

Supplementary information

1- X-ray diffraction and x-ray fluorescence analysis of the brucite sample

The polycrystalline sample loaded in 0.3mm diameter borosilicate capillaries was analyzed by X-ray diffraction et X-ray fluorescence at the X-ray diffraction platform of the *Institut de Minéralogie, de Physique des Matériaux et Cosmochimie* (IMPMC), Sorbonne Université (Paris, France).

For both XRD and XRF, we used a Rigaku MM007HF diffractometer equipped with Varimax focusing optics, a RAXIS4++ image plate detector and a Mo rotating anode ($\lambda K\alpha 1 = 0.709319 \text{ \AA}$ and $\lambda K\alpha 2 = 0.713609 \text{ \AA}$) at 50 KeV and 24 mA. A home-made collimator allowed us to get a very low divergent x-ray beam ($<0.1\text{mrad}$) with a size at sample of $80\mu\text{m}$ FWHM ($200\mu\text{m}$ at the total).

The XRD data were collected for 15 minutes in transmission geometry. The Fit2D program (Hammersley, 2016) was used for the integration of 2D images into 1D patterns (from 3 to $45^\circ 2\theta$) after a calibration with a LaB6 standard. A Rietveld refinement of the XRD pattern was the performed with the FullProf software (Rodriguez-Carvajal, 1993), starting with the brucite and calcite crystal structures from Von Dreele (1994, amcsd code 0001637) and Graf (1961, amcsd code 0000098), respectively. Scale factors, cell parameters, isotropic pseudo-Voigt line-profile functions (Thompson-Cox-Hastings) and overall B factors were first refined for the two phases. The peak widths were significantly larger than the instrument resolution ($\sim 0.1^\circ 2\theta$). The instrumental resolution function (IRF) was determined over the 2θ range measured from the LaB6 crystallographic standard Rietveld refinement. Assuming that the lorentzian part of the peak broadening is preferentially due to size effect and the Gaussian part to the microstrain, lorentzian isotropic size (Y) and gaussian isotropic

strain (U) parameters were refined taking into account the IRF. The refined pattern is presented in Fig. 1 and the corresponding refined crystallographic data are summarized in the Table 1.

The XRF measurement were performed with the same diffractometer and same set-up. A Si-drift KETEK™ detector (Ketek Vitus H80) was installed at 90° relatively to the Mo x-ray source. After a calibration for the energy, 30min measurements allowed to determine the presence of Fe and Mn, notably (Fig. 2).

Table S1: Results of the Rietveld refinement from X-ray diffraction analysis of brucite sample

Brucite				
<i>P</i> -3 <i>m</i> 1	<i>a</i> = <i>b</i> = 3.1473 (1) Å	<i>c</i> = 4.7694 (3) Å	Vol = 40.914 Å ³	
Atom	<i>x</i>	<i>y</i>	<i>z</i>	occupation
Mg	0	0	0	1/12
O	1/3	2/3	0.22030	1/6
Rietveld refinement		R _{Bragg} = 4.06 %	Fract. (%) = 97	

Calcite				
<i>R</i> -3 <i>c</i>	<i>a</i> = <i>b</i> = 4.9852 (32) Å	<i>c</i> = 17.0217(8) Å	Vol = 366.358 Å ³	
Atom	<i>x</i>	<i>y</i>	<i>z</i>	occupation
Ca	0	0	0	1/6
C	0	0	0.25	1/6
O	0.2578	0	0.25	1/2
Rietveld refinement		R _{Bragg} = 14.5 %	Fract. (%) = 3	

Fig. S1: Rietveld refinement of XRD pattern of the investigated brucite sample revealing the presence of 3% of calcite.

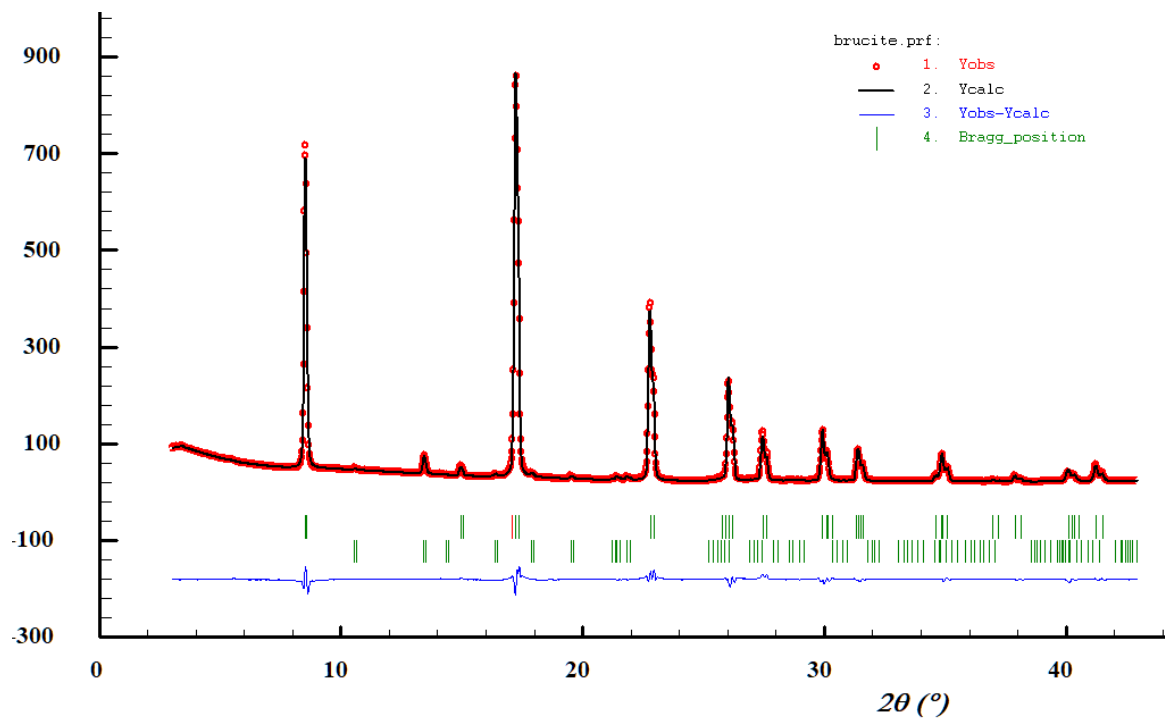
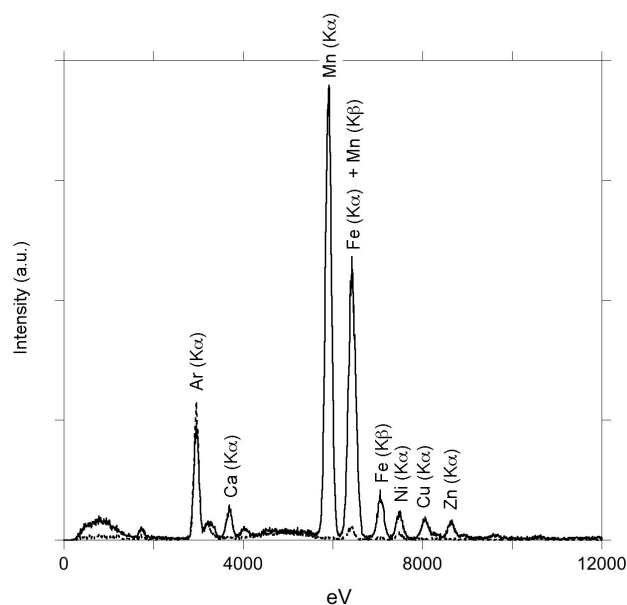


Fig. S2: Enlarged view of the-ray fluorescence spectrum of the investigated brucite sample. The dotted line is the spectrum of the empty capillary.



2- Theoretical vibrational properties of talc, brucite and lizardite

- Tables S2, S3 and S4 report the theoretical normalized eigendisplacements of the vibrational modes calculated at the Brillouin zone center ($q = 0.0, 0.0, 0.0$) of talc, brucite and lizardite, respectively.

- Atoms are ordered as in the corresponding structure files (.cif).

- Vibrational modes are numbered from 1 to $3n$, n being the number of atoms in the cell.

- Displacement coordinates are reported in cartesian reference frames (X,Y,Z) defined such as the crystal cell axes have the coordinates specified in the heading of the Table.

Table S2 : vibrational modes of talc

alat= 9.990000 a.u.

crystal axes: (cart. coord. in units of alat)

a(1)= (1.013600 0.000109 0.001716)

a(2)= (0.505317 0.878304 0.032081)

a(3)= (-0.281340 -0.076695 1.788127)

freq (1) = -0.008186 [THz] = -0.273060 [cm-1]

(-0.000195	0.000000	0.027650	0.000000	-0.216453	0.000000)
(-0.000195	0.000000	0.027650	0.000000	-0.216453	0.000000)
(-0.000205	0.000000	0.027673	0.000000	-0.216453	0.000000)
(-0.000205	0.000000	0.027673	0.000000	-0.216453	0.000000)
(-0.000609	0.000000	0.027451	0.000000	-0.216519	0.000000)
(-0.000581	0.000000	0.027538	0.000000	-0.216443	0.000000)
(-0.000581	0.000000	0.027538	0.000000	-0.216443	0.000000)
(-0.000535	0.000000	0.027614	0.000000	-0.216464	0.000000)
(-0.000535	0.000000	0.027614	0.000000	-0.216464	0.000000)
(-0.000582	0.000000	0.027493	0.000000	-0.216485	0.000000)
(-0.000582	0.000000	0.027493	0.000000	-0.216485	0.000000)
(-0.000445	0.000000	0.027522	0.000000	-0.216453	0.000000)
(-0.000445	0.000000	0.027522	0.000000	-0.216453	0.000000)
(-0.000186	0.000000	0.027644	0.000000	-0.216422	0.000000)
(-0.000186	0.000000	0.027644	0.000000	-0.216422	0.000000)
(-0.000164	0.000000	0.027591	0.000000	-0.216481	0.000000)
(-0.000164	0.000000	0.027591	0.000000	-0.216481	0.000000)
(0.000038	0.000000	0.027645	0.000000	-0.216457	0.000000)
(0.000038	0.000000	0.027645	0.000000	-0.216457	0.000000)
(-0.001230	0.000000	0.028087	0.000000	-0.216460	0.000000)
(-0.001230	0.000000	0.028087	0.000000	-0.216460	0.000000)

freq (2) = -0.004804 [THz] = -0.160258 [cm-1]

(-0.110231	0.000000	-0.186843	0.000000	-0.023649	0.000000)
(-0.110231	0.000000	-0.186843	0.000000	-0.023649	0.000000)
(-0.110232	0.000000	-0.186838	0.000000	-0.023673	0.000000)
(-0.110232	0.000000	-0.186838	0.000000	-0.023673	0.000000)
(-0.110188	0.000000	-0.186869	0.000000	-0.023477	0.000000)
(-0.110286	0.000000	-0.186826	0.000000	-0.023633	0.000000)
(-0.110286	0.000000	-0.186826	0.000000	-0.023633	0.000000)
(-0.110248	0.000000	-0.186829	0.000000	-0.023657	0.000000)
(-0.110248	0.000000	-0.186829	0.000000	-0.023657	0.000000)
(-0.110227	0.000000	-0.186835	0.000000	-0.023577	0.000000)
(-0.110227	0.000000	-0.186835	0.000000	-0.023577	0.000000)
(-0.110253	0.000000	-0.186837	0.000000	-0.023627	0.000000)
(-0.110253	0.000000	-0.186837	0.000000	-0.023627	0.000000)
(-0.109943	0.000000	-0.186359	0.000000	-0.023707	0.000000)
(-0.109943	0.000000	-0.186359	0.000000	-0.023707	0.000000)
(-0.109916	0.000000	-0.187386	0.000000	-0.023714	0.000000)
(-0.109916	0.000000	-0.187386	0.000000	-0.023714	0.000000)
(-0.110842	0.000000	-0.186833	0.000000	-0.023718	0.000000)

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( -0.110842  0.000000  -0.186833  0.000000  -0.023718  0.000000  )
( -0.110199  0.000000  -0.186768  0.000000  -0.023579  0.000000  )
( -0.110199  0.000000  -0.186768  0.000000  -0.023579  0.000000  )
  freq ( 3) =   -0.003428 [THz] =   -0.114347 [cm-1]
(  0.188346  0.000000  -0.109313  0.000000  -0.014200  0.000000  )
(  0.188346  0.000000  -0.109313  0.000000  -0.014200  0.000000  )
(  0.188321  0.000000  -0.109337  0.000000  -0.014207  0.000000  )
(  0.188321  0.000000  -0.109337  0.000000  -0.014207  0.000000  )
(  0.188354  0.000000  -0.109272  0.000000  -0.014234  0.000000  )
(  0.188310  0.000000  -0.109343  0.000000  -0.014323  0.000000  )
(  0.188310  0.000000  -0.109343  0.000000  -0.014323  0.000000  )
(  0.188298  0.000000  -0.109353  0.000000  -0.014242  0.000000  )
(  0.188298  0.000000  -0.109353  0.000000  -0.014242  0.000000  )
(  0.188357  0.000000  -0.109255  0.000000  -0.014364  0.000000  )
(  0.188357  0.000000  -0.109255  0.000000  -0.014364  0.000000  )
(  0.188350  0.000000  -0.109322  0.000000  -0.014205  0.000000  )
(  0.188350  0.000000  -0.109322  0.000000  -0.014205  0.000000  )
(  0.188393  0.000000  -0.109225  0.000000  -0.014146  0.000000  )
(  0.188393  0.000000  -0.109225  0.000000  -0.014146  0.000000  )
(  0.188367  0.000000  -0.109370  0.000000  -0.014211  0.000000  )
(  0.188367  0.000000  -0.109370  0.000000  -0.014211  0.000000  )
(  0.188213  0.000000  -0.109332  0.000000  -0.014145  0.000000  )
(  0.188213  0.000000  -0.109332  0.000000  -0.014145  0.000000  )
(  0.188380  0.000000  -0.109151  0.000000  -0.014389  0.000000  )
(  0.188380  0.000000  -0.109151  0.000000  -0.014389  0.000000  )
  freq ( 4) =    2.899728 [THz] =    96.724525 [cm-1]
( -0.000059  0.000000   0.000213  0.000000  -0.008217  0.000000  )
( -0.000059  0.000000   0.000213  0.000000  -0.008217  0.000000  )
(  0.000726  0.000000   0.000438  0.000000  -0.009145  0.000000  )
(  0.000726  0.000000   0.000438  0.000000  -0.009145  0.000000  )
( -0.000909  0.000000  -0.001549  0.000000  -0.014160  0.000000  )
(  0.000803  0.000000   0.000654  0.000000  -0.011417  0.000000  )
(  0.000803  0.000000   0.000654  0.000000  -0.011417  0.000000  )
(  0.001573  0.000000   0.000169  0.000000  -0.007680  0.000000  )
(  0.001573  0.000000   0.000169  0.000000  -0.007680  0.000000  )
( -0.001457  0.000000  -0.003694  0.000000   0.006849  0.000000  )
( -0.001457  0.000000  -0.003694  0.000000   0.006849  0.000000  )
(  0.000741  0.000000   0.002770  0.000000  -0.006822  0.000000  )
(  0.000741  0.000000   0.002770  0.000000  -0.006822  0.000000  )
( -0.204125  0.000000  -0.355193  0.000000   0.010496  0.000000  )
( -0.204125  0.000000  -0.355193  0.000000   0.010496  0.000000  )
( -0.204450  0.000000   0.352244  0.000000   0.031186  0.000000  )
( -0.204450  0.000000   0.352244  0.000000   0.031186  0.000000  )
(  0.404967  0.000000  -0.000175  0.000000   0.024043  0.000000  )
(  0.404967  0.000000  -0.000175  0.000000   0.024043  0.000000  )
( -0.003177  0.000000  -0.004552  0.000000   0.006465  0.000000  )
( -0.003177  0.000000  -0.004552  0.000000   0.006465  0.000000  )
  freq ( 5) =    3.031868 [THz] =   101.132246 [cm-1]
(  0.150355  0.000000   0.035593  0.000000   0.016234  0.000000  )
( -0.150355  0.000000  -0.035593  0.000000  -0.016234  0.000000  )

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( 0.155349 0.000000 0.036472 0.000000 0.015414 0.000000 )
( -0.155349 0.000000 -0.036472 0.000000 -0.015414 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.002364 0.000000 0.001421 0.000000 -0.019942 0.000000 )
( -0.002364 0.000000 -0.001421 0.000000 0.019942 0.000000 )
( 0.074892 0.000000 0.014346 0.000000 0.015133 0.000000 )
( -0.074892 0.000000 -0.014346 0.000000 -0.015133 0.000000 )
( 0.018174 0.000000 0.007354 0.000000 -0.017930 0.000000 )
( -0.018174 0.000000 -0.007354 0.000000 0.017930 0.000000 )
( 0.060509 0.000000 0.014424 0.000000 0.013843 0.000000 )
( -0.060509 0.000000 -0.014424 0.000000 -0.013843 0.000000 )
( 0.336450 0.000000 0.354742 0.000000 -0.001250 0.000000 )
( -0.336450 0.000000 -0.354742 0.000000 0.001250 0.000000 )
( 0.325769 0.000000 -0.261057 0.000000 -0.007653 0.000000 )
( -0.325769 0.000000 0.261057 0.000000 0.007653 0.000000 )
( -0.154215 0.000000 0.036535 0.000000 0.000834 0.000000 )
( 0.154215 0.000000 -0.036535 0.000000 -0.000834 0.000000 )
( 0.008494 0.000000 0.007924 0.000000 -0.017775 0.000000 )
( -0.008494 0.000000 -0.007924 0.000000 0.017775 0.000000 )
  freq ( 6 ) = 3.244403 [THz] = 108.221645 [cm-1]
( -0.186484 0.000000 -0.122066 0.000000 0.000020 0.000000 )
( 0.186484 0.000000 0.122066 0.000000 -0.000020 0.000000 )
( -0.190007 0.000000 -0.123638 0.000000 0.000748 0.000000 )
( 0.190007 0.000000 0.123638 0.000000 -0.000748 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( -0.000888 0.000000 -0.002088 0.000000 0.018823 0.000000 )
( 0.000888 0.000000 0.002088 0.000000 -0.018823 0.000000 )
( -0.086136 0.000000 -0.055447 0.000000 0.001706 0.000000 )
( 0.086136 0.000000 0.055447 0.000000 -0.001706 0.000000 )
( -0.028761 0.000000 -0.027689 0.000000 -0.002216 0.000000 )
( 0.028761 0.000000 0.027689 0.000000 0.002216 0.000000 )
( -0.077573 0.000000 -0.049621 0.000000 0.002755 0.000000 )
( 0.077573 0.000000 0.049621 0.000000 -0.002755 0.000000 )
( -0.083713 0.000000 0.056918 0.000000 0.003050 0.000000 )
( 0.083713 0.000000 -0.056918 0.000000 -0.003050 0.000000 )
( -0.061327 0.000000 -0.339492 0.000000 -0.027853 0.000000 )
( 0.061327 0.000000 0.339492 0.000000 0.027853 0.000000 )
( -0.480154 0.000000 -0.122423 0.000000 -0.016866 0.000000 )
( 0.480154 0.000000 0.122423 0.000000 0.016866 0.000000 )
( -0.022041 0.000000 -0.040385 0.000000 -0.002654 0.000000 )
( 0.022041 0.000000 0.040385 0.000000 0.002654 0.000000 )
  freq ( 7 ) = 3.418539 [THz] = 114.030198 [cm-1]
( 0.124608 0.000000 -0.255578 0.000000 -0.014673 0.000000 )
( -0.124608 0.000000 0.255578 0.000000 0.014673 0.000000 )
( 0.126819 0.000000 -0.247578 0.000000 -0.013008 0.000000 )
( -0.126819 0.000000 0.247578 0.000000 0.013008 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.000755 0.000000 0.004265 0.000000 -0.044702 0.000000 )
( -0.000755 0.000000 -0.004265 0.000000 0.044702 0.000000 )
( 0.060106 0.000000 -0.101613 0.000000 -0.006296 0.000000 )

