486686	4.508512	0.000134	-0.033745	-0.000541
Si	1.821370	10.314915	1.858278	0.000166	-0.033712	-0.000509
Si	-0.333059	10.387486	5.041673	0.000150	-0.033751	-0.000529
Si	2.786201	3.414115	1.325117	0.000123	-0.033712	-0.000556
O	0.061445	3.072947	3.041906	0.000055	-0.033556	-0.000559
O	2.391697	10.728653	3.324884	0.000104	-0.033556	-0.000525
O	4.546126	9.973747	0.141489	0.000226	-0.033579	-0.000517
O	-2.092984	3.827853	6.225301	0.000179	-0.033547	-0.000534
O	2.197450	3.933608	4.519003	0.000257	-0.034127	-0.000742
O	0.255692	9.867992	1.847787	0.000291	-0.034104	-0.000692
O	-1.898737	10.834409	5.031182	0.000029	-0.034129	-0.000327
O	4.351879	2.967192	1.335608	-0.000003	-0.034112	-0.000379
O	-0.212316	4.798696	5.055280	0.000266	-0.033639	-0.000457
O	2.665458	9.002905	1.311510	0.000292	-0.033599	-0.000440
O	0.511030	11.699496	4.494905	0.000023	-0.033639	-0.000594
O	1.942113	2.102105	1.871885	-0.000008	-0.033594	-0.000623
O	0.525580	2.169271	5.472081	-0.000025	-0.033695	-0.000500
O	1.927562	11.632329	0.894709	0.000005	-0.033655	-0.000463
O	-0.226867	9.070071	4.078104	0.000311	-0.033694	-0.000578
O	2.680009	4.731529	2.288686	0.000297	-0.033653	-0.000605
O	0.058846	0.698526	2.444964	0.000149	-0.033552	-0.000445
O	2.394296	13.103075	3.921826	0.000142	-0.033556	-0.000416
O	4.548725	7.599326	0.738431	0.000128	-0.033569	-0.000613
O	-2.095583	6.202275	5.628359	0.000147	-0.033551	-0.000657

O	-2.459230	13.184059	5.445139	0.000324	-0.033999	-0.000644
O	4.912372	0.617542	0.921651	0.000304	-0.033998	-0.000644
O	2.757943	6.283259	4.105046	-0.000036	-0.033998	-0.000427
O	-0.304801	7.518342	2.261744	-0.000007	-0.033992	-0.000442
O	-0.175430	2.374756	0.744070	0.000011	-0.033672	-0.000533
O	2.628573	11.426844	5.622720	0.000042	-0.033670	-0.000499
O	4.783002	9.275557	2.439325	0.000277	-0.033672	-0.000540
O	-2.329859	4.526044	3.927465	0.000247	-0.033673	-0.000562
O	-1.223866	12.517207	2.155216	0.000589	-0.033762	-0.000341
O	3.677009	1.284394	4.211574	0.000585	-0.033764	-0.000333
O	5.831438	5.616407	1.028179	-0.000287	-0.033765	-0.000731
O	-3.378295	8.185194	5.338611	-0.000298	-0.033764	-0.000730
H	-0.637445	12.195109	2.878812	0.000679	-0.033631	-0.000335
H	3.090587	1.606491	3.487978	0.000669	-0.033625	-0.000314
H	5.245016	5.294309	0.304583	-0.000379	-0.033633	-0.000738
H	-2.791874	8.507292	6.062207	-0.000384	-0.033626	-0.000747

180 f/i=	0.073215 THz	0.460024 2PiTHz	2.442191 cm-1	0.302793 meV		
	X	Y	Z	dx	dy	dz
Li	3.769818	9.645336	4.001386	-0.033734	-0.000177	0.000288
Li	-1.316675	4.156264	2.365404	-0.033717	-0.000199	0.000257
Li	-3.471104	2.744536	5.548798	-0.033713	-0.000113	0.000269
Li	5.924247	11.057064	0.817991	-0.033742	-0.000113	0.000294
Na	2.049025	6.784862	1.629696	-0.033110	-0.000034	0.000356
Na	0.404117	7.016739	4.737094	-0.032733	0.000016	0.000398
Na	2.558546	13.685662	1.553699	-0.032717	-0.000316	0.000409
Na	-0.105403	0.115939	4.813091	-0.033115	-0.000266	0.000362
B	4.155007	8.978944	1.168663	-0.033796	0.000025	0.000532
B	-1.701865	4.822656	5.198127	-0.033759	0.000030	0.000485
B	0.452564	2.078144	2.014732	-0.033766	-0.000334	0.000488
B	2.000578	11.723457	4.352058	-0.033789	-0.000316	0.000540
B	-2.733891	11.746082	5.839177	-0.033656	-0.000114	0.000342
B	5.187034	2.055518	0.527613	-0.033636	-0.000125	0.000286
B	3.032605	4.845282	3.711007	-0.033629	-0.000187	0.000288
B	-0.579463	8.956318	2.655782	-0.033661	-0.000177	0.000335