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( -0.060106 0.000000 0.101613 0.000000 0.006296 0.000000 )
( 0.008132 0.000000 -0.036248 0.000000 0.008076 0.000000 )
( -0.008132 0.000000 0.036248 0.000000 -0.008076 0.000000 )
( 0.055350 0.000000 -0.121944 0.000000 -0.012165 0.000000 )
( -0.055350 0.000000 0.121944 0.000000 0.012165 0.000000 )
( 0.070082 0.000000 -0.342213 0.000000 -0.007195 0.000000 )
( -0.070082 0.000000 0.342213 0.000000 0.007195 0.000000 )
( 0.118248 0.000000 -0.238489 0.000000 -0.006764 0.000000 )
( -0.118248 0.000000 0.238489 0.000000 0.006764 0.000000 )
( 0.221842 0.000000 -0.249694 0.000000 -0.018334 0.000000 )
( -0.221842 0.000000 0.249694 0.000000 0.018334 0.000000 )
( -0.013462 0.000000 -0.027239 0.000000 0.008342 0.000000 )
( 0.013462 0.000000 0.027239 0.000000 -0.008342 0.000000 )
freq ( 8) = 5.055900 [THz] = 168.646680 [cm-1]
( -0.080365 0.000000 -0.122811 0.000000 0.003562 0.000000 )
( -0.080365 0.000000 -0.122811 0.000000 0.003562 0.000000 )
( -0.065109 0.000000 -0.132051 0.000000 0.000849 0.000000 )
( -0.065109 0.000000 -0.132051 0.000000 0.000849 0.000000 )
( 0.128061 0.000000 0.221755 0.000000 0.133425 0.000000 )
( 0.128133 0.000000 0.227375 0.000000 -0.069973 0.000000 )
( 0.128133 0.000000 0.227375 0.000000 -0.069973 0.000000 )
( 0.069299 0.000000 0.074615 0.000000 0.009381 0.000000 )
( 0.069299 0.000000 0.074615 0.000000 0.009381 0.000000 )
( 0.143546 0.000000 0.253814 0.000000 -0.031871 0.000000 )
( 0.143546 0.000000 0.253814 0.000000 -0.031871 0.000000 )
( 0.030839 0.000000 0.099847 0.000000 0.011669 0.000000 )
( 0.030839 0.000000 0.099847 0.000000 0.011669 0.000000 )
( -0.122393 0.000000 -0.214463 0.000000 -0.007195 0.000000 )
( -0.122393 0.000000 -0.214463 0.000000 -0.007195 0.000000 )
( -0.047162 0.000000 -0.171633 0.000000 0.005095 0.000000 )
( -0.047162 0.000000 -0.171633 0.000000 0.005095 0.000000 )
( -0.121001 0.000000 -0.126481 0.000000 0.010404 0.000000 )
( -0.121001 0.000000 -0.126481 0.000000 0.010404 0.000000 )
( 0.162838 0.000000 0.289140 0.000000 -0.030158 0.000000 )
( 0.162838 0.000000 0.289140 0.000000 -0.030158 0.000000 )
freq ( 9) = 5.275886 [THz] = 175.984624 [cm-1]
( -0.144509 0.000000 0.073752 0.000000 -0.000715 0.000000 )
( -0.144509 0.000000 0.073752 0.000000 -0.000715 0.000000 )
( -0.135105 0.000000 0.084319 0.000000 0.004802 0.000000 )
( -0.135105 0.000000 0.084319 0.000000 0.004802 0.000000 )
( 0.250507 0.000000 -0.142680 0.000000 0.001184 0.000000 )
( 0.260638 0.000000 -0.149048 0.000000 -0.006792 0.000000 )
( 0.260638 0.000000 -0.149048 0.000000 -0.006792 0.000000 )
( 0.130469 0.000000 -0.050822 0.000000 0.005768 0.000000 )
( 0.130469 0.000000 -0.050822 0.000000 0.005768 0.000000 )
( 0.236884 0.000000 -0.133838 0.000000 -0.002566 0.000000 )
( 0.236884 0.000000 -0.133838 0.000000 -0.002566 0.000000 )
( 0.101459 0.000000 -0.082247 0.000000 -0.010986 0.000000 )
( 0.101459 0.000000 -0.082247 0.000000 -0.010986 0.000000 )
( -0.140115 0.000000 0.082602 0.000000 -0.005969 0.000000 )

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( -0.140115  0.000000  0.082602  0.000000  -0.005969  0.000000 )
( -0.191426  0.000000  0.169314  0.000000  0.045429  0.000000 )
( -0.191426  0.000000  0.169314  0.000000  0.045429  0.000000 )
( -0.244380  0.000000  0.078903  0.000000  -0.031163  0.000000 )
( -0.244380  0.000000  0.078903  0.000000  -0.031163  0.000000 )
(  0.185443  0.000000  -0.102545  0.000000  -0.001454  0.000000 )
(  0.185443  0.000000  -0.102545  0.000000  -0.001454  0.000000 )
  freq ( 10) =   5.738969 [THz] =  191.431409 [cm-1]
(  0.020867  0.000000  0.013044  0.000000  -0.250722  0.000000 )
( -0.020867  0.000000  -0.013044  0.000000  0.250722  0.000000 )
( -0.010618  0.000000  0.017443  0.000000  -0.253804  0.000000 )
(  0.010618  0.000000  -0.017443  0.000000  0.253804  0.000000 )
( -0.000000  0.000000  0.000000  0.000000  -0.000000  0.000000 )
(  0.050005  0.000000  -0.028638  0.000000  0.011100  0.000000 )
( -0.050005  0.000000  0.028638  0.000000  -0.011100  0.000000 )
( -0.051680  0.000000  0.013027  0.000000  -0.214123  0.000000 )
(  0.051680  0.000000  -0.013027  0.000000  0.214123  0.000000 )
(  0.024670  0.000000  0.027204  0.000000  0.124230  0.000000 )
( -0.024670  0.000000  -0.027204  0.000000  -0.124230  0.000000 )
(  0.042042  0.000000  -0.014103  0.000000  -0.213050  0.000000 )
( -0.042042  0.000000  0.014103  0.000000  0.213050  0.000000 )
(  0.013050  0.000000  0.025156  0.000000  -0.226636  0.000000 )
( -0.013050  0.000000  -0.025156  0.000000  0.226636  0.000000 )
(  0.009640  0.000000  0.005562  0.000000  -0.318062  0.000000 )
( -0.009640  0.000000  -0.005562  0.000000  0.318062  0.000000 )
( -0.005572  0.000000  0.014553  0.000000  -0.280711  0.000000 )
(  0.005572  0.000000  -0.014553  0.000000  0.280711  0.000000 )
(  0.056171  0.000000  0.063863  0.000000  0.125291  0.000000 )
( -0.056171  0.000000  -0.063863  0.000000  -0.125291  0.000000 )
  freq ( 11) =   6.975723 [THz] =  232.685067 [cm-1]
( -0.042364  0.000000  -0.052729  0.000000  -0.004950  0.000000 )
(  0.042364  0.000000  0.052729  0.000000  0.004950  0.000000 )
(  0.022427  0.000000  0.069873  0.000000  -0.011449  0.000000 )
( -0.022427  0.000000  -0.069873  0.000000  0.011449  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.000000  0.000000 )
(  0.003332  0.000000  0.013790  0.000000  -0.387708  0.000000 )
( -0.003332  0.000000  -0.013790  0.000000  0.387708  0.000000 )
(  0.085466  0.000000  0.143905  0.000000  -0.007551  0.000000 )
( -0.085466  0.000000  -0.143905  0.000000  0.007551  0.000000 )
( -0.163377  0.000000  0.098555  0.000000  0.008838  0.000000 )
(  0.163377  0.000000  -0.098555  0.000000  -0.008838  0.000000 )
( -0.064972  0.000000  -0.149730  0.000000  -0.007501  0.000000 )
(  0.064972  0.000000  0.149730  0.000000  0.007501  0.000000 )
( -0.014456  0.000000  0.007170  0.000000  0.005743  0.000000 )
(  0.014456  0.000000  -0.007170  0.000000  -0.005743  0.000000 )
( -0.019318  0.000000  0.007816  0.000000  0.159518  0.000000 )
(  0.019318  0.000000  -0.007816  0.000000  -0.159518  0.000000 )
( -0.027367  0.000000  0.019606  0.000000  -0.188417  0.000000 )
(  0.027367  0.000000  -0.019606  0.000000  0.188417  0.000000 )
( -0.367797  0.000000  0.223278  0.000000  0.013387  0.000000 )

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( 0.367797 0.000000 -0.223278 0.000000 -0.013387 0.000000 )
freq ( 12) = 7.033440 [THz] = 234.610301 [cm-1]
( -0.055037 0.000000 0.053828 0.000000 -0.012960 0.000000 )
( -0.055037 0.000000 0.053828 0.000000 -0.012960 0.000000 )
( 0.086552 0.000000 -0.019063 0.000000 -0.023725 0.000000 )
( 0.086552 0.000000 -0.019063 0.000000 -0.023725 0.000000 )
( -0.042045 0.000000 -0.070764 0.000000 0.480444 0.000000 )
( -0.051872 0.000000 -0.073399 0.000000 -0.193451 0.000000 )
( -0.051872 0.000000 -0.073399 0.000000 -0.193451 0.000000 )
( 0.140733 0.000000 -0.144074 0.000000 -0.023215 0.000000 )
( 0.140733 0.000000 -0.144074 0.000000 -0.023215 0.000000 )
( 0.033257 0.000000 0.066661 0.000000 0.100624 0.000000 )
( 0.033257 0.000000 0.066661 0.000000 0.100624 0.000000 )
( -0.206012 0.000000 0.036117 0.000000 -0.011578 0.000000 )
( -0.206012 0.000000 0.036117 0.000000 -0.011578 0.000000 )
( 0.038891 0.000000 0.062935 0.000000 -0.269308 0.000000 )
( 0.038891 0.000000 0.062935 0.000000 -0.269308 0.000000 )
( 0.003651 0.000000 0.042433 0.000000 0.111514 0.000000 )
( 0.003651 0.000000 0.042433 0.000000 0.111514 0.000000 )
( 0.034521 0.000000 0.022582 0.000000 0.078437 0.000000 )
( 0.034521 0.000000 0.022582 0.000000 0.078437 0.000000 )
( 0.167195 0.000000 0.283457 0.000000 0.110108 0.000000 )
( 0.167195 0.000000 0.283457 0.000000 0.110108 0.000000 )
freq ( 13) = 7.607100 [THz] = 253.745542 [cm-1]
( 0.020779 0.000000 0.007979 0.000000 0.077958 0.000000 )
( 0.020779 0.000000 0.007979 0.000000 0.077958 0.000000 )
( -0.005298 0.000000 0.019211 0.000000 0.081470 0.000000 )
( -0.005298 0.000000 0.019211 0.000000 0.081470 0.000000 )
( -0.075825 0.000000 -0.138859 0.000000 0.014679 0.000000 )
( 0.000252 0.000000 0.007589 0.000000 -0.222732 0.000000 )
( 0.000252 0.000000 0.007589 0.000000 -0.222732 0.000000 )
( -0.076943 0.000000 -0.022994 0.000000 0.058883 0.000000 )
( -0.076943 0.000000 -0.022994 0.000000 0.058883 0.000000 )
( 0.033066 0.000000 0.065910 0.000000 -0.387804 0.000000 )
( 0.033066 0.000000 0.065910 0.000000 -0.387804 0.000000 )
( 0.024883 0.000000 -0.073289 0.000000 0.055660 0.000000 )
( 0.024883 0.000000 -0.073289 0.000000 0.055660 0.000000 )
( 0.020853 0.000000 0.034208 0.000000 0.166445 0.000000 )
( 0.020853 0.000000 0.034208 0.000000 0.166445 0.000000 )
( 0.003617 0.000000 0.018415 0.000000 0.083449 0.000000 )
( 0.003617 0.000000 0.018415 0.000000 0.083449 0.000000 )
( 0.016918 0.000000 0.010530 0.000000 0.094995 0.000000 )
( 0.016918 0.000000 0.010530 0.000000 0.094995 0.000000 )
( 0.111483 0.000000 0.213979 0.000000 -0.380796 0.000000 )
( 0.111483 0.000000 0.213979 0.000000 -0.380796 0.000000 )
freq ( 14) = 8.561605 [THz] = 285.584400 [cm-1]
( 0.099332 0.000000 -0.059546 0.000000 0.052363 0.000000 )
( -0.099332 0.000000 0.059546 0.000000 -0.052363 0.000000 )
( -0.060869 0.000000 0.084489 0.000000 0.013727 0.000000 )
( 0.060869 0.000000 -0.084489 0.000000 -0.013727 0.000000 )

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( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( -0.011949 0.000000 0.014606 0.000000 0.086458 0.000000 )
( 0.011949 0.000000 -0.014606 0.000000 -0.086458 0.000000 )
( -0.131194 0.000000 0.207184 0.000000 0.001006 0.000000 )
( 0.131194 0.000000 -0.207184 0.000000 -0.001006 0.000000 )
( 0.117135 0.000000 0.061559 0.000000 0.096876 0.000000 )
( -0.117135 0.000000 -0.061559 0.000000 -0.096876 0.000000 )
( 0.230177 0.000000 -0.137836 0.000000 0.033452 0.000000 )
( -0.230177 0.000000 0.137836 0.000000 -0.033452 0.000000 )
( -0.017353 0.000000 -0.073436 0.000000 0.417404 0.000000 )
( 0.017353 0.000000 0.073436 0.000000 -0.417404 0.000000 )
( 0.009877 0.000000 -0.007115 0.000000 -0.068003 0.000000 )
( -0.009877 0.000000 0.007115 0.000000 0.068003 0.000000 )
( -0.059829 0.000000 0.021496 0.000000 -0.232789 0.000000 )
( 0.059829 0.000000 -0.021496 0.000000 0.232789 0.000000 )
( 0.208787 0.000000 0.093145 0.000000 0.098273 0.000000 )
( -0.208787 0.000000 -0.093145 0.000000 -0.098273 0.000000 )
  freq ( 15) = 8.612871 [THz] = 287.294469 [cm-1]
( -0.045447 0.000000 -0.121262 0.000000 -0.024306 0.000000 )
( -0.045447 0.000000 -0.121262 0.000000 -0.024306 0.000000 )
( 0.087540 0.000000 0.081352 0.000000 0.040409 0.000000 )
( 0.087540 0.000000 0.081352 0.000000 0.040409 0.000000 )
( -0.048689 0.000000 0.026427 0.000000 -0.063597 0.000000 )
( -0.016934 0.000000 0.035691 0.000000 0.019185 0.000000 )
( -0.016934 0.000000 0.035691 0.000000 0.019185 0.000000 )
( 0.133144 0.000000 0.239843 0.000000 0.053482 0.000000 )
( 0.133144 0.000000 0.239843 0.000000 0.053482 0.000000 )
( 0.005473 0.000000 -0.009713 0.000000 -0.034675 0.000000 )
( 0.005473 0.000000 -0.009713 0.000000 -0.034675 0.000000 )
( -0.164683 0.000000 -0.224077 0.000000 -0.043914 0.000000 )
( -0.164683 0.000000 -0.224077 0.000000 -0.043914 0.000000 )
( 0.005754 0.000000 0.003433 0.000000 -0.028134 0.000000 )
( 0.005754 0.000000 0.003433 0.000000 -0.028134 0.000000 )
( 0.006051 0.000000 0.003520 0.000000 0.400184 0.000000 )
( 0.006051 0.000000 0.003520 0.000000 0.400184 0.000000 )
( -0.001680 0.000000 -0.011470 0.000000 -0.353591 0.000000 )
( -0.001680 0.000000 -0.011470 0.000000 -0.353591 0.000000 )
( 0.078169 0.000000 -0.093764 0.000000 -0.038024 0.000000 )
( 0.078169 0.000000 -0.093764 0.000000 -0.038024 0.000000 )
  freq ( 16) = 8.833615 [THz] = 294.657670 [cm-1]
( -0.064187 0.000000 -0.065015 0.000000 0.006087 0.000000 )
( 0.064187 0.000000 0.065015 0.000000 -0.006087 0.000000 )
( 0.079340 0.000000 0.046636 0.000000 -0.037847 0.000000 )
( -0.079340 0.000000 -0.046636 0.000000 0.037847 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.003723 0.000000 -0.024247 0.000000 0.225552 0.000000 )
( -0.003723 0.000000 0.024247 0.000000 -0.225552 0.000000 )
( 0.209972 0.000000 0.097198 0.000000 -0.041322 0.000000 )
( -0.209972 0.000000 -0.097198 0.000000 0.041322 0.000000 )
( 0.151185 0.000000 -0.131152 0.000000 -0.029690 0.000000 )

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( -0.151185 0.000000 0.131152 0.000000 0.029690 0.000000 )
( -0.122626 0.000000 -0.183072 0.000000 0.019177 0.000000 )
( 0.122626 0.000000 0.183072 0.000000 -0.019177 0.000000 )
( 0.019446 0.000000 0.011064 0.000000 -0.129253 0.000000 )
( -0.019446 0.000000 -0.011064 0.000000 0.129253 0.000000 )
( -0.034329 0.000000 0.029606 0.000000 0.307083 0.000000 )
( 0.034329 0.000000 -0.029606 0.000000 -0.307083 0.000000 )
( -0.034293 0.000000 0.015144 0.000000 -0.225465 0.000000 )
( 0.034293 0.000000 -0.015144 0.000000 0.225465 0.000000 )
( 0.265323 0.000000 -0.218773 0.000000 -0.032803 0.000000 )
( -0.265323 0.000000 0.218773 0.000000 0.032803 0.000000 )
  freq ( 17) = 9.093304 [THz] = 303.319984 [cm-1]
( -0.074613 0.000000 0.037878 0.000000 0.059786 0.000000 )
( -0.074613 0.000000 0.037878 0.000000 0.059786 0.000000 )
( 0.060632 0.000000 -0.073437 0.000000 0.011770 0.000000 )
( 0.060632 0.000000 -0.073437 0.000000 0.011770 0.000000 )
( -0.031000 0.000000 0.007831 0.000000 -0.405442 0.000000 )
( 0.067069 0.000000 0.098688 0.000000 0.094743 0.000000 )
( 0.067069 0.000000 0.098688 0.000000 0.094743 0.000000 )
( 0.157654 0.000000 -0.151850 0.000000 -0.007314 0.000000 )
( 0.157654 0.000000 -0.151850 0.000000 -0.007314 0.000000 )
( -0.033965 0.000000 -0.047892 0.000000 -0.151076 0.000000 )
( -0.033965 0.000000 -0.047892 0.000000 -0.151076 0.000000 )
( -0.160922 0.000000 0.115361 0.000000 0.042402 0.000000 )
( -0.160922 0.000000 0.115361 0.000000 0.042402 0.000000 )
( 0.018147 0.000000 0.018421 0.000000 -0.274600 0.000000 )
( 0.018147 0.000000 0.018421 0.000000 -0.274600 0.000000 )
( -0.019487 0.000000 -0.003045 0.000000 0.179795 0.000000 )
( -0.019487 0.000000 -0.003045 0.000000 0.179795 0.000000 )
( -0.007209 0.000000 -0.011907 0.000000 0.258960 0.000000 )
( -0.007209 0.000000 -0.011907 0.000000 0.258960 0.000000 )
( -0.130014 0.000000 -0.202732 0.000000 -0.158154 0.000000 )
( -0.130014 0.000000 -0.202732 0.000000 -0.158154 0.000000 )
  freq ( 18) = 9.699489 [THz] = 323.540118 [cm-1]
( 0.003725 0.000000 0.032328 0.000000 -0.092715 0.000000 )
( -0.003725 0.000000 -0.032328 0.000000 0.092715 0.000000 )
( 0.030324 0.000000 -0.016029 0.000000 0.086144 0.000000 )
( -0.030324 0.000000 0.016029 0.000000 -0.086144 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( -0.127843 0.000000 -0.140117 0.000000 -0.129765 0.000000 )
( 0.127843 0.000000 0.140117 0.000000 0.129765 0.000000 )
( 0.271609 0.000000 0.010711 0.000000 0.072434 0.000000 )
( -0.271609 0.000000 -0.010711 0.000000 -0.072434 0.000000 )
( 0.354200 0.000000 0.083819 0.000000 -0.016022 0.000000 )
( -0.354200 0.000000 -0.083819 0.000000 0.016022 0.000000 )
( 0.233267 0.000000 0.129357 0.000000 -0.069816 0.000000 )
( -0.233267 0.000000 -0.129357 0.000000 0.069816 0.000000 )
( -0.091476 0.000000 -0.120925 0.000000 -0.065192 0.000000 )
( 0.091476 0.000000 0.120925 0.000000 0.065192 0.000000 )
( 0.004913 0.000000 0.062298 0.000000 -0.005793 0.000000 )

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( -0.004913  0.000000  -0.062298  0.000000   0.005793  0.000000 )
( -0.205193  0.000000  -0.019650  0.000000   0.048705  0.000000 )
(  0.205193  0.000000   0.019650  0.000000  -0.048705  0.000000 )
(  0.232400  0.000000   0.103694  0.000000  -0.015306  0.000000 )
( -0.232400  0.000000  -0.103694  0.000000   0.015306  0.000000 )
  freq ( 19) =    9.766541 [THz] =   325.776732 [cm-1]
( -0.031430  0.000000   0.018801  0.000000   0.045632  0.000000 )
(  0.031430  0.000000  -0.018801  0.000000  -0.045632  0.000000 )
(  0.031134  0.000000   0.009480  0.000000  -0.055957  0.000000 )
( -0.031134  0.000000  -0.009480  0.000000   0.055957  0.000000 )
( -0.000000  0.000000   0.000000  0.000000  -0.000000  0.000000 )
(  0.018819  0.000000   0.139200  0.000000   0.109836  0.000000 )
( -0.018819  0.000000  -0.139200  0.000000  -0.109836  0.000000 )
(  0.051940  0.000000   0.271238  0.000000  -0.033506  0.000000 )
( -0.051940  0.000000  -0.271238  0.000000   0.033506  0.000000 )
( -0.030355  0.000000   0.380834  0.000000  -0.010478  0.000000 )
(  0.030355  0.000000  -0.380834  0.000000   0.010478  0.000000 )
( -0.081683  0.000000   0.270369  0.000000   0.047242  0.000000 )
(  0.081683  0.000000  -0.270369  0.000000  -0.047242  0.000000 )
( -0.079015  0.000000  -0.151893  0.000000  -0.087574  0.000000 )
(  0.079015  0.000000   0.151893  0.000000   0.087574  0.000000 )
(  0.088896  0.000000  -0.171217  0.000000   0.048970  0.000000 )
( -0.088896  0.000000   0.171217  0.000000  -0.048970  0.000000 )
(  0.012606  0.000000   0.019926  0.000000   0.002491  0.000000 )
( -0.012606  0.000000  -0.019926  0.000000  -0.002491  0.000000 )
(  0.017887  0.000000   0.278303  0.000000  -0.014034  0.000000 )
( -0.017887  0.000000  -0.278303  0.000000   0.014034  0.000000 )
  freq ( 20) =   10.079531 [THz] =   336.216951 [cm-1]
( -0.011140  0.000000   0.016837  0.000000  -0.236984  0.000000 )
( -0.011140  0.000000   0.016837  0.000000  -0.236984  0.000000 )
( -0.004698  0.000000  -0.033673  0.000000   0.240649  0.000000 )
( -0.004698  0.000000  -0.033673  0.000000   0.240649  0.000000 )
(  0.575883  0.000000  -0.324644  0.000000  -0.029819  0.000000 )
( -0.163217  0.000000   0.122505  0.000000   0.013775  0.000000 )
( -0.163217  0.000000   0.122505  0.000000   0.013775  0.000000 )
( -0.028688  0.000000  -0.027517  0.000000   0.191197  0.000000 )
( -0.028688  0.000000  -0.027517  0.000000   0.191197  0.000000 )
( -0.122511  0.000000   0.067051  0.000000  -0.004845  0.000000 )
( -0.122511  0.000000   0.067051  0.000000  -0.004845  0.000000 )
( -0.046611  0.000000   0.034722  0.000000  -0.190048  0.000000 )
( -0.046611  0.000000   0.034722  0.000000  -0.190048  0.000000 )
( -0.040488  0.000000   0.057559  0.000000  -0.022359  0.000000 )
( -0.040488  0.000000   0.057559  0.000000  -0.022359  0.000000 )
(  0.048331  0.000000   0.023761  0.000000  -0.005364  0.000000 )
(  0.048331  0.000000   0.023761  0.000000  -0.005364  0.000000 )
(  0.034967  0.000000  -0.067012  0.000000   0.027176  0.000000 )
(  0.034967  0.000000  -0.067012  0.000000   0.027176  0.000000 )
( -0.104594  0.000000   0.024233  0.000000  -0.006525  0.000000 )
( -0.104594  0.000000   0.024233  0.000000  -0.006525  0.000000 )
  freq ( 21) =   10.211711 [THz] =   340.626022 [cm-1]

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( 0.030380 0.000000 0.009853 0.000000 0.203835 0.000000 )
( -0.030380 0.000000 -0.009853 0.000000 -0.203835 0.000000 )
( 0.020273 0.000000 -0.045371 0.000000 -0.209119 0.000000 )
( -0.020273 0.000000 0.045371 0.000000 0.209119 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.173454 0.000000 0.341790 0.000000 -0.087232 0.000000 )
( -0.173454 0.000000 -0.341790 0.000000 0.087232 0.000000 )
( 0.175847 0.000000 -0.151327 0.000000 -0.167472 0.000000 )
( -0.175847 0.000000 0.151327 0.000000 0.167472 0.000000 )
( 0.116664 0.000000 -0.047882 0.000000 -0.038324 0.000000 )
( -0.116664 0.000000 0.047882 0.000000 0.038324 0.000000 )
( 0.199827 0.000000 -0.030824 0.000000 0.163238 0.000000 )
( -0.199827 0.000000 0.030824 0.000000 -0.163238 0.000000 )
( 0.059761 0.000000 -0.040816 0.000000 -0.025836 0.000000 )
( -0.059761 0.000000 0.040816 0.000000 0.025836 0.000000 )
( -0.126097 0.000000 0.128541 0.000000 -0.048314 0.000000 )
( 0.126097 0.000000 -0.128541 0.000000 0.048314 0.000000 )
( -0.173749 0.000000 0.039835 0.000000 0.061859 0.000000 )
( 0.173749 0.000000 -0.039835 0.000000 -0.061859 0.000000 )
( 0.094996 0.000000 -0.056217 0.000000 -0.038696 0.000000 )
( -0.094996 0.000000 0.056217 0.000000 0.038696 0.000000 )

```

freq (22) = 10.696471 [THz] = 356.795879 [cm-1]

```

( -0.016255 0.000000 0.009957 0.000000 0.038623 0.000000 )
( 0.016255 0.000000 -0.009957 0.000000 -0.038623 0.000000 )
( 0.016284 0.000000 -0.011400 0.000000 0.024497 0.000000 )
( -0.016284 0.000000 0.011400 0.000000 -0.024497 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.281255 0.000000 -0.143624 0.000000 -0.010409 0.000000 )
( -0.281255 0.000000 0.143624 0.000000 0.010409 0.000000 )
( 0.011027 0.000000 -0.017825 0.000000 -0.005153 0.000000 )
( -0.011027 0.000000 0.017825 0.000000 0.005153 0.000000 )
( 0.046102 0.000000 0.056348 0.000000 0.421440 0.000000 )
( -0.046102 0.000000 -0.056348 0.000000 -0.421440 0.000000 )
( -0.007235 0.000000 0.002193 0.000000 0.006806 0.000000 )
( 0.007235 0.000000 -0.002193 0.000000 -0.006806 0.000000 )
( 0.001417 0.000000 0.000785 0.000000 -0.011637 0.000000 )
( -0.001417 0.000000 -0.000785 0.000000 0.011637 0.000000 )
( -0.000179 0.000000 -0.007742 0.000000 0.095855 0.000000 )
( 0.000179 0.000000 0.007742 0.000000 -0.095855 0.000000 )
( -0.010945 0.000000 -0.002443 0.000000 0.100568 0.000000 )
( 0.010945 0.000000 0.002443 0.000000 -0.100568 0.000000 )
( 0.076573 0.000000 0.104077 0.000000 0.421315 0.000000 )
( -0.076573 0.000000 -0.104077 0.000000 -0.421315 0.000000 )

```

freq (23) = 10.930832 [THz] = 364.613310 [cm-1]

```

( -0.040874 0.000000 0.107887 0.000000 0.026727 0.000000 )
( -0.040874 0.000000 0.107887 0.000000 0.026727 0.000000 )
( 0.017332 0.000000 0.113578 0.000000 -0.000975 0.000000 )
( 0.017332 0.000000 0.113578 0.000000 -0.000975 0.000000 )
( -0.047669 0.000000 -0.318877 0.000000 0.032513 0.000000 )
( 0.102714 0.000000 -0.076847 0.000000 -0.007885 0.000000 )

```

```

( 0.102714 0.000000 -0.076847 0.000000 -0.007885 0.000000 )
( 0.043059 0.000000 0.259290 0.000000 0.002318 0.000000 )
( 0.043059 0.000000 0.259290 0.000000 0.002318 0.000000 )
( -0.085348 0.000000 -0.106577 0.000000 -0.028944 0.000000 )
( -0.085348 0.000000 -0.106577 0.000000 -0.028944 0.000000 )
( -0.063503 0.000000 0.239571 0.000000 0.017494 0.000000 )
( -0.063503 0.000000 0.239571 0.000000 0.017494 0.000000 )
( -0.188978 0.000000 -0.240075 0.000000 -0.029632 0.000000 )
( -0.188978 0.000000 -0.240075 0.000000 -0.029632 0.000000 )
( 0.192594 0.000000 -0.275812 0.000000 -0.017615 0.000000 )
( 0.192594 0.000000 -0.275812 0.000000 -0.017615 0.000000 )
( 0.031233 0.000000 0.083967 0.000000 -0.000128 0.000000 )
( 0.031233 0.000000 0.083967 0.000000 -0.000128 0.000000 )
( -0.115820 0.000000 0.154917 0.000000 -0.017424 0.000000 )
( -0.115820 0.000000 0.154917 0.000000 -0.017424 0.000000 )
  freq ( 24 ) = 11.002103 [THz] = 366.990658 [cm-1]
( -0.096310 0.000000 -0.034796 0.000000 0.015594 0.000000 )
( -0.096310 0.000000 -0.034796 0.000000 0.015594 0.000000 )
( -0.105209 0.000000 0.006548 0.000000 -0.024573 0.000000 )
( -0.105209 0.000000 0.006548 0.000000 -0.024573 0.000000 )
( 0.071675 0.000000 -0.010334 0.000000 0.098408 0.000000 )
( 0.270791 0.000000 0.113940 0.000000 0.023157 0.000000 )
( 0.270791 0.000000 0.113940 0.000000 0.023157 0.000000 )
( -0.228560 0.000000 -0.015472 0.000000 -0.013828 0.000000 )
( -0.228560 0.000000 -0.015472 0.000000 -0.013828 0.000000 )
( -0.042496 0.000000 -0.076117 0.000000 0.003270 0.000000 )
( -0.042496 0.000000 -0.076117 0.000000 0.003270 0.000000 )
( -0.218756 0.000000 -0.103017 0.000000 0.009342 0.000000 )
( -0.218756 0.000000 -0.103017 0.000000 0.009342 0.000000 )
( 0.062968 0.000000 0.216179 0.000000 -0.005509 0.000000 )
( 0.062968 0.000000 0.216179 0.000000 -0.005509 0.000000 )
( -0.006641 0.000000 -0.127484 0.000000 -0.058615 0.000000 )
( -0.006641 0.000000 -0.127484 0.000000 -0.058615 0.000000 )
( 0.338553 0.000000 -0.005144 0.000000 -0.028718 0.000000 )
( 0.338553 0.000000 -0.005144 0.000000 -0.028718 0.000000 )
( -0.269809 0.000000 -0.075294 0.000000 0.003645 0.000000 )
( -0.269809 0.000000 -0.075294 0.000000 0.003645 0.000000 )
  freq ( 25 ) = 11.025586 [THz] = 367.773956 [cm-1]
( -0.061794 0.000000 0.010051 0.000000 0.007960 0.000000 )
( -0.061794 0.000000 0.010051 0.000000 0.007960 0.000000 )
( -0.041554 0.000000 0.029690 0.000000 -0.010481 0.000000 )
( -0.041554 0.000000 0.029690 0.000000 -0.010481 0.000000 )
( 0.232633 0.000000 0.263475 0.000000 -0.221043 0.000000 )
( -0.083958 0.000000 -0.365698 0.000000 -0.031216 0.000000 )
( -0.083958 0.000000 -0.365698 0.000000 -0.031216 0.000000 )
( -0.079914 0.000000 0.062908 0.000000 -0.003605 0.000000 )
( -0.079914 0.000000 0.062908 0.000000 -0.003605 0.000000 )
( 0.155032 0.000000 0.271826 0.000000 0.022145 0.000000 )
( 0.155032 0.000000 0.271826 0.000000 0.022145 0.000000 )
( -0.132596 0.000000 0.027283 0.000000 0.003713 0.000000 )

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( -0.132596 0.000000 0.027283 0.000000 0.003713 0.000000 )
( -0.021055 0.000000 0.036434 0.000000 0.034050 0.000000 )
( -0.021055 0.000000 0.036434 0.000000 0.034050 0.000000 )
( 0.051634 0.000000 -0.143846 0.000000 0.072991 0.000000 )
( 0.051634 0.000000 -0.143846 0.000000 0.072991 0.000000 )
( 0.158917 0.000000 0.014078 0.000000 0.089356 0.000000 )
( 0.158917 0.000000 0.014078 0.000000 0.089356 0.000000 )
( -0.000413 0.000000 0.269882 0.000000 0.018469 0.000000 )
( -0.000413 0.000000 0.269882 0.000000 0.018469 0.000000 )
  freq ( 26) = 11.148261 [THz] = 371.865959 [cm-1]
( -0.086872 0.000000 -0.071465 0.000000 0.063696 0.000000 )
( 0.086872 0.000000 0.071465 0.000000 -0.063696 0.000000 )
( -0.090595 0.000000 -0.049117 0.000000 -0.046384 0.000000 )
( 0.090595 0.000000 0.049117 0.000000 0.046384 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( -0.190243 0.000000 0.053042 0.000000 -0.077975 0.000000 )
( 0.190243 0.000000 -0.053042 0.000000 0.077975 0.000000 )
( -0.145237 0.000000 -0.035318 0.000000 -0.060865 0.000000 )
( 0.145237 0.000000 0.035318 0.000000 0.060865 0.000000 )
( 0.372595 0.000000 0.216127 0.000000 0.117003 0.000000 )
( -0.372595 0.000000 -0.216127 0.000000 -0.117003 0.000000 )
( -0.091717 0.000000 -0.097728 0.000000 0.052285 0.000000 )
( 0.091717 0.000000 0.097728 0.000000 -0.052285 0.000000 )
( 0.117001 0.000000 0.235720 0.000000 -0.051069 0.000000 )
( -0.117001 0.000000 -0.235720 0.000000 0.051069 0.000000 )
( -0.090697 0.000000 -0.036045 0.000000 0.025639 0.000000 )
( 0.090697 0.000000 0.036045 0.000000 -0.025639 0.000000 )
( 0.237823 0.000000 -0.024770 0.000000 0.056128 0.000000 )
( -0.237823 0.000000 0.024770 0.000000 -0.056128 0.000000 )
( 0.142513 0.000000 0.067649 0.000000 0.110487 0.000000 )
( -0.142513 0.000000 -0.067649 0.000000 -0.110487 0.000000 )
  freq ( 27) = 11.273217 [THz] = 376.034038 [cm-1]
( 0.049406 0.000000 -0.075029 0.000000 -0.098283 0.000000 )
( -0.049406 0.000000 0.075029 0.000000 0.098283 0.000000 )
( 0.037544 0.000000 -0.088874 0.000000 0.105019 0.000000 )
( -0.037544 0.000000 0.088874 0.000000 -0.105019 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 )
( -0.060663 0.000000 0.115726 0.000000 0.145645 0.000000 )
( 0.060663 0.000000 -0.115726 0.000000 -0.145645 0.000000 )
( 0.058630 0.000000 -0.146292 0.000000 0.098664 0.000000 )
( -0.058630 0.000000 0.146292 0.000000 -0.098664 0.000000 )
( -0.219664 0.000000 0.352740 0.000000 0.087220 0.000000 )
( 0.219664 0.000000 -0.352740 0.000000 -0.087220 0.000000 )
( 0.111272 0.000000 -0.140259 0.000000 -0.112247 0.000000 )
( -0.111272 0.000000 0.140259 0.000000 0.112247 0.000000 )
( 0.091747 0.000000 0.115360 0.000000 -0.033737 0.000000 )
( -0.091747 0.000000 -0.115360 0.000000 0.033737 0.000000 )
( -0.107540 0.000000 0.249779 0.000000 0.065057 0.000000 )
( 0.107540 0.000000 -0.249779 0.000000 -0.065057 0.000000 )
( -0.128507 0.000000 -0.092401 0.000000 -0.010300 0.000000 )