B	-0.983708	0.054306	1.827988	-0.034020	-0.000166	0.000127
B	3.436850	13.747295	4.538802	-0.034029	-0.000173	0.000164
B	5.591279	6.955106	1.355407	-0.034053	-0.000125	0.000162
B	-3.138137	6.846495	5.011383	-0.034010	-0.000136	0.000117
Si	0.631772	3.486686	4.508512	-0.033695	0.000035	0.000414
Si	1.821370	10.314915	1.858278	-0.033721	0.000039	0.000459
Si	-0.333059	10.387486	5.041673	-0.033722	-0.000329	0.000454
Si	2.786201	3.414115	1.325117	-0.033702	-0.000342	0.000414
O	0.061445	3.072947	3.041906	-0.033692	-0.000233	0.000473
O	2.391697	10.728653	3.324884	-0.033727	-0.000232	0.000526
O	4.546126	9.973747	0.141489	-0.033732	-0.000060	0.000521
O	-2.092984	3.827853	6.225301	-0.033693	-0.000066	0.000472
O	2.197450	3.933608	4.519003	-0.033710	0.000021	0.000362
O	0.255692	9.867992	1.847787	-0.033744	0.000037	0.000405
O	-1.898737	10.834409	5.031182	-0.033744	-0.000318	0.000399
O	4.351879	2.967192	1.335608	-0.033723	-0.000341	0.000364
O	-0.212316	4.798696	5.055280	-0.033697	0.000046	0.000624
O	2.665458	9.002905	1.311510	-0.033734	0.000033	0.000674
O	0.511030	11.699496	4.494905	-0.033728	-0.000323	0.000681
O	1.942113	2.102105	1.871885	-0.033706	-0.000355	0.000613
O	0.525580	2.169271	5.472081	-0.033526	0.000010	0.000330
O	1.927562	11.632329	0.894709	-0.033532	0.000023	0.000381
O	-0.226867	9.070071	4.078104	-0.033543	-0.000313	0.000376
O	2.680009	4.731529	2.288686	-0.033522	-0.000316	0.000332
O	0.058846	0.698526	2.444964	-0.034013	-0.000406	0.000362
O	2.394296	13.103075	3.921826	-0.034005	-0.000413	0.000389
O	4.548725	7.599326	0.738431	-0.034021	0.000124	0.000384
O	-2.095583	6.202275	5.628359	-0.033998	0.000110	0.000349
O	-2.459230	13.184059	5.445139	-0.033752	-0.000118	0.000008
O	4.912372	0.617542	0.921651	-0.033731	-0.000130	-0.000055
O	2.757943	6.283259	4.105046	-0.033733	-0.000185	-0.000044
O	-0.304801	7.518342	2.261744	-0.033763	-0.000179	-0.000003
O	-0.175430	2.374756	0.744070	-0.033618	-0.000250	0.000477
O	2.628573	11.426844	5.622720	-0.033632	-0.000240	0.000527
O	4.783002	9.275557	2.439325	-0.033635	-0.000050	0.000517
O	-2.329859	4.526044	3.927465	-0.033607	-0.000052	0.000471

O	-1.223866	12.517207	2.155216	-0.034863	-0.000097	-0.000197
O	3.677009	1.284394	4.211574	-0.034809	-0.000122	-0.000208
O	5.831438	5.616407	1.028179	-0.034867	-0.000182	-0.000207
O	-3.378295	8.185194	5.338611	-0.034842	-0.000198	-0.000220
H	-0.637445	12.195109	2.878812	-0.035461	-0.000443	0.000110
H	3.090587	1.606491	3.487978	-0.035416	-0.000452	0.000113
H	5.245016	5.294309	0.304583	-0.035483	0.000160	0.000114
H	-2.791874	8.507292	6.062207	-0.035438	0.000146	0.000086