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( 0.128507 0.000000 0.092401 0.000000 0.010300 0.000000 )
( -0.100636 0.000000 0.146684 0.000000 0.079272 0.000000 )
( 0.100636 0.000000 -0.146684 0.000000 -0.079272 0.000000 )
freq ( 28) = 11.534002 [THz] = 384.732887 [cm-1]
( 0.037973 0.000000 -0.039306 0.000000 0.128436 0.000000 )
( 0.037973 0.000000 -0.039306 0.000000 0.128436 0.000000 )
( 0.035298 0.000000 -0.004346 0.000000 -0.131929 0.000000 )
( 0.035298 0.000000 -0.004346 0.000000 -0.131929 0.000000 )
( 0.258374 0.000000 -0.119670 0.000000 -0.000618 0.000000 )
( 0.087287 0.000000 -0.048603 0.000000 -0.010605 0.000000 )
( 0.087287 0.000000 -0.048603 0.000000 -0.010605 0.000000 )
( 0.005571 0.000000 -0.025009 0.000000 -0.133542 0.000000 )
( 0.005571 0.000000 -0.025009 0.000000 -0.133542 0.000000 )
( -0.399334 0.000000 0.219276 0.000000 0.011524 0.000000 )
( -0.399334 0.000000 0.219276 0.000000 0.011524 0.000000 )
( 0.044646 0.000000 -0.023554 0.000000 0.130864 0.000000 )
( 0.044646 0.000000 -0.023554 0.000000 0.130864 0.000000 )
( 0.067024 0.000000 -0.030737 0.000000 0.007450 0.000000 )
( 0.067024 0.000000 -0.030737 0.000000 0.007450 0.000000 )
( -0.070980 0.000000 0.060024 0.000000 0.068733 0.000000 )
( -0.070980 0.000000 0.060024 0.000000 0.068733 0.000000 )
( -0.084128 0.000000 0.030400 0.000000 -0.062908 0.000000 )
( -0.084128 0.000000 0.030400 0.000000 -0.062908 0.000000 )
( -0.322161 0.000000 0.175119 0.000000 0.009866 0.000000 )
( -0.322161 0.000000 0.175119 0.000000 0.009866 0.000000 )
freq ( 29) = 12.258016 [THz] = 408.883401 [cm-1]
( -0.003120 0.000000 -0.021024 0.000000 0.007057 0.000000 )
( -0.003120 0.000000 -0.021024 0.000000 0.007057 0.000000 )
( -0.018496 0.000000 -0.016905 0.000000 -0.006729 0.000000 )
( -0.018496 0.000000 -0.016905 0.000000 -0.006729 0.000000 )
( -0.208429 0.000000 -0.377189 0.000000 -0.003980 0.000000 )
( -0.001879 0.000000 -0.018325 0.000000 0.244537 0.000000 )
( -0.001879 0.000000 -0.018325 0.000000 0.244537 0.000000 )
( -0.017403 0.000000 -0.037651 0.000000 0.012592 0.000000 )
( -0.017403 0.000000 -0.037651 0.000000 0.012592 0.000000 )
( 0.194116 0.000000 0.369832 0.000000 -0.063497 0.000000 )
( 0.194116 0.000000 0.369832 0.000000 -0.063497 0.000000 )
( -0.011298 0.000000 -0.027840 0.000000 0.027741 0.000000 )
( -0.011298 0.000000 -0.027840 0.000000 0.027741 0.000000 )
( 0.022376 0.000000 0.037830 0.000000 -0.109807 0.000000 )
( 0.022376 0.000000 0.037830 0.000000 -0.109807 0.000000 )
( -0.034308 0.000000 0.028760 0.000000 -0.113429 0.000000 )
( -0.034308 0.000000 0.028760 0.000000 -0.113429 0.000000 )
( 0.036300 0.000000 -0.009283 0.000000 -0.118605 0.000000 )
( 0.036300 0.000000 -0.009283 0.000000 -0.118605 0.000000 )
( 0.150164 0.000000 0.304897 0.000000 -0.062776 0.000000 )
( 0.150164 0.000000 0.304897 0.000000 -0.062776 0.000000 )
freq ( 30) = 12.666584 [THz] = 422.511748 [cm-1]
( -0.117165 0.000000 0.041705 0.000000 -0.148684 0.000000 )
( 0.117165 0.000000 -0.041705 0.000000 0.148684 0.000000 )

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( -0.112407  0.000000   0.081213  0.000000   0.150327  0.000000 )
(  0.112407  0.000000  -0.081213  0.000000  -0.150327  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.000000  0.000000 )
(  0.165109  0.000000   0.266511  0.000000   0.011560  0.000000 )
( -0.165109  0.000000  -0.266511  0.000000  -0.011560  0.000000 )
(  0.137197  0.000000  -0.046338  0.000000   0.137493  0.000000 )
( -0.137197  0.000000   0.046338  0.000000  -0.137493  0.000000 )
(  0.100273  0.000000  -0.062941  0.000000  -0.013491  0.000000 )
( -0.100273  0.000000   0.062941  0.000000   0.013491  0.000000 )
(  0.135739  0.000000  -0.093234  0.000000  -0.142976  0.000000 )
( -0.135739  0.000000   0.093234  0.000000   0.142976  0.000000 )
( -0.119602  0.000000   0.079360  0.000000   0.007010  0.000000 )
(  0.119602  0.000000  -0.079360  0.000000  -0.007010  0.000000 )
(  0.106604  0.000000  -0.172570  0.000000   0.000798  0.000000 )
( -0.106604  0.000000   0.172570  0.000000  -0.000798  0.000000 )
(  0.209137  0.000000  -0.010791  0.000000  -0.010237  0.000000 )
( -0.209137  0.000000   0.010791  0.000000   0.010237  0.000000 )
( -0.302061  0.000000   0.153332  0.000000  -0.005780  0.000000 )
(  0.302061  0.000000  -0.153332  0.000000   0.005780  0.000000 )
  freq ( 31) = 12.770044 [THz] = 425.962826 [cm-1]
( -0.035406  0.000000  -0.118892  0.000000  -0.006260  0.000000 )
(  0.035406  0.000000   0.118892  0.000000   0.006260  0.000000 )
( -0.084902  0.000000  -0.090181  0.000000  -0.017260  0.000000 )
(  0.084902  0.000000   0.090181  0.000000   0.017260  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.000000  0.000000 )
(  0.211708  0.000000  -0.150782  0.000000   0.005287  0.000000 )
( -0.211708  0.000000   0.150782  0.000000  -0.005287  0.000000 )
(  0.095048  0.000000   0.137726  0.000000   0.008580  0.000000 )
( -0.095048  0.000000  -0.137726  0.000000  -0.008580  0.000000 )
(  0.009232  0.000000   0.076551  0.000000  -0.249067  0.000000 )
( -0.009232  0.000000  -0.076551  0.000000   0.249067  0.000000 )
(  0.094542  0.000000   0.129312  0.000000   0.015283  0.000000 )
( -0.094542  0.000000  -0.129312  0.000000  -0.015283  0.000000 )
(  0.107757  0.000000   0.179044  0.000000   0.057872  0.000000 )
( -0.107757  0.000000  -0.179044  0.000000  -0.057872  0.000000 )
( -0.123191  0.000000   0.064402  0.000000  -0.035751  0.000000 )
(  0.123191  0.000000  -0.064402  0.000000   0.035751  0.000000 )
(  0.108200  0.000000  -0.068591  0.000000  -0.031899  0.000000 )
( -0.108200  0.000000   0.068591  0.000000   0.031899  0.000000 )
( -0.205505  0.000000  -0.284989  0.000000  -0.266272  0.000000 )
(  0.205505  0.000000   0.284989  0.000000   0.266272  0.000000 )
  freq ( 32) = 12.958044 [THz] = 432.233838 [cm-1]
(  0.068305  0.000000  -0.043050  0.000000  -0.181288  0.000000 )
(  0.068305  0.000000  -0.043050  0.000000  -0.181288  0.000000 )
(  0.047392  0.000000  -0.103620  0.000000   0.176957  0.000000 )
(  0.047392  0.000000  -0.103620  0.000000   0.176957  0.000000 )
( -0.291329  0.000000   0.109800  0.000000  -0.003934  0.000000 )
(  0.304314  0.000000  -0.199032  0.000000  -0.026163  0.000000 )
(  0.304314  0.000000  -0.199032  0.000000  -0.026163  0.000000 )
( -0.057576  0.000000   0.115717  0.000000   0.162006  0.000000 )

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( -0.057576 0.000000 0.115717 0.000000 0.162006 0.000000 )
( -0.230257 0.000000 0.129917 0.000000 0.015350 0.000000 )
( -0.230257 0.000000 0.129917 0.000000 0.015350 0.000000 )
( -0.052591 0.000000 0.133994 0.000000 -0.158760 0.000000 )
( -0.052591 0.000000 0.133994 0.000000 -0.158760 0.000000 )
( 0.023242 0.000000 0.045353 0.000000 0.000741 0.000000 )
( 0.023242 0.000000 0.045353 0.000000 0.000741 0.000000 )
( -0.013952 0.000000 0.174407 0.000000 -0.017960 0.000000 )
( -0.013952 0.000000 0.174407 0.000000 -0.017960 0.000000 )
( -0.110237 0.000000 -0.116183 0.000000 0.048423 0.000000 )
( -0.110237 0.000000 -0.116183 0.000000 0.048423 0.000000 )
( -0.045924 0.000000 -0.110738 0.000000 0.005740 0.000000 )
( -0.045924 0.000000 -0.110738 0.000000 0.005740 0.000000 )
freq ( 33 ) = 13.095475 [THz] = 436.818025 [cm-1]
( 0.070794 0.000000 0.110491 0.000000 -0.024498 0.000000 )
( 0.070794 0.000000 0.110491 0.000000 -0.024498 0.000000 )
( 0.080263 0.000000 0.097217 0.000000 0.032176 0.000000 )
( 0.080263 0.000000 0.097217 0.000000 0.032176 0.000000 )
( 0.026608 0.000000 0.134613 0.000000 -0.001539 0.000000 )
( 0.073644 0.000000 0.028159 0.000000 0.062960 0.000000 )
( 0.073644 0.000000 0.028159 0.000000 0.062960 0.000000 )
( -0.100062 0.000000 -0.240024 0.000000 0.024401 0.000000 )
( -0.100062 0.000000 -0.240024 0.000000 0.024401 0.000000 )
( -0.020316 0.000000 0.039321 0.000000 -0.028479 0.000000 )
( -0.020316 0.000000 0.039321 0.000000 -0.028479 0.000000 )
( -0.180541 0.000000 -0.195745 0.000000 -0.025051 0.000000 )
( -0.180541 0.000000 -0.195745 0.000000 -0.025051 0.000000 )
( -0.103500 0.000000 -0.179048 0.000000 0.023721 0.000000 )
( -0.103500 0.000000 -0.179048 0.000000 0.023721 0.000000 )
( 0.113896 0.000000 -0.019809 0.000000 -0.056109 0.000000 )
( 0.113896 0.000000 -0.019809 0.000000 -0.056109 0.000000 )
( -0.121973 0.000000 0.060163 0.000000 -0.045619 0.000000 )
( -0.121973 0.000000 0.060163 0.000000 -0.045619 0.000000 )
( 0.241932 0.000000 0.405011 0.000000 -0.011763 0.000000 )
( 0.241932 0.000000 0.405011 0.000000 -0.011763 0.000000 )
freq ( 34 ) = 13.246795 [THz] = 441.865535 [cm-1]
( 0.074191 0.000000 -0.051603 0.000000 -0.092380 0.000000 )
( -0.074191 0.000000 0.051603 0.000000 0.092380 0.000000 )
( 0.072093 0.000000 -0.047833 0.000000 0.087160 0.000000 )
( -0.072093 0.000000 0.047833 0.000000 -0.087160 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.103549 0.000000 0.146435 0.000000 -0.073519 0.000000 )
( -0.103549 0.000000 -0.146435 0.000000 0.073519 0.000000 )
( -0.223879 0.000000 0.070917 0.000000 0.070015 0.000000 )
( 0.223879 0.000000 -0.070917 0.000000 -0.070015 0.000000 )
( 0.153016 0.000000 -0.072398 0.000000 -0.024058 0.000000 )
( -0.153016 0.000000 0.072398 0.000000 0.024058 0.000000 )
( -0.173759 0.000000 0.155294 0.000000 -0.062917 0.000000 )
( 0.173759 0.000000 -0.155294 0.000000 0.062917 0.000000 )
( 0.029592 0.000000 0.000375 0.000000 0.003109 0.000000 )

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( -0.029592  0.000000  -0.000375  0.000000  -0.003109  0.000000  )
( -0.012682  0.000000   0.129132  0.000000   0.061202  0.000000  )
(  0.012682  0.000000  -0.129132  0.000000  -0.061202  0.000000  )
( -0.103051  0.000000  -0.059838  0.000000  -0.064924  0.000000  )
(  0.103051  0.000000   0.059838  0.000000   0.064924  0.000000  )
(  0.420328  0.000000  -0.256088  0.000000  -0.030869  0.000000  )
( -0.420328  0.000000   0.256088  0.000000   0.030869  0.000000  )
  freq ( 35) =   13.553174 [THz] =   452.085232 [cm-1]
(  0.098332  0.000000  -0.039920  0.000000   0.052555  0.000000  )
(  0.098332  0.000000  -0.039920  0.000000   0.052555  0.000000  )
(  0.077098  0.000000  -0.059846  0.000000  -0.057537  0.000000  )
(  0.077098  0.000000  -0.059846  0.000000  -0.057537  0.000000  )
(  0.127277  0.000000  -0.076025  0.000000   0.000070  0.000000  )
( -0.004986  0.000000   0.004945  0.000000   0.000973  0.000000  )
( -0.004986  0.000000   0.004945  0.000000   0.000973  0.000000  )
( -0.235439  0.000000   0.136936  0.000000  -0.029961  0.000000  )
( -0.235439  0.000000   0.136936  0.000000  -0.029961  0.000000  )
(  0.147036  0.000000  -0.082827  0.000000  -0.002141  0.000000  )
(  0.147036  0.000000  -0.082827  0.000000  -0.002141  0.000000  )
( -0.224142  0.000000   0.124433  0.000000   0.038923  0.000000  )
( -0.224142  0.000000   0.124433  0.000000   0.038923  0.000000  )
(  0.070794  0.000000  -0.041496  0.000000  -0.004031  0.000000  )
(  0.070794  0.000000  -0.041496  0.000000  -0.004031  0.000000  )
( -0.051555  0.000000   0.119756  0.000000  -0.004686  0.000000  )
( -0.051555  0.000000   0.119756  0.000000  -0.004686  0.000000  )
( -0.131082  0.000000  -0.015686  0.000000   0.009478  0.000000  )
( -0.131082  0.000000  -0.015686  0.000000   0.009478  0.000000  )
(  0.433996  0.000000  -0.248175  0.000000  -0.007929  0.000000  )
(  0.433996  0.000000  -0.248175  0.000000  -0.007929  0.000000  )
  freq ( 36) =   13.802086 [THz] =   460.388036 [cm-1]
(  0.027524  0.000000   0.062844  0.000000   0.001586  0.000000  )
( -0.027524  0.000000  -0.062844  0.000000  -0.001586  0.000000  )
(  0.033573  0.000000   0.058214  0.000000  -0.001847  0.000000  )
( -0.033573  0.000000  -0.058214  0.000000   0.001847  0.000000  )
( -0.000000  0.000000  -0.000000  0.000000  -0.000000  0.000000  )
(  0.141147  0.000000  -0.085639  0.000000   0.000718  0.000000  )
( -0.141147  0.000000   0.085639  0.000000  -0.000718  0.000000  )
( -0.069752  0.000000  -0.216139  0.000000  -0.006289  0.000000  )
(  0.069752  0.000000   0.216139  0.000000   0.006289  0.000000  )
(  0.113359  0.000000   0.214833  0.000000  -0.221739  0.000000  )
( -0.113359  0.000000  -0.214833  0.000000   0.221739  0.000000  )
( -0.141586  0.000000  -0.174272  0.000000  -0.002135  0.000000  )
(  0.141586  0.000000   0.174272  0.000000   0.002135  0.000000  )
( -0.047491  0.000000  -0.080785  0.000000   0.047366  0.000000  )
(  0.047491  0.000000   0.080785  0.000000  -0.047366  0.000000  )
(  0.055292  0.000000  -0.024263  0.000000  -0.023430  0.000000  )
( -0.055292  0.000000   0.024263  0.000000   0.023430  0.000000  )
( -0.037393  0.000000   0.039065  0.000000  -0.020759  0.000000  )
(  0.037393  0.000000  -0.039065  0.000000   0.020759  0.000000  )
(  0.193259  0.000000   0.388926  0.000000  -0.214737  0.000000  )

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```

( -0.193259  0.000000  -0.388926  0.000000   0.214737  0.000000 )
  freq ( 37) =   14.219025 [THz] =   474.295621 [cm-1]
(  0.017217  0.000000  -0.016695  0.000000  -0.030132  0.000000 )
(  0.017217  0.000000  -0.016695  0.000000  -0.030132  0.000000 )
( -0.018754  0.000000   0.014277  0.000000  -0.041351  0.000000 )
( -0.018754  0.000000   0.014277  0.000000  -0.041351  0.000000 )
( -0.117976  0.000000  -0.213613  0.000000  -0.253104  0.000000 )
(  0.039139  0.000000   0.087121  0.000000  -0.179362  0.000000 )
(  0.039139  0.000000   0.087121  0.000000  -0.179362  0.000000 )
(  0.150779  0.000000  -0.114300  0.000000  -0.061602  0.000000 )
(  0.150779  0.000000  -0.114300  0.000000  -0.061602  0.000000 )
(  0.061368  0.000000   0.093633  0.000000   0.304756  0.000000 )
(  0.061368  0.000000   0.093633  0.000000   0.304756  0.000000 )
( -0.192215  0.000000   0.039280  0.000000  -0.047933  0.000000 )
( -0.192215  0.000000   0.039280  0.000000  -0.047933  0.000000 )
(  0.018710  0.000000   0.019828  0.000000   0.326786  0.000000 )
(  0.018710  0.000000   0.019828  0.000000   0.326786  0.000000 )
( -0.002870  0.000000  -0.005619  0.000000   0.018002  0.000000 )
( -0.002870  0.000000  -0.005619  0.000000   0.018002  0.000000 )
( -0.006406  0.000000  -0.002842  0.000000   0.031152  0.000000 )
( -0.006406  0.000000  -0.002842  0.000000   0.031152  0.000000 )
(  0.054651  0.000000   0.065479  0.000000   0.301950  0.000000 )
(  0.054651  0.000000   0.065479  0.000000   0.301950  0.000000 )
  freq ( 38) =   14.797964 [THz] =   493.606955 [cm-1]
( -0.047275  0.000000  -0.018530  0.000000   0.028109  0.000000 )
(  0.047275  0.000000   0.018530  0.000000  -0.028109  0.000000 )
( -0.006905  0.000000   0.046876  0.000000  -0.032726  0.000000 )
(  0.006905  0.000000  -0.046876  0.000000   0.032726  0.000000 )
(  0.000000  0.000000   0.000000  0.000000   0.000000  0.000000 )
( -0.022693  0.000000  -0.033371  0.000000  -0.009766  0.000000 )
(  0.022693  0.000000   0.033371  0.000000   0.009766  0.000000 )
( -0.152526  0.000000  -0.353437  0.000000  -0.019484  0.000000 )
(  0.152526  0.000000   0.353437  0.000000   0.019484  0.000000 )
( -0.033913  0.000000   0.017794  0.000000   0.002119  0.000000 )
(  0.033913  0.000000  -0.017794  0.000000  -0.002119  0.000000 )
(  0.217829  0.000000   0.321238  0.000000   0.011631  0.000000 )
( -0.217829  0.000000  -0.321238  0.000000  -0.011631  0.000000 )
( -0.006943  0.000000   0.007762  0.000000   0.006816  0.000000 )
(  0.006943  0.000000  -0.007762  0.000000  -0.006816  0.000000 )
(  0.012234  0.000000  -0.069879  0.000000   0.288469  0.000000 )
( -0.012234  0.000000   0.069879  0.000000  -0.288469  0.000000 )
(  0.060927  0.000000   0.028495  0.000000  -0.295062  0.000000 )
( -0.060927  0.000000  -0.028495  0.000000   0.295062  0.000000 )
( -0.094150  0.000000   0.043800  0.000000   0.003158  0.000000 )
(  0.094150  0.000000  -0.043800  0.000000  -0.003158  0.000000 )
  freq ( 39) =   15.066761 [THz] =   502.573034 [cm-1]
( -0.020133  0.000000  -0.009077  0.000000  -0.032755  0.000000 )
( -0.020133  0.000000  -0.009077  0.000000  -0.032755  0.000000 )
(  0.010797  0.000000   0.030986  0.000000   0.021572  0.000000 )
(  0.010797  0.000000   0.030986  0.000000   0.021572  0.000000 )

```

```

( -0.042342  0.000000  -0.012164  0.000000  -0.030299  0.000000  )
(  0.027536  0.000000   0.002004  0.000000  -0.029358  0.000000  )
(  0.027536  0.000000   0.002004  0.000000  -0.029358  0.000000  )
( -0.286702  0.000000  -0.309745  0.000000  -0.019127  0.000000  )
( -0.286702  0.000000  -0.309745  0.000000  -0.019127  0.000000  )
(  0.054158  0.000000  -0.010854  0.000000   0.052651  0.000000  )
(  0.054158  0.000000  -0.010854  0.000000   0.052651  0.000000  )
(  0.201889  0.000000   0.327550  0.000000   0.000983  0.000000  )
(  0.201889  0.000000   0.327550  0.000000   0.000983  0.000000  )
( -0.017192  0.000000  -0.003886  0.000000  -0.019107  0.000000  )
( -0.017192  0.000000  -0.003886  0.000000  -0.019107  0.000000  )
(  0.028602  0.000000  -0.045010  0.000000   0.307880  0.000000  )
(  0.028602  0.000000  -0.045010  0.000000   0.307880  0.000000  )
(  0.027318  0.000000   0.007142  0.000000  -0.239452  0.000000  )
(  0.027318  0.000000   0.007142  0.000000  -0.239452  0.000000  )
( -0.021303  0.000000   0.040320  0.000000   0.054239  0.000000  )
( -0.021303  0.000000   0.040320  0.000000   0.054239  0.000000  )
  freq ( 40) =  15.080014 [THz] =  503.015128 [cm-1]
( -0.007397  0.000000   0.045495  0.000000  -0.033550  0.000000  )
( -0.007397  0.000000   0.045495  0.000000  -0.033550  0.000000  )
(  0.036111  0.000000   0.012359  0.000000  -0.030652  0.000000  )
(  0.036111  0.000000   0.012359  0.000000  -0.030652  0.000000  )
( -0.069398  0.000000  -0.117600  0.000000  -0.109313  0.000000  )
(  0.032474  0.000000   0.063170  0.000000  -0.100295  0.000000  )
(  0.032474  0.000000   0.063170  0.000000  -0.100295  0.000000  )
( -0.271986  0.000000   0.155650  0.000000  -0.019214  0.000000  )
( -0.271986  0.000000   0.155650  0.000000  -0.019214  0.000000  )
(  0.037645  0.000000   0.076565  0.000000   0.213307  0.000000  )
(  0.037645  0.000000   0.076565  0.000000   0.213307  0.000000  )
(  0.218522  0.000000  -0.282608  0.000000  -0.046372  0.000000  )
(  0.218522  0.000000  -0.282608  0.000000  -0.046372  0.000000  )
( -0.027898  0.000000  -0.041489  0.000000  -0.199650  0.000000  )
( -0.027898  0.000000  -0.041489  0.000000  -0.199650  0.000000  )
(  0.032974  0.000000  -0.030229  0.000000   0.143218  0.000000  )
(  0.032974  0.000000  -0.030229  0.000000   0.143218  0.000000  )
( -0.039838  0.000000   0.008245  0.000000   0.243481  0.000000  )
( -0.039838  0.000000   0.008245  0.000000   0.243481  0.000000  )
(  0.057101  0.000000   0.090056  0.000000   0.213659  0.000000  )
(  0.057101  0.000000   0.090056  0.000000   0.213659  0.000000  )
  freq ( 41) =  15.184971 [THz] =  506.516111 [cm-1]
( -0.013576  0.000000   0.026492  0.000000   0.007232  0.000000  )
(  0.013576  0.000000  -0.026492  0.000000  -0.007232  0.000000  )
(  0.033779  0.000000   0.003885  0.000000  -0.005256  0.000000  )
( -0.033779  0.000000  -0.003885  0.000000   0.005256  0.000000  )
( -0.000000  0.000000  -0.000000  0.000000  -0.000000  0.000000  )
(  0.047524  0.000000  -0.032425  0.000000  -0.001317  0.000000  )
( -0.047524  0.000000   0.032425  0.000000   0.001317  0.000000  )
( -0.346565  0.000000   0.190659  0.000000  -0.004164  0.000000  )
(  0.346565  0.000000  -0.190659  0.000000   0.004164  0.000000  )
( -0.008035  0.000000  -0.006000  0.000000  -0.121480  0.000000  )

```

```
( 0.008035 0.000000 0.006000 0.000000 0.121480 0.000000 )
( 0.346469 0.000000 -0.190691 0.000000 -0.005598 0.000000 )
( -0.346469 0.000000 0.190691 0.000000 0.005598 0.000000 )
( -0.023215 0.000000 -0.033372 0.000000 -0.303079 0.000000 )
( 0.023215 0.000000 0.033372 0.000000 0.303079 0.000000 )
( 0.017410 0.000000 -0.020942 0.000000 0.163669 0.000000 )
( -0.017410 0.000000 0.020942 0.000000 -0.163669 0.000000 )
( -0.028176 0.000000 0.003821 0.000000 0.154247 0.000000 )
( 0.028176 0.000000 -0.003821 0.000000 -0.154247 0.000000 )
( 0.042844 0.000000 0.072644 0.000000 -0.118515 0.000000 )
( -0.042844 0.000000 -0.072644 0.000000 0.118515 0.000000 )
```

freq (42) = 19.543291 [THz] = 651.894014 [cm-1]

```
( -0.001933 0.000000 -0.006913 0.000000 0.166207 0.000000 )
( 0.001933 0.000000 0.006913 0.000000 -0.166207 0.000000 )
( 0.002799 0.000000 0.001765 0.000000 0.166478 0.000000 )
( -0.002799 0.000000 -0.001765 0.000000 -0.166478 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.027331 0.000000 -0.015783 0.000000 -0.000578 0.000000 )
( -0.027331 0.000000 0.015783 0.000000 0.000578 0.000000 )
( -0.016217 0.000000 -0.013216 0.000000 0.271332 0.000000 )
( 0.016217 0.000000 0.013216 0.000000 -0.271332 0.000000 )
( 0.007769 0.000000 0.012413 0.000000 0.050657 0.000000 )
( -0.007769 0.000000 -0.012413 0.000000 -0.050657 0.000000 )
( 0.007245 0.000000 -0.020650 0.000000 0.270452 0.000000 )
( -0.007245 0.000000 0.020650 0.000000 -0.270452 0.000000 )
( -0.011322 0.000000 -0.010111 0.000000 -0.310839 0.000000 )
( 0.011322 0.000000 0.010111 0.000000 0.310839 0.000000 )
( -0.005527 0.000000 0.023371 0.000000 -0.302420 0.000000 )
( 0.005527 0.000000 -0.023371 0.000000 0.302420 0.000000 )
( 0.017283 0.000000 0.012448 0.000000 -0.307047 0.000000 )
( -0.017283 0.000000 -0.012448 0.000000 0.307047 0.000000 )
( -0.041908 0.000000 -0.078794 0.000000 0.039459 0.000000 )
( 0.041908 0.000000 0.078794 0.000000 -0.039459 0.000000 )
```

freq (43) = 19.907964 [THz] = 664.058197 [cm-1]

```
( 0.013047 0.000000 0.003972 0.000000 0.208945 0.000000 )
( 0.013047 0.000000 0.003972 0.000000 0.208945 0.000000 )
( -0.012728 0.000000 -0.013603 0.000000 0.206662 0.000000 )
( -0.012728 0.000000 -0.013603 0.000000 0.206662 0.000000 )
( 0.008184 0.000000 0.020565 0.000000 -0.213353 0.000000 )
( -0.002844 0.000000 0.002654 0.000000 -0.222143 0.000000 )
( -0.002844 0.000000 0.002654 0.000000 -0.222143 0.000000 )
( -0.003372 0.000000 -0.008404 0.000000 0.195608 0.000000 )
( -0.003372 0.000000 -0.008404 0.000000 0.195608 0.000000 )
( 0.004534 0.000000 0.005126 0.000000 0.149780 0.000000 )
( 0.004534 0.000000 0.005126 0.000000 0.149780 0.000000 )
( -0.002266 0.000000 -0.015707 0.000000 0.197390 0.000000 )
( -0.002266 0.000000 -0.015707 0.000000 0.197390 0.000000 )
( -0.009446 0.000000 -0.007884 0.000000 -0.262071 0.000000 )
( -0.009446 0.000000 -0.007884 0.000000 -0.262071 0.000000 )
( -0.004313 0.000000 0.020802 0.000000 -0.256214 0.000000 )
```

```

( -0.004313  0.000000  0.020802  0.000000  -0.256214  0.000000 )
(  0.015240  0.000000  0.011231  0.000000  -0.263068  0.000000 )
(  0.015240  0.000000  0.011231  0.000000  -0.263068  0.000000 )
( -0.044038  0.000000  -0.126689  0.000000   0.134947  0.000000 )
( -0.044038  0.000000  -0.126689  0.000000   0.134947  0.000000 )
  freq ( 44) = 20.623179 [THz] = 687.915189 [cm-1]
( -0.010569  0.000000  0.013152  0.000000   0.001691  0.000000 )
( -0.010569  0.000000  0.013152  0.000000   0.001691  0.000000 )
(  0.016977  0.000000  0.006405  0.000000  -0.000318  0.000000 )
(  0.016977  0.000000  0.006405  0.000000  -0.000318  0.000000 )
(  0.000221  0.000000  -0.000469  0.000000   0.023184  0.000000 )
(  0.000211  0.000000  0.000232  0.000000  -0.006170  0.000000 )
(  0.000211  0.000000  0.000232  0.000000  -0.006170  0.000000 )
( -0.005079  0.000000  -0.014102  0.000000  -0.003627  0.000000 )
( -0.005079  0.000000  -0.014102  0.000000  -0.003627  0.000000 )
(  0.014199  0.000000  0.045539  0.000000  -0.005788  0.000000 )
(  0.014199  0.000000  0.045539  0.000000  -0.005788  0.000000 )
( -0.003699  0.000000  -0.010664  0.000000  -0.005567  0.000000 )
( -0.003699  0.000000  -0.010664  0.000000  -0.005567  0.000000 )
( -0.012084  0.000000  -0.016196  0.000000   0.011132  0.000000 )
( -0.012084  0.000000  -0.016196  0.000000   0.011132  0.000000 )
(  0.013988  0.000000  -0.007450  0.000000  -0.004222  0.000000 )
(  0.013988  0.000000  -0.007450  0.000000  -0.004222  0.000000 )
( -0.006408  0.000000  0.010988  0.000000  -0.000330  0.000000 )
( -0.006408  0.000000  0.010988  0.000000  -0.000330  0.000000 )
( -0.200727  0.000000  -0.673621  0.000000  -0.036756  0.000000 )
( -0.200727  0.000000  -0.673621  0.000000  -0.036756  0.000000 )
  freq ( 45) = 20.726129 [THz] = 691.349232 [cm-1]
(  0.013872  0.000000  0.007506  0.000000  -0.003495  0.000000 )
(  0.013872  0.000000  0.007506  0.000000  -0.003495  0.000000 )
(  0.005697  0.000000  -0.012994  0.000000   0.003770  0.000000 )
(  0.005697  0.000000  -0.012994  0.000000   0.003770  0.000000 )
( -0.000006  0.000000  -0.000076  0.000000   0.005113  0.000000 )
( -0.000315  0.000000  0.000381  0.000000  -0.001840  0.000000 )
( -0.000315  0.000000  0.000381  0.000000  -0.001840  0.000000 )
( -0.006695  0.000000  0.008211  0.000000  -0.005875  0.000000 )
( -0.006695  0.000000  0.008211  0.000000  -0.005875  0.000000 )
(  0.042405  0.000000  -0.012065  0.000000  -0.001485  0.000000 )
(  0.042405  0.000000  -0.012065  0.000000  -0.001485  0.000000 )
( -0.013852  0.000000  -0.003258  0.000000   0.004156  0.000000 )
( -0.013852  0.000000  -0.003258  0.000000   0.004156  0.000000 )
(  0.006356  0.000000  -0.009453  0.000000   0.001706  0.000000 )
(  0.006356  0.000000  -0.009453  0.000000   0.001706  0.000000 )
( -0.000070  0.000000  0.016413  0.000000   0.005197  0.000000 )
( -0.000070  0.000000  0.016413  0.000000   0.005197  0.000000 )
( -0.019534  0.000000  -0.003592  0.000000  -0.005424  0.000000 )
( -0.019534  0.000000  -0.003592  0.000000  -0.005424  0.000000 )
( -0.674354  0.000000  0.203872  0.000000   0.004963  0.000000 )
( -0.674354  0.000000  0.203872  0.000000   0.004963  0.000000 )
  freq ( 46) = 20.813365 [THz] = 694.259128 [cm-1]

```



```

( 0.013890 0.000000 0.004699 0.000000 0.004721 0.000000 )
( -0.013890 0.000000 -0.004699 0.000000 -0.004721 0.000000 )
( 0.002474 0.000000 -0.017339 0.000000 -0.004239 0.000000 )
( -0.002474 0.000000 0.017339 0.000000 0.004239 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( -0.000041 0.000000 -0.000612 0.000000 0.016609 0.000000 )
( 0.000041 0.000000 0.000612 0.000000 -0.016609 0.000000 )
( -0.013892 0.000000 0.010802 0.000000 0.006281 0.000000 )
( 0.013892 0.000000 -0.010802 0.000000 -0.006281 0.000000 )
( 0.036805 0.000000 -0.026530 0.000000 -0.001062 0.000000 )
( -0.036805 0.000000 0.026530 0.000000 0.001062 0.000000 )
( -0.015386 0.000000 0.009764 0.000000 -0.004832 0.000000 )
( 0.015386 0.000000 -0.009764 0.000000 0.004832 0.000000 )
( 0.011478 0.000000 -0.003472 0.000000 -0.000859 0.000000 )
( -0.011478 0.000000 0.003472 0.000000 0.000859 0.000000 )
( -0.005996 0.000000 0.017734 0.000000 0.007155 0.000000 )
( 0.005996 0.000000 -0.017734 0.000000 -0.007155 0.000000 )
( -0.015880 0.000000 -0.005796 0.000000 -0.007790 0.000000 )
( 0.015880 0.000000 0.005796 0.000000 0.007790 0.000000 )
( -0.563997 0.000000 0.420917 0.000000 0.015543 0.000000 )
( 0.563997 0.000000 -0.420917 0.000000 -0.015543 0.000000 )

```

freq (47) = 20.951738 [THz] = 698.874753 [cm-1]

```

( -0.005439 0.000000 0.017180 0.000000 -0.001711 0.000000 )
( 0.005439 0.000000 -0.017180 0.000000 0.001711 0.000000 )
( 0.016232 0.000000 -0.001830 0.000000 -0.003052 0.000000 )
( -0.016232 0.000000 0.001830 0.000000 0.003052 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( -0.000214 0.000000 0.000165 0.000000 0.001741 0.000000 )
( 0.000214 0.000000 -0.000165 0.000000 -0.001741 0.000000 )
( -0.013460 0.000000 -0.006871 0.000000 -0.001448 0.000000 )
( 0.013460 0.000000 0.006871 0.000000 0.001448 0.000000 )
( 0.022932 0.000000 0.029739 0.000000 0.007616 0.000000 )
( -0.022932 0.000000 -0.029739 0.000000 -0.007616 0.000000 )
( -0.003113 0.000000 -0.013943 0.000000 -0.003361 0.000000 )
( 0.003113 0.000000 0.013943 0.000000 0.003361 0.000000 )
( -0.008186 0.000000 -0.017069 0.000000 0.010088 0.000000 )
( 0.008186 0.000000 0.017069 0.000000 -0.010088 0.000000 )
( 0.012530 0.000000 -0.001951 0.000000 0.000092 0.000000 )
( -0.012530 0.000000 0.001951 0.000000 -0.000092 0.000000 )
( -0.011022 0.000000 0.008774 0.000000 -0.001756 0.000000 )
( 0.011022 0.000000 -0.008774 0.000000 0.001756 0.000000 )
( -0.417132 0.000000 -0.567699 0.000000 -0.019377 0.000000 )
( 0.417132 0.000000 0.567699 0.000000 0.019377 0.000000 )

```

freq (48) = 22.423367 [THz] = 747.963028 [cm-1]

```

( -0.339576 0.000000 -0.167720 0.000000 -0.009138 0.000000 )
( -0.339576 0.000000 -0.167720 0.000000 -0.009138 0.000000 )
( 0.363560 0.000000 0.118322 0.000000 0.011704 0.000000 )
( 0.363560 0.000000 0.118322 0.000000 0.011704 0.000000 )
( 0.005109 0.000000 0.000849 0.000000 -0.026693 0.000000 )
( -0.002079 0.000000 -0.001403 0.000000 0.003440 0.000000 )

```

```
( -0.002079 0.000000 -0.001403 0.000000 0.003440 0.000000 )
( -0.070898 0.000000 -0.017466 0.000000 0.012731 0.000000 )
( -0.070898 0.000000 -0.017466 0.000000 0.012731 0.000000 )
( 0.007769 0.000000 -0.022243 0.000000 0.003802 0.000000 )
( 0.007769 0.000000 -0.022243 0.000000 0.003802 0.000000 )
( 0.063581 0.000000 0.035660 0.000000 0.031243 0.000000 )
( 0.063581 0.000000 0.035660 0.000000 0.031243 0.000000 )
( 0.015499 0.000000 0.022907 0.000000 0.101910 0.000000 )
( 0.015499 0.000000 0.022907 0.000000 0.101910 0.000000 )
( -0.027905 0.000000 0.052284 0.000000 -0.198504 0.000000 )
( -0.027905 0.000000 0.052284 0.000000 -0.198504 0.000000 )
( -0.023553 0.000000 -0.005298 0.000000 0.058222 0.000000 )
( -0.023553 0.000000 -0.005298 0.000000 0.058222 0.000000 )
( -0.116185 0.000000 0.354263 0.000000 0.019481 0.000000 )
( -0.116185 0.000000 0.354263 0.000000 0.019481 0.000000 )
```

freq (49) = 22.541634 [THz] = 751.907963 [cm-1]

```
( 0.152389 0.000000 -0.328025 0.000000 -0.007944 0.000000 )
( -0.152389 0.000000 0.328025 0.000000 0.007944 0.000000 )
( -0.102941 0.000000 0.347827 0.000000 0.003373 0.000000 )
( 0.102941 0.000000 -0.347827 0.000000 -0.003373 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.002985 0.000000 -0.001376 0.000000 0.017463 0.000000 )
( -0.002985 0.000000 0.001376 0.000000 -0.017463 0.000000 )
( 0.013419 0.000000 -0.069027 0.000000 -0.023675 0.000000 )
( -0.013419 0.000000 0.069027 0.000000 0.023675 0.000000 )
( 0.020087 0.000000 0.008187 0.000000 0.004295 0.000000 )
( -0.020087 0.000000 -0.008187 0.000000 -0.004295 0.000000 )
( -0.035027 0.000000 0.061067 0.000000 0.017631 0.000000 )
( 0.035027 0.000000 -0.061067 0.000000 -0.017631 0.000000 )
( -0.022039 0.000000 -0.029832 0.000000 -0.137039 0.000000 )
( 0.022039 0.000000 0.029832 0.000000 0.137039 0.000000 )
( 0.004282 0.000000 0.011865 0.000000 -0.025999 0.000000 )
( -0.004282 0.000000 -0.011865 0.000000 0.025999 0.000000 )
( -0.048754 0.000000 -0.009058 0.000000 0.172342 0.000000 )
( 0.048754 0.000000 0.009058 0.000000 -0.172342 0.000000 )
( -0.387097 0.000000 -0.151436 0.000000 -0.004103 0.000000 )
( 0.387097 0.000000 0.151436 0.000000 0.004103 0.000000 )
```

freq (50) = 22.655103 [THz] = 755.692882 [cm-1]

```
( 0.168007 0.000000 -0.357452 0.000000 -0.018302 0.000000 )
( 0.168007 0.000000 -0.357452 0.000000 -0.018302 0.000000 )
( -0.128503 0.000000 0.372587 0.000000 0.020639 0.000000 )
( -0.128503 0.000000 0.372587 0.000000 0.020639 0.000000 )
( -0.000199 0.000000 -0.004479 0.000000 0.025483 0.000000 )
( 0.001638 0.000000 0.002809 0.000000 -0.012530 0.000000 )
( 0.001638 0.000000 0.002809 0.000000 -0.012530 0.000000 )
( 0.020015 0.000000 -0.075624 0.000000 0.020084 0.000000 )
( 0.020015 0.000000 -0.075624 0.000000 0.020084 0.000000 )
( 0.016446 0.000000 0.008916 0.000000 -0.003153 0.000000 )
( 0.016446 0.000000 0.008916 0.000000 -0.003153 0.000000 )
( -0.036735 0.000000 0.067539 0.000000 -0.013464 0.000000 )
```

```
( -0.036735 0.000000 0.067539 0.000000 -0.013464 0.000000 )
( -0.009272 0.000000 -0.028603 0.000000 -0.161636 0.000000 )
( -0.009272 0.000000 -0.028603 0.000000 -0.161636 0.000000 )
( -0.002291 0.000000 0.006976 0.000000 -0.031019 0.000000 )
( -0.002291 0.000000 0.006976 0.000000 -0.031019 0.000000 )
( -0.041405 0.000000 0.003295 0.000000 0.185494 0.000000 )
( -0.041405 0.000000 0.003295 0.000000 0.185494 0.000000 )
( -0.292102 0.000000 -0.157474 0.000000 -0.011290 0.000000 )
( -0.292102 0.000000 -0.157474 0.000000 -0.011290 0.000000 )
```

freq (51) = 22.752533 [THz] = 758.942801 [cm-1]

```
( 0.360976 0.000000 0.161432 0.000000 0.001088 0.000000 )
( -0.360976 0.000000 -0.161432 0.000000 -0.001088 0.000000 )
( -0.373864 0.000000 -0.117634 0.000000 -0.002964 0.000000 )
( 0.373864 0.000000 0.117634 0.000000 0.002964 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.000610 0.000000 -0.003524 0.000000 -0.020448 0.000000 )
( -0.000610 0.000000 0.003524 0.000000 0.020448 0.000000 )
( 0.073139 0.000000 0.015632 0.000000 -0.002049 0.000000 )
( -0.073139 0.000000 -0.015632 0.000000 0.002049 0.000000 )
( -0.005190 0.000000 0.017938 0.000000 0.003216 0.000000 )
( 0.005190 0.000000 -0.017938 0.000000 -0.003216 0.000000 )
( -0.065715 0.000000 -0.036733 0.000000 0.009269 0.000000 )
( 0.065715 0.000000 0.036733 0.000000 -0.009269 0.000000 )
( -0.017314 0.000000 -0.020779 0.000000 -0.132799 0.000000 )
( 0.017314 0.000000 0.020779 0.000000 0.132799 0.000000 )
( 0.022410 0.000000 -0.042769 0.000000 0.200625 0.000000 )
( -0.022410 0.000000 0.042769 0.000000 -0.200625 0.000000 )
( 0.010587 0.000000 0.005075 0.000000 -0.075364 0.000000 )
( -0.010587 0.000000 -0.005075 0.000000 0.075364 0.000000 )
( 0.086137 0.000000 -0.321843 0.000000 -0.010193 0.000000 )
( -0.086137 0.000000 0.321843 0.000000 0.010193 0.000000 )
```

freq (52) = 25.542176 [THz] = 851.995282 [cm-1]

```
( -0.007169 0.000000 0.015134 0.000000 -0.197158 0.000000 )
( 0.007169 0.000000 -0.015134 0.000000 0.197158 0.000000 )
( 0.003965 0.000000 -0.018352 0.000000 0.198200 0.000000 )
( -0.003965 0.000000 0.018352 0.000000 -0.198200 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.004958 0.000000 0.008856 0.000000 0.004023 0.000000 )
( -0.004958 0.000000 -0.008856 0.000000 -0.004023 0.000000 )
( -0.001032 0.000000 -0.007440 0.000000 -0.433868 0.000000 )
( 0.001032 0.000000 0.007440 0.000000 0.433868 0.000000 )
( -0.013599 0.000000 0.007345 0.000000 -0.000107 0.000000 )
( 0.013599 0.000000 -0.007345 0.000000 0.000107 0.000000 )
( 0.022408 0.000000 -0.002921 0.000000 0.432442 0.000000 )
( -0.022408 0.000000 0.002921 0.000000 -0.432442 0.000000 )
( -0.043512 0.000000 0.027243 0.000000 0.007103 0.000000 )
( 0.043512 0.000000 -0.027243 0.000000 -0.007103 0.000000 )
( 0.050054 0.000000 0.031668 0.000000 0.002412 0.000000 )
( -0.050054 0.000000 -0.031668 0.000000 -0.002412 0.000000 )
( -0.000293 0.000000 -0.055077 0.000000 -0.010674 0.000000 )
```

```

( 0.000293 0.000000 0.055077 0.000000 0.010674 0.000000 )
( -0.159612 0.000000 0.101023 0.000000 0.003313 0.000000 )
( 0.159612 0.000000 -0.101023 0.000000 -0.003313 0.000000 )
freq ( 53) = 25.561087 [THz] = 852.626072 [cm-1]
( -0.005195 0.000000 0.000419 0.000000 0.195765 0.000000 )
( -0.005195 0.000000 0.000419 0.000000 0.195765 0.000000 )
( 0.008828 0.000000 -0.002097 0.000000 -0.202279 0.000000 )
( 0.008828 0.000000 -0.002097 0.000000 -0.202279 0.000000 )
( 0.011405 0.000000 -0.006549 0.000000 -0.001242 0.000000 )
( -0.004009 0.000000 0.002536 0.000000 -0.000011 0.000000 )
( -0.004009 0.000000 0.002536 0.000000 -0.000011 0.000000 )
( -0.005331 0.000000 -0.039328 0.000000 0.437907 0.000000 )
( -0.005331 0.000000 -0.039328 0.000000 0.437907 0.000000 )
( -0.013488 0.000000 0.007173 0.000000 -0.000195 0.000000 )
( -0.013488 0.000000 0.007173 0.000000 -0.000195 0.000000 )
( 0.021749 0.000000 0.028780 0.000000 -0.424473 0.000000 )
( 0.021749 0.000000 0.028780 0.000000 -0.424473 0.000000 )
( 0.048931 0.000000 -0.025702 0.000000 0.005380 0.000000 )
( 0.048931 0.000000 -0.025702 0.000000 0.005380 0.000000 )
( -0.050053 0.000000 -0.026001 0.000000 -0.000119 0.000000 )
( -0.050053 0.000000 -0.026001 0.000000 -0.000119 0.000000 )
( -0.000407 0.000000 0.052934 0.000000 -0.006278 0.000000 )
( -0.000407 0.000000 0.052934 0.000000 -0.006278 0.000000 )
( -0.163672 0.000000 0.097904 0.000000 0.003155 0.000000 )
( -0.163672 0.000000 0.097904 0.000000 0.003155 0.000000 )
freq ( 54) = 26.541321 [THz] = 885.323158 [cm-1]
( 0.006706 0.000000 0.016587 0.000000 -0.240499 0.000000 )
( 0.006706 0.000000 0.016587 0.000000 -0.240499 0.000000 )
( -0.007204 0.000000 0.004207 0.000000 -0.233000 0.000000 )
( -0.007204 0.000000 0.004207 0.000000 -0.233000 0.000000 )
( -0.003624 0.000000 -0.004837 0.000000 -0.023937 0.000000 )
( 0.002531 0.000000 0.004741 0.000000 -0.027285 0.000000 )
( 0.002531 0.000000 0.004741 0.000000 -0.027285 0.000000 )
( 0.011681 0.000000 -0.015266 0.000000 0.426113 0.000000 )
( 0.011681 0.000000 -0.015266 0.000000 0.426113 0.000000 )
( -0.003994 0.000000 -0.006314 0.000000 -0.011448 0.000000 )
( -0.003994 0.000000 -0.006314 0.000000 -0.011448 0.000000 )
( -0.008377 0.000000 -0.006692 0.000000 0.439291 0.000000 )
( -0.008377 0.000000 -0.006692 0.000000 0.439291 0.000000 )
( -0.000202 0.000000 -0.001433 0.000000 0.010184 0.000000 )
( -0.000202 0.000000 -0.001433 0.000000 0.010184 0.000000 )
( 0.004904 0.000000 -0.004341 0.000000 0.020086 0.000000 )
( 0.004904 0.000000 -0.004341 0.000000 0.020086 0.000000 )
( -0.001448 0.000000 -0.000118 0.000000 0.007309 0.000000 )
( -0.001448 0.000000 -0.000118 0.000000 0.007309 0.000000 )
( -0.043072 0.000000 -0.092702 0.000000 -0.011259 0.000000 )
( -0.043072 0.000000 -0.092702 0.000000 -0.011259 0.000000 )
freq ( 55) = 28.737754 [THz] = 958.588297 [cm-1]
( -0.125923 0.000000 -0.152775 0.000000 -0.003997 0.000000 )
( -0.125923 0.000000 -0.152775 0.000000 -0.003997 0.000000 )

```

```

( -0.137419  0.000000  -0.144754  0.000000  -0.006973  0.000000  )
( -0.137419  0.000000  -0.144754  0.000000  -0.006973  0.000000  )
(  0.000283  0.000000  -0.000771  0.000000  -0.004080  0.000000  )
(  0.001133  0.000000   0.001811  0.000000   0.001889  0.000000  )
(  0.001133  0.000000   0.001811  0.000000   0.001889  0.000000  )
( -0.012475  0.000000  -0.009481  0.000000   0.001213  0.000000  )
( -0.012475  0.000000  -0.009481  0.000000   0.001213  0.000000  )
( -0.002131  0.000000  -0.002356  0.000000   0.000176  0.000000  )
( -0.002131  0.000000  -0.002356  0.000000   0.000176  0.000000  )
( -0.007594  0.000000  -0.013531  0.000000  -0.002428  0.000000  )
( -0.007594  0.000000  -0.013531  0.000000  -0.002428  0.000000  )
(  0.069544  0.000000  -0.087550  0.000000   0.000724  0.000000  )
(  0.069544  0.000000  -0.087550  0.000000   0.000724  0.000000  )
(  0.438881  0.000000   0.238842  0.000000   0.008774  0.000000  )
(  0.438881  0.000000   0.238842  0.000000   0.008774  0.000000  )
( -0.028556  0.000000   0.391158  0.000000   0.010851  0.000000  )
( -0.028556  0.000000   0.391158  0.000000   0.010851  0.000000  )
(  0.042580  0.000000   0.048801  0.000000   0.002521  0.000000  )
(  0.042580  0.000000   0.048801  0.000000   0.002521  0.000000  )
  freq ( 56) =   28.740466 [THz] =   958.678765 [cm-1]
(  0.154349  0.000000   0.125512  0.000000   0.002624  0.000000  )
( -0.154349  0.000000  -0.125512  0.000000  -0.002624  0.000000  )
(  0.166515  0.000000   0.108283  0.000000   0.007833  0.000000  )
( -0.166515  0.000000  -0.108283  0.000000  -0.007833  0.000000  )
( -0.000000  0.000000   0.000000  0.000000   0.000000  0.000000  )
( -0.001594  0.000000   0.000338  0.000000   0.001389  0.000000  )
(  0.001594  0.000000  -0.000338  0.000000  -0.001389  0.000000  )
(  0.013718  0.000000   0.007032  0.000000  -0.003551  0.000000  )
( -0.013718  0.000000  -0.007032  0.000000   0.003551  0.000000  )
(  0.002270  0.000000   0.001692  0.000000   0.000226  0.000000  )
( -0.002270  0.000000  -0.001692  0.000000  -0.000226  0.000000  )
(  0.010913  0.000000   0.010921  0.000000   0.001297  0.000000  )
( -0.010913  0.000000  -0.010921  0.000000  -0.001297  0.000000  )
( -0.161560  0.000000   0.137215  0.000000   0.005385  0.000000  )
(  0.161560  0.000000  -0.137215  0.000000  -0.005385  0.000000  )
( -0.457184  0.000000  -0.259649  0.000000  -0.009861  0.000000  )
(  0.457184  0.000000   0.259649  0.000000   0.009861  0.000000  )
(  0.033423  0.000000  -0.305081  0.000000  -0.011762  0.000000  )
( -0.033423  0.000000   0.305081  0.000000   0.011762  0.000000  )
( -0.054637  0.000000  -0.039880  0.000000  -0.001821  0.000000  )
(  0.054637  0.000000   0.039880  0.000000   0.001821  0.000000  )
  freq ( 57) =   28.805323 [THz] =   960.842153 [cm-1]
(  0.157335  0.000000  -0.123760  0.000000  -0.007160  0.000000  )
(  0.157335  0.000000  -0.123760  0.000000  -0.007160  0.000000  )
(  0.139900  0.000000  -0.139295  0.000000  -0.002867  0.000000  )
(  0.139900  0.000000  -0.139295  0.000000  -0.002867  0.000000  )
( -0.003095  0.000000   0.001662  0.000000  -0.000814  0.000000  )
(  0.000048  0.000000   0.000508  0.000000   0.000147  0.000000  )
(  0.000048  0.000000   0.000508  0.000000   0.000147  0.000000  )
(  0.010485  0.000000  -0.012219  0.000000  -0.000396  0.000000  )

```

```

( 0.010485 0.000000 -0.012219 0.000000 -0.000396 0.000000 )
( 0.002211 0.000000 -0.001972 0.000000 0.000064 0.000000 )
( 0.002211 0.000000 -0.001972 0.000000 0.000064 0.000000 )
( 0.013057 0.000000 -0.008949 0.000000 0.001641 0.000000 )
( 0.013057 0.000000 -0.008949 0.000000 0.001641 0.000000 )
( -0.445351 0.000000 0.247173 0.000000 0.006398 0.000000 )
( -0.445351 0.000000 0.247173 0.000000 0.006398 0.000000 )
( -0.128270 0.000000 -0.120368 0.000000 -0.003594 0.000000 )
( -0.128270 0.000000 -0.120368 0.000000 -0.003594 0.000000 )
( 0.031307 0.000000 0.353506 0.000000 0.013753 0.000000 )
( 0.031307 0.000000 0.353506 0.000000 0.013753 0.000000 )
( -0.046447 0.000000 0.040535 0.000000 0.001661 0.000000 )
( -0.046447 0.000000 0.040535 0.000000 0.001661 0.000000 )
freq ( 58) = 28.860380 [THz] = 962.678659 [cm-1]
( 0.123834 0.000000 -0.153601 0.000000 -0.009026 0.000000 )
( -0.123834 0.000000 0.153601 0.000000 0.009026 0.000000 )
( 0.109484 0.000000 -0.164995 0.000000 -0.006191 0.000000 )
( -0.109484 0.000000 0.164995 0.000000 0.006191 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( -0.000079 0.000000 -0.001570 0.000000 0.003045 0.000000 )
( 0.000079 0.000000 0.001570 0.000000 -0.003045 0.000000 )
( 0.006647 0.000000 -0.014202 0.000000 0.002894 0.000000 )
( -0.006647 0.000000 0.014202 0.000000 -0.002894 0.000000 )
( 0.001718 0.000000 -0.002220 0.000000 0.000123 0.000000 )
( -0.001718 0.000000 0.002220 0.000000 -0.000123 0.000000 )
( 0.011456 0.000000 -0.010994 0.000000 0.004395 0.000000 )
( -0.011456 0.000000 0.010994 0.000000 -0.004395 0.000000 )
( -0.419998 0.000000 0.223299 0.000000 0.007766 0.000000 )
( 0.419998 0.000000 -0.223299 0.000000 -0.007766 0.000000 )
( -0.031372 0.000000 -0.066656 0.000000 -0.003584 0.000000 )
( 0.031372 0.000000 0.066656 0.000000 0.003584 0.000000 )
( 0.023468 0.000000 0.429521 0.000000 0.015614 0.000000 )
( -0.023468 0.000000 -0.429521 0.000000 -0.015614 0.000000 )
( -0.037140 0.000000 0.052603 0.000000 0.002472 0.000000 )
( 0.037140 0.000000 -0.052603 0.000000 -0.002472 0.000000 )
freq ( 59) = 29.902659 [THz] = 997.445332 [cm-1]
( 0.001728 0.000000 -0.009963 0.000000 0.262854 0.000000 )
( -0.001728 0.000000 0.009963 0.000000 -0.262854 0.000000 )
( -0.001883 0.000000 -0.011849 0.000000 0.263014 0.000000 )
( 0.001883 0.000000 0.011849 0.000000 -0.263014 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.002827 0.000000 -0.001518 0.000000 -0.000092 0.000000 )
( -0.002827 0.000000 0.001518 0.000000 0.000092 0.000000 )
( 0.011258 0.000000 0.014487 0.000000 -0.409751 0.000000 )
( -0.011258 0.000000 -0.014487 0.000000 0.409751 0.000000 )
( -0.003300 0.000000 -0.004538 0.000000 -0.031938 0.000000 )
( 0.003300 0.000000 0.004538 0.000000 0.031938 0.000000 )
( -0.005412 0.000000 0.022039 0.000000 -0.411287 0.000000 )
( 0.005412 0.000000 -0.022039 0.000000 0.411287 0.000000 )
( -0.004211 0.000000 -0.000437 0.000000 -0.076553 0.000000 )

```

```

( 0.004211 0.000000 0.000437 0.000000 0.076553 0.000000 )
( -0.001168 0.000000 0.004648 0.000000 -0.076141 0.000000 )
( 0.001168 0.000000 -0.004648 0.000000 0.076141 0.000000 )
( 0.004233 0.000000 0.010347 0.000000 -0.077735 0.000000 )
( -0.004233 0.000000 -0.010347 0.000000 0.077735 0.000000 )
( -0.023007 0.000000 -0.041046 0.000000 -0.049385 0.000000 )
( 0.023007 0.000000 0.041046 0.000000 0.049385 0.000000 )
  freq ( 60 ) = 31.334355 [THz] = 1045.201569 [cm-1]
( 0.000680 0.000000 -0.000331 0.000000 0.103034 0.000000 )
( -0.000680 0.000000 0.000331 0.000000 -0.103034 0.000000 )
( 0.004397 0.000000 -0.001676 0.000000 -0.101052 0.000000 )
( -0.004397 0.000000 0.001676 0.000000 0.101052 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 )
( -0.009314 0.000000 -0.016096 0.000000 -0.000680 0.000000 )
( 0.009314 0.000000 0.016096 0.000000 0.000680 0.000000 )
( 0.000514 0.000000 0.004505 0.000000 -0.007240 0.000000 )
( -0.000514 0.000000 -0.004505 0.000000 0.007240 0.000000 )
( 0.001699 0.000000 -0.001161 0.000000 -0.000169 0.000000 )
( -0.001699 0.000000 0.001161 0.000000 0.000169 0.000000 )
( -0.001993 0.000000 -0.002862 0.000000 0.004522 0.000000 )
( 0.001993 0.000000 0.002862 0.000000 -0.004522 0.000000 )
( -0.352149 0.000000 0.204437 0.000000 0.009956 0.000000 )
( 0.352149 0.000000 -0.204437 0.000000 -0.009956 0.000000 )
( 0.340122 0.000000 0.196397 0.000000 0.007651 0.000000 )
( -0.340122 0.000000 -0.196397 0.000000 -0.007651 0.000000 )
( 0.002020 0.000000 -0.397040 0.000000 -0.019306 0.000000 )
( -0.002020 0.000000 0.397040 0.000000 0.019306 0.000000 )
( 0.020030 0.000000 -0.007692 0.000000 -0.000388 0.000000 )
( -0.020030 0.000000 0.007692 0.000000 0.000388 0.000000 )
  freq ( 61 ) = 31.350880 [THz] = 1045.752792 [cm-1]
( 0.004522 0.000000 -0.009285 0.000000 0.100431 0.000000 )
( 0.004522 0.000000 -0.009285 0.000000 0.100431 0.000000 )
( 0.001314 0.000000 0.007494 0.000000 -0.101130 0.000000 )
( 0.001314 0.000000 0.007494 0.000000 -0.101130 0.000000 )
( 0.018341 0.000000 -0.010580 0.000000 -0.000236 0.000000 )
( -0.009373 0.000000 0.005452 0.000000 -0.000037 0.000000 )
( -0.009373 0.000000 0.005452 0.000000 -0.000037 0.000000 )
( 0.000629 0.000000 -0.004186 0.000000 -0.006106 0.000000 )
( 0.000629 0.000000 -0.004186 0.000000 -0.006106 0.000000 )
( -0.001699 0.000000 0.000994 0.000000 0.000042 0.000000 )
( -0.001699 0.000000 0.000994 0.000000 0.000042 0.000000 )
( 0.002956 0.000000 0.002471 0.000000 0.006925 0.000000 )
( 0.002956 0.000000 0.002471 0.000000 0.006925 0.000000 )
( -0.352543 0.000000 0.201746 0.000000 0.002136 0.000000 )
( -0.352543 0.000000 0.201746 0.000000 0.002136 0.000000 )
( 0.342447 0.000000 0.197663 0.000000 0.006912 0.000000 )
( 0.342447 0.000000 0.197663 0.000000 0.006912 0.000000 )
( -0.000505 0.000000 -0.396386 0.000000 -0.008474 0.000000 )
( -0.000505 0.000000 -0.396386 0.000000 -0.008474 0.000000 )
( -0.019763 0.000000 0.009639 0.000000 0.000352 0.000000 )

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( -0.019763  0.000000  0.009639  0.000000  0.000352  0.000000 )
  freq ( 62) = 110.536106 [THz] = 3687.087627 [cm-1]
( 0.000009  0.000000  0.000023  0.000000  -0.000405  0.000000 )
( -0.000009  0.000000  -0.000023  0.000000  0.000405  0.000000 )
( -0.000012  0.000000  0.000006  0.000000  -0.000401  0.000000 )
( 0.000012  0.000000  -0.000006  0.000000  0.000401  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  0.000000  0.000000 )
( -0.000155  0.000000  0.000092  0.000000  0.000002  0.000000 )
( 0.000155  0.000000  -0.000092  0.000000  -0.000002  0.000000 )
( 0.000027  0.000000  -0.000010  0.000000  0.000328  0.000000 )
( -0.000027  0.000000  0.000010  0.000000  -0.000328  0.000000 )
( -0.000177  0.000000  -0.001884  0.000000  0.044372  0.000000 )
( 0.000177  0.000000  0.001884  0.000000  -0.044372  0.000000 )
( -0.000017  0.000000  0.000008  0.000000  0.000329  0.000000 )
( 0.000017  0.000000  -0.000008  0.000000  -0.000329  0.000000 )
( 0.000002  0.000000  0.000007  0.000000  0.000262  0.000000 )
( -0.000002  0.000000  -0.000007  0.000000  -0.000262  0.000000 )
( 0.000017  0.000000  -0.000035  0.000000  0.000283  0.000000 )
( -0.000017  0.000000  0.000035  0.000000  -0.000283  0.000000 )
( -0.000016  0.000000  -0.000009  0.000000  0.000257  0.000000 )
( 0.000016  0.000000  0.000009  0.000000  -0.000257  0.000000 )
( 0.002776  0.000000  0.029912  0.000000  -0.705070  0.000000 )
( -0.002776  0.000000  -0.029912  0.000000  0.705070  0.000000 )
  freq ( 63) = 110.544790 [THz] = 3687.377276 [cm-1]
( 0.000010  0.000000  0.000002  0.000000  0.000207  0.000000 )
( 0.000010  0.000000  0.000002  0.000000  0.000207  0.000000 )
( -0.000011  0.000000  -0.000010  0.000000  0.000210  0.000000 )
( -0.000011  0.000000  -0.000010  0.000000  0.000210  0.000000 )
( 0.000104  0.000000  0.000192  0.000000  -0.000258  0.000000 )
( -0.000048  0.000000  -0.000082  0.000000  -0.000263  0.000000 )
( -0.000048  0.000000  -0.000082  0.000000  -0.000263  0.000000 )
( 0.000031  0.000000  0.000003  0.000000  -0.000014  0.000000 )
( 0.000031  0.000000  0.000003  0.000000  -0.000014  0.000000 )
( 0.000147  0.000000  0.001833  0.000000  -0.044192  0.000000 )
( 0.000147  0.000000  0.001833  0.000000  -0.044192  0.000000 )
( -0.000015  0.000000  0.000024  0.000000  -0.000013  0.000000 )
( -0.000015  0.000000  0.000024  0.000000  -0.000013  0.000000 )
( -0.000014  0.000000  -0.000015  0.000000  -0.000120  0.000000 )
( -0.000014  0.000000  -0.000015  0.000000  -0.000120  0.000000 )
( -0.000002  0.000000  0.000009  0.000000  -0.000099  0.000000 )
( -0.000002  0.000000  0.000009  0.000000  -0.000099  0.000000 )
( 0.000019  0.000000  0.000007  0.000000  -0.000120  0.000000 )
( 0.000019  0.000000  0.000007  0.000000  -0.000120  0.000000 )
( -0.002627  0.000000  -0.029722  0.000000  0.705091  0.000000 )
( -0.002627  0.000000  -0.029722  0.000000  0.705091  0.000000 )
*****

```


Table S3: vibrational modes of brucite

alat= 6.026781 a.u.

crystal axes: (cart. coord. in units of alat)

a(1)= (1.000000 0.000000 0.000000)

a(2)= (-0.500000 0.866025 0.000000)

a(3)= (0.000000 0.000000 1.534564)

freq (1)= -0.000000 [THz] = -0.000008 [cm-1]

(-0.435353 0.000000 -0.084573 0.000000 -0.057577 0.000000)
 (-0.435353 0.000000 -0.084573 0.000000 -0.057577 0.000000)
 (-0.435353 0.000000 -0.084573 0.000000 -0.057577 0.000000)
 (-0.435353 0.000000 -0.084573 0.000000 -0.057577 0.000000)
 (-0.435353 0.000000 -0.084573 0.000000 -0.057577 0.000000)

freq (2)= 0.000000 [THz] = 0.000005 [cm-1]

(-0.085284 0.000000 0.439006 0.000000 0.000004 0.000000)
 (-0.085284 0.000000 0.439006 0.000000 0.000004 0.000000)
 (-0.085284 0.000000 0.439006 0.000000 0.000004 0.000000)
 (-0.085284 0.000000 0.439006 0.000000 0.000004 0.000000)
 (-0.085284 0.000000 0.439006 0.000000 0.000004 0.000000)

freq (3)= 0.000001 [THz] = 0.000039 [cm-1]

(-0.056520 0.000000 -0.010984 0.000000 0.443492 0.000000)
 (-0.056520 0.000000 -0.010984 0.000000 0.443492 0.000000)
 (-0.056520 0.000000 -0.010984 0.000000 0.443492 0.000000)
 (-0.056520 0.000000 -0.010984 0.000000 0.443492 0.000000)
 (-0.056520 0.000000 -0.010984 0.000000 0.443492 0.000000)

freq (4)= 8.230415 [THz] = 274.537104 [cm-1]

(-0.067911 0.000000 0.267775 0.000000 -0.000000 0.000000)
 (0.067911 0.000000 -0.267775 0.000000 -0.000000 0.000000)
 (0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000)
 (-0.160012 0.000000 0.630936 0.000000 -0.000000 0.000000)
 (0.160012 0.000000 -0.630936 0.000000 -0.000000 0.000000)

freq (5)= 8.230415 [THz] = 274.537104 [cm-1]

(-0.267775 0.000000 -0.067911 0.000000 -0.000000 0.000000)
 (0.267775 0.000000 0.067911 0.000000 -0.000000 0.000000)
 (0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000)
 (-0.630936 0.000000 -0.160012 0.000000 -0.000000 0.000000)
 (0.630936 0.000000 0.160012 0.000000 -0.000000 0.000000)

freq (6)= 10.587551 [THz] = 353.162671 [cm-1]

(0.185295 0.000000 0.462708 0.000000 -0.000000 0.000000)
 (0.185295 0.000000 0.462708 0.000000 0.000000 0.000000)
 (-0.187746 0.000000 -0.468831 0.000000 0.000000 0.000000)
 (0.130931 0.000000 0.326953 0.000000 -0.000000 0.000000)
 (0.130931 0.000000 0.326953 0.000000 0.000000 0.000000)

freq (7)= 10.587551 [THz] = 353.162671 [cm-1]

(0.462708 0.000000 -0.185295 0.000000 -0.000000 0.000000)
 (0.462708 0.000000 -0.185295 0.000000 -0.000000 0.000000)
 (-0.468831 0.000000 0.187746 0.000000 0.000000 0.000000)
 (0.326953 0.000000 -0.130931 0.000000 -0.000000 0.000000)
 (0.326953 0.000000 -0.130931 0.000000 -0.000000 0.000000)

freq (8)= 13.373582 [THz] = 446.094682 [cm-1]

```

( 0.000000 0.000000 0.000000 0.000000 0.499380 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.499380 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.500620 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.500620 0.000000 )
freq ( 9) = 13.393022 [THz] = 446.743128 [cm-1]
( -0.633304 0.000000 0.310116 0.000000 0.000000 0.000000 )
( -0.633304 0.000000 0.310116 0.000000 -0.000000 0.000000 )
( -0.008961 0.000000 0.004388 0.000000 0.000000 0.000000 )
( 0.046706 0.000000 -0.022871 0.000000 0.000000 0.000000 )
( 0.046706 0.000000 -0.022871 0.000000 -0.000000 0.000000 )
freq ( 10) = 13.393022 [THz] = 446.743128 [cm-1]
( -0.310116 0.000000 -0.633304 0.000000 0.000000 0.000000 )
( -0.310116 0.000000 -0.633304 0.000000 -0.000000 0.000000 )
( -0.004388 0.000000 -0.008961 0.000000 0.000000 0.000000 )
( 0.022871 0.000000 0.046706 0.000000 0.000000 0.000000 )
( 0.022871 0.000000 0.046706 0.000000 -0.000000 0.000000 )
freq ( 11) = 14.342579 [THz] = 478.416948 [cm-1]
( -0.000000 0.000000 0.000000 0.000000 0.390485 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.390485 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.585185 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.419882 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.419882 0.000000 )
freq ( 12) = 22.449868 [THz] = 748.846988 [cm-1]
( 0.580360 0.000000 0.403516 0.000000 0.000000 0.000000 )
( -0.580360 0.000000 -0.403516 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( -0.015518 0.000000 -0.010790 0.000000 0.000000 0.000000 )
( 0.015518 0.000000 0.010790 0.000000 0.000000 0.000000 )
freq ( 13) = 22.449868 [THz] = 748.846988 [cm-1]
( -0.403516 0.000000 0.580360 0.000000 -0.000000 0.000000 )
( 0.403516 0.000000 -0.580360 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.010790 0.000000 -0.015518 0.000000 -0.000000 0.000000 )
( -0.010790 0.000000 0.015518 0.000000 -0.000000 0.000000 )
freq ( 14) = 110.505184 [THz] = 3686.056186 [cm-1]
( -0.000000 0.000000 0.000000 0.000000 0.705714 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.705714 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.044352 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.044352 0.000000 )
freq ( 15) = 110.992568 [THz] = 3702.313554 [cm-1]
( 0.000000 0.000000 0.000000 0.000000 -0.705787 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.705787 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.001712 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.043166 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.043166 0.000000 )

```

Table S4: vibrational modes of lizardite

alat= 10.174957 a.u.

crystal axes: (cart. coord. in units of alat)

a(1)= (1.000000 0.000000 0.000000)

a(2)= (-0.500000 0.866025 0.000000)

a(3)= (0.000000 0.000000 1.371497)

freq (1) = -0.008805 [THz] = -0.293709 [cm-1]					
(0.000037	0.000000	0.000000	0.000000	0.235671	0.000000)
(-0.000011	0.000000	0.000028	0.000000	0.235671	0.000000)
(-0.000011	0.000000	-0.000028	0.000000	0.235671	0.000000)
(0.000005	0.000000	0.000000	0.000000	0.235755	0.000000)
(0.000005	0.000000	0.000000	0.000000	0.235755	0.000000)
(0.000005	0.000000	0.000000	0.000000	0.235770	0.000000)
(0.000005	0.000000	-0.000000	0.000000	0.235770	0.000000)
(-0.000302	0.000000	0.000000	0.000000	0.235767	0.000000)
(0.000158	0.000000	-0.000265	0.000000	0.235767	0.000000)
(0.000158	0.000000	0.000265	0.000000	0.235767	0.000000)
(0.000180	0.000000	0.000000	0.000000	0.235677	0.000000)
(-0.000083	0.000000	0.000151	0.000000	0.235677	0.000000)
(-0.000083	0.000000	-0.000151	0.000000	0.235677	0.000000)
(0.000005	0.000000	0.000000	0.000000	0.235538	0.000000)
(0.000991	0.000000	0.000000	0.000000	0.235722	0.000000)
(-0.000488	0.000000	0.000854	0.000000	0.235722	0.000000)
(-0.000488	0.000000	-0.000854	0.000000	0.235722	0.000000)
(0.000005	0.000000	0.000000	0.000000	0.235537	0.000000)
freq (2) = -0.004234 [THz] = -0.141214 [cm-1]					
(0.000000	0.000000	0.235742	0.000000	-0.000000	0.000000)
(0.000030	0.000000	0.235690	0.000000	0.000057	0.000000)
(-0.000030	0.000000	0.235690	0.000000	-0.000057	0.000000)
(-0.000028	0.000000	0.235679	0.000000	-0.000000	0.000000)
(0.000028	0.000000	0.235679	0.000000	0.000000	0.000000)
(-0.000168	0.000000	0.235680	0.000000	-0.000000	0.000000)
(0.000168	0.000000	0.235680	0.000000	0.000000	0.000000)
(0.000000	0.000000	0.235676	0.000000	-0.000000	0.000000)
(0.000002	0.000000	0.235673	0.000000	-0.000049	0.000000)
(-0.000001	0.000000	0.235673	0.000000	0.000049	0.000000)
(0.000000	0.000000	0.235681	0.000000	-0.000000	0.000000)
(-0.000023	0.000000	0.235721	0.000000	-0.000176	0.000000)
(0.000023	0.000000	0.235721	0.000000	0.000176	0.000000)
(0.000000	0.000000	0.235748	0.000000	-0.000000	0.000000)
(0.000000	0.000000	0.235633	0.000000	-0.000000	0.000000)
(-0.000051	0.000000	0.235723	0.000000	-0.000200	0.000000)
(0.000052	0.000000	0.235723	0.000000	0.000200	0.000000)
(0.000000	0.000000	0.235830	0.000000	-0.000000	0.000000)
freq (3) = -0.004233 [THz] = -0.141203 [cm-1]					
(0.235672	0.000000	-0.000000	0.000000	0.000061	0.000000)
(0.235725	0.000000	0.000030	0.000000	-0.000038	0.000000)
(0.235725	0.000000	-0.000030	0.000000	-0.000038	0.000000)
(0.235679	0.000000	0.000028	0.000000	-0.000005	0.000000)

```

( 0.235679 0.000000 -0.000028 0.000000 -0.000005 0.000000 )
( 0.235680 0.000000 0.000168 0.000000 -0.000005 0.000000 )
( 0.235680 0.000000 -0.000168 0.000000 -0.000005 0.000000 )
( 0.235672 0.000000 -0.000000 0.000000 -0.000061 0.000000 )
( 0.235675 0.000000 0.000002 0.000000 0.000023 0.000000 )
( 0.235675 0.000000 -0.000002 0.000000 0.000023 0.000000 )
( 0.235734 0.000000 -0.000000 0.000000 -0.000208 0.000000 )
( 0.235694 0.000000 -0.000023 0.000000 0.000097 0.000000 )
( 0.235694 0.000000 0.000023 0.000000 0.000097 0.000000 )
( 0.235748 0.000000 -0.000000 0.000000 -0.000005 0.000000 )
( 0.235753 0.000000 -0.000000 0.000000 -0.000236 0.000000 )
( 0.235663 0.000000 -0.000052 0.000000 0.000111 0.000000 )
( 0.235663 0.000000 0.000051 0.000000 0.000111 0.000000 )
( 0.235830 0.000000 -0.000000 0.000000 -0.000005 0.000000 )
freq ( 4) = 3.628835 [THz] = 121.044916 [cm-1]
( 0.002008 0.000000 0.000000 0.000000 -0.000159 0.000000 )
( -0.001004 0.000000 0.001739 0.000000 -0.000159 0.000000 )
( -0.001004 0.000000 -0.001739 0.000000 -0.000159 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.005528 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.005528 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.007246 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.007246 0.000000 )
( -0.576715 0.000000 -0.000000 0.000000 -0.011962 0.000000 )
( 0.288357 0.000000 -0.499449 0.000000 -0.011962 0.000000 )
( 0.288357 0.000000 0.499449 0.000000 -0.011962 0.000000 )
( 0.000376 0.000000 0.000000 0.000000 0.001083 0.000000 )
( -0.000188 0.000000 0.000326 0.000000 0.001083 0.000000 )
( -0.000188 0.000000 -0.000326 0.000000 0.001083 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.002250 0.000000 )
( -0.022858 0.000000 -0.000000 0.000000 -0.002011 0.000000 )
( 0.011429 0.000000 -0.019796 0.000000 -0.002011 0.000000 )
( 0.011429 0.000000 0.019796 0.000000 -0.002011 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.002284 0.000000 )
freq ( 5) = 3.870221 [THz] = 129.096689 [cm-1]
( -0.000000 0.000000 0.246328 0.000000 -0.000000 0.000000 )
( 0.010071 0.000000 0.228885 0.000000 0.058825 0.000000 )
( -0.010071 0.000000 0.228885 0.000000 -0.058825 0.000000 )
( -0.007003 0.000000 -0.284040 0.000000 -0.000000 0.000000 )
( 0.007003 0.000000 -0.284040 0.000000 0.000000 0.000000 )
( -0.008537 0.000000 -0.027089 0.000000 -0.000000 0.000000 )
( 0.008537 0.000000 -0.027089 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.282314 0.000000 0.000000 0.000000 )
( 0.036415 0.000000 -0.345386 0.000000 -0.013589 0.000000 )
( -0.036415 0.000000 -0.345386 0.000000 0.013589 0.000000 )
( -0.000000 0.000000 0.225503 0.000000 0.000000 0.000000 )
( -0.023565 0.000000 0.266318 0.000000 -0.016636 0.000000 )
( 0.023565 0.000000 0.266318 0.000000 0.016636 0.000000 )
( -0.000000 0.000000 0.155995 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 0.084090 0.000000 0.000000 0.000000 )
( -0.071700 0.000000 0.208278 0.000000 -0.018873 0.000000 )

```

```

( 0.071700 0.000000 0.208278 0.000000 0.018873 0.000000 )
( -0.000000 0.000000 0.139721 0.000000 -0.000000 0.000000 )
freq ( 6) = 3.870223 [THz] = 129.096745 [cm-1]
( 0.223071 0.000000 0.000000 0.000000 0.067925 0.000000 )
( 0.240514 0.000000 0.010071 0.000000 -0.033963 0.000000 )
( 0.240514 0.000000 -0.010071 0.000000 -0.033963 0.000000 )
( -0.284040 0.000000 0.007003 0.000000 0.000000 0.000000 )
( -0.284040 0.000000 -0.007003 0.000000 0.000000 0.000000 )
( -0.027089 0.000000 0.008537 0.000000 0.000000 0.000000 )
( -0.027089 0.000000 -0.008537 0.000000 0.000000 0.000000 )
( -0.366410 0.000000 -0.000000 0.000000 -0.015691 0.000000 )
( -0.303338 0.000000 0.036416 0.000000 0.007846 0.000000 )
( -0.303338 0.000000 -0.036416 0.000000 0.007846 0.000000 )
( 0.279923 0.000000 0.000000 0.000000 -0.019210 0.000000 )
( 0.239108 0.000000 -0.023565 0.000000 0.009605 0.000000 )
( 0.239108 0.000000 0.023565 0.000000 0.009605 0.000000 )
( 0.155995 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.249674 0.000000 0.000000 0.000000 -0.021792 0.000000 )
( 0.125486 0.000000 -0.071700 0.000000 0.010896 0.000000 )
( 0.125486 0.000000 0.071700 0.000000 0.010896 0.000000 )
( 0.139721 0.000000 0.000000 0.000000 -0.000000 0.000000 )
freq ( 7) = 6.166981 [THz] = 205.708359 [cm-1]
( -0.056102 0.000000 0.000000 0.000000 0.432532 0.000000 )
( -0.031105 0.000000 0.014432 0.000000 -0.216266 0.000000 )
( -0.031105 0.000000 -0.014432 0.000000 -0.216266 0.000000 )
( 0.018037 0.000000 0.030330 0.000000 -0.000000 0.000000 )
( 0.018037 0.000000 -0.030330 0.000000 -0.000000 0.000000 )
( -0.000515 0.000000 0.051595 0.000000 -0.000000 0.000000 )
( -0.000515 0.000000 -0.051595 0.000000 -0.000000 0.000000 )
( 0.030400 0.000000 -0.000000 0.000000 -0.052071 0.000000 )
( 0.020260 0.000000 -0.005854 0.000000 0.026035 0.000000 )
( 0.020260 0.000000 0.005854 0.000000 0.026035 0.000000 )
( 0.102661 0.000000 0.000000 0.000000 -0.037238 0.000000 )
( -0.115216 0.000000 -0.125791 0.000000 0.018619 0.000000 )
( -0.115216 0.000000 0.125791 0.000000 0.018619 0.000000 )
( 0.142729 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.401514 0.000000 0.000000 0.000000 -0.018726 0.000000 )
( -0.165527 0.000000 -0.327382 0.000000 0.009363 0.000000 )
( -0.165527 0.000000 0.327382 0.000000 0.009363 0.000000 )
( 0.422016 0.000000 -0.000000 0.000000 0.000000 0.000000 )
freq ( 8) = 6.166983 [THz] = 205.708401 [cm-1]
( -0.000000 0.000000 -0.022773 0.000000 0.000000 0.000000 )
( 0.014432 0.000000 -0.047770 0.000000 0.374584 0.000000 )
( -0.014432 0.000000 -0.047770 0.000000 -0.374584 0.000000 )
( -0.030330 0.000000 0.018037 0.000000 0.000000 0.000000 )
( 0.030330 0.000000 0.018037 0.000000 -0.000000 0.000000 )
( -0.051595 0.000000 -0.000515 0.000000 0.000000 0.000000 )
( 0.051595 0.000000 -0.000515 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.016881 0.000000 -0.000000 0.000000 )
( -0.005854 0.000000 0.027020 0.000000 -0.045095 0.000000 )

```

```

( 0.005854 0.000000 0.027020 0.000000 0.045095 0.000000 )
( 0.000000 0.000000 -0.187842 0.000000 -0.000000 0.000000 )
( -0.125791 0.000000 0.030035 0.000000 -0.032249 0.000000 )
( 0.125791 0.000000 0.030035 0.000000 0.032249 0.000000 )
( 0.000000 0.000000 0.142729 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 -0.354541 0.000000 -0.000000 0.000000 )
( -0.327381 0.000000 0.212501 0.000000 -0.016217 0.000000 )
( 0.327381 0.000000 0.212501 0.000000 0.016217 0.000000 )
( 0.000000 0.000000 0.422015 0.000000 -0.000000 0.000000 )
freq ( 9) = 6.821431 [THz] = 227.538432 [cm-1]
( -0.002624 0.000000 -0.000000 0.000000 -0.173626 0.000000 )
( 0.001312 0.000000 -0.002272 0.000000 -0.173626 0.000000 )
( 0.001312 0.000000 0.002272 0.000000 -0.173626 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.188202 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.188202 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.168024 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.168024 0.000000 )
( -0.001612 0.000000 -0.000000 0.000000 0.245721 0.000000 )
( 0.000806 0.000000 -0.001396 0.000000 0.245721 0.000000 )
( 0.000806 0.000000 0.001396 0.000000 0.245721 0.000000 )
( 0.072790 0.000000 0.000000 0.000000 -0.158411 0.000000 )
( -0.036395 0.000000 0.063038 0.000000 -0.158411 0.000000 )
( -0.036395 0.000000 -0.063038 0.000000 -0.158411 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.413612 0.000000 )
( 0.179617 0.000000 0.000000 0.000000 -0.153247 0.000000 )
( -0.089808 0.000000 0.155552 0.000000 -0.153247 0.000000 )
( -0.089808 0.000000 -0.155552 0.000000 -0.153247 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.414248 0.000000 )
freq ( 10) = 8.028713 [THz] = 267.809028 [cm-1]
( 0.136683 0.000000 0.000000 0.000000 -0.044848 0.000000 )
( -0.079270 0.000000 -0.124681 0.000000 0.022424 0.000000 )
( -0.079270 0.000000 0.124681 0.000000 0.022424 0.000000 )
( 0.002546 0.000000 0.120195 0.000000 -0.000000 0.000000 )
( 0.002546 0.000000 -0.120195 0.000000 -0.000000 0.000000 )
( 0.085643 0.000000 0.382780 0.000000 -0.000000 0.000000 )
( 0.085643 0.000000 -0.382780 0.000000 -0.000000 0.000000 )
( -0.049865 0.000000 0.000000 0.000000 -0.383079 0.000000 )
( -0.014106 0.000000 0.020645 0.000000 0.191539 0.000000 )
( -0.014106 0.000000 -0.020645 0.000000 0.191539 0.000000 )
( 0.031964 0.000000 0.000000 0.000000 0.334939 0.000000 )
( -0.005225 0.000000 -0.021471 0.000000 -0.167470 0.000000 )
( -0.005225 0.000000 0.021471 0.000000 -0.167470 0.000000 )
( -0.070274 0.000000 0.000000 0.000000 0.000000 0.000000 )
( -0.073185 0.000000 0.000000 0.000000 0.325190 0.000000 )
( -0.035862 0.000000 0.021549 0.000000 -0.162595 0.000000 )
( -0.035862 0.000000 -0.021549 0.000000 -0.162595 0.000000 )
( -0.177402 0.000000 0.000000 0.000000 0.000000 0.000000 )
freq ( 11) = 8.028713 [THz] = 267.809038 [cm-1]
( -0.000000 0.000000 0.151255 0.000000 0.000000 0.000000 )
( 0.124681 0.000000 -0.064699 0.000000 0.038839 0.000000 )

```

```
( -0.124681  0.000000  -0.064699  0.000000  -0.038839  0.000000  )
(  0.120195  0.000000  -0.002546  0.000000  -0.000000  0.000000  )
( -0.120195  0.000000  -0.002546  0.000000   0.000000  0.000000  )
(  0.382780  0.000000  -0.085643  0.000000  -0.000000  0.000000  )
( -0.382780  0.000000  -0.085643  0.000000   0.000000  0.000000  )
(  0.000000  0.000000   0.002187  0.000000   0.000000  0.000000  )
( -0.020645  0.000000   0.037945  0.000000   0.331756  0.000000  )
(  0.020645  0.000000   0.037945  0.000000  -0.331756  0.000000  )
( -0.000000  0.000000   0.017622  0.000000  -0.000000  0.000000  )
(  0.021471  0.000000  -0.019567  0.000000  -0.290066  0.000000  )
( -0.021471  0.000000  -0.019567  0.000000   0.290066  0.000000  )
(  0.000000  0.000000   0.070274  0.000000  -0.000000  0.000000  )
(  0.000000  0.000000   0.023421  0.000000  -0.000000  0.000000  )
( -0.021549  0.000000   0.060744  0.000000  -0.281623  0.000000  )
(  0.021549  0.000000   0.060744  0.000000   0.281623  0.000000  )
(  0.000000  0.000000   0.177402  0.000000  -0.000000  0.000000  )
```

freq (12) = 8.973052 [THz] = 299.308786 [cm-1]

```
( -0.000000  0.000000  -0.074571  0.000000  -0.000000  0.000000  )
( -0.013713  0.000000  -0.050819  0.000000  -0.071640  0.000000  )
(  0.013713  0.000000  -0.050819  0.000000   0.071640  0.000000  )
(  0.010357  0.000000  -0.010070  0.000000  -0.000000  0.000000  )
( -0.010357  0.000000  -0.010070  0.000000   0.000000  0.000000  )
(  0.029656  0.000000   0.381501  0.000000  -0.000000  0.000000  )
( -0.029656  0.000000   0.381501  0.000000   0.000000  0.000000  )
( -0.000000  0.000000  -0.015696  0.000000  -0.000000  0.000000  )
(  0.107345  0.000000  -0.201622  0.000000  -0.004107  0.000000  )
( -0.107345  0.000000  -0.201622  0.000000   0.004107  0.000000  )
( -0.000000  0.000000  -0.154460  0.000000  -0.000000  0.000000  )
(  0.029125  0.000000  -0.204905  0.000000  -0.058196  0.000000  )
( -0.029125  0.000000  -0.204905  0.000000   0.058196  0.000000  )
(  0.000000  0.000000   0.520177  0.000000  -0.000000  0.000000  )
( -0.000000  0.000000  -0.003554  0.000000  -0.000000  0.000000  )
(  0.085711  0.000000  -0.152009  0.000000  -0.057258  0.000000  )
( -0.085711  0.000000  -0.152009  0.000000   0.057258  0.000000  )
(  0.000000  0.000000   0.355502  0.000000  -0.000000  0.000000  )
```

freq (13) = 8.973052 [THz] = 299.308792 [cm-1]

```
(  0.042902  0.000000  -0.000000  0.000000   0.082723  0.000000  )
(  0.066654  0.000000   0.013713  0.000000  -0.041362  0.000000  )
(  0.066654  0.000000  -0.013713  0.000000  -0.041362  0.000000  )
(  0.010070  0.000000   0.010357  0.000000   0.000000  0.000000  )
(  0.010070  0.000000  -0.010357  0.000000   0.000000  0.000000  )
( -0.381501  0.000000   0.029656  0.000000  -0.000000  0.000000  )
( -0.381501  0.000000  -0.029656  0.000000  -0.000000  0.000000  )
(  0.263597  0.000000  -0.000000  0.000000   0.004742  0.000000  )
(  0.077671  0.000000  -0.107345  0.000000  -0.002371  0.000000  )
(  0.077671  0.000000   0.107345  0.000000  -0.002371  0.000000  )
(  0.221720  0.000000  -0.000000  0.000000   0.067198  0.000000  )
(  0.171275  0.000000  -0.029125  0.000000  -0.033599  0.000000  )
(  0.171275  0.000000   0.029125  0.000000  -0.033599  0.000000  )
( -0.520176  0.000000   0.000000  0.000000  -0.000000  0.000000  )
```

```

( 0.201495 0.000000 -0.000000 0.000000 0.066116 0.000000 )
( 0.053039 0.000000 -0.085711 0.000000 -0.033058 0.000000 )
( 0.053039 0.000000 0.085711 0.000000 -0.033058 0.000000 )
( -0.355503 0.000000 0.000000 0.000000 -0.000000 0.000000 )
freq ( 14) = 9.472737 [THz] = 315.976502 [cm-1]
( 0.177931 0.000000 0.000000 0.000000 0.107091 0.000000 )
( -0.105523 0.000000 -0.163653 0.000000 -0.053546 0.000000 )
( -0.105523 0.000000 0.163653 0.000000 -0.053546 0.000000 )
( -0.019676 0.000000 -0.099301 0.000000 0.000000 0.000000 )
( -0.019676 0.000000 0.099301 0.000000 0.000000 0.000000 )
( 0.104992 0.000000 -0.193363 0.000000 0.000000 0.000000 )
( 0.104992 0.000000 0.193363 0.000000 0.000000 0.000000 )
( -0.024439 0.000000 0.000000 0.000000 0.316235 0.000000 )
( -0.013292 0.000000 0.006436 0.000000 -0.158118 0.000000 )
( -0.013292 0.000000 -0.006436 0.000000 -0.158118 0.000000 )
( 0.028624 0.000000 -0.000000 0.000000 0.431505 0.000000 )
( 0.009527 0.000000 -0.011026 0.000000 -0.215753 0.000000 )
( 0.009527 0.000000 0.011026 0.000000 -0.215753 0.000000 )
( -0.073554 0.000000 0.000000 0.000000 0.000000 0.000000 )
( 0.031927 0.000000 0.000000 0.000000 0.428466 0.000000 )
( -0.012174 0.000000 -0.025462 0.000000 -0.214233 0.000000 )
( -0.012174 0.000000 0.025462 0.000000 -0.214233 0.000000 )
( -0.207378 0.000000 0.000000 0.000000 0.000000 0.000000 )
freq ( 15) = 9.472738 [THz] = 315.976512 [cm-1]
( 0.000000 0.000000 -0.200008 0.000000 0.000000 0.000000 )
( -0.163653 0.000000 0.083446 0.000000 0.092743 0.000000 )
( 0.163653 0.000000 0.083446 0.000000 -0.092743 0.000000 )
( 0.099301 0.000000 -0.019676 0.000000 0.000000 0.000000 )
( -0.099301 0.000000 -0.019676 0.000000 -0.000000 0.000000 )
( 0.193363 0.000000 0.104992 0.000000 0.000000 0.000000 )
( -0.193363 0.000000 0.104992 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.009576 0.000000 0.000000 0.000000 )
( 0.006436 0.000000 -0.020723 0.000000 0.273868 0.000000 )
( -0.006436 0.000000 -0.020723 0.000000 -0.273868 0.000000 )
( 0.000000 0.000000 0.003161 0.000000 0.000000 0.000000 )
( -0.011026 0.000000 0.022258 0.000000 0.373695 0.000000 )
( 0.011026 0.000000 0.022258 0.000000 -0.373695 0.000000 )
( -0.000000 0.000000 -0.073554 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.026874 0.000000 0.000000 0.000000 )
( -0.025462 0.000000 0.017227 0.000000 0.371063 0.000000 )
( 0.025462 0.000000 0.017227 0.000000 -0.371063 0.000000 )
( -0.000000 0.000000 -0.207377 0.000000 0.000000 0.000000 )
freq ( 16) = 9.832137 [THz] = 327.964805 [cm-1]
( -0.000000 0.000000 0.324416 0.000000 -0.000000 0.000000 )
( -0.280952 0.000000 -0.162208 0.000000 -0.000000 0.000000 )
( 0.280952 0.000000 -0.162208 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.136525 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.136525 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.083859 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.083859 0.000000 )

```



```

( -0.000000  0.000000  -0.029270  0.000000  -0.000000  0.000000 )
(  0.025349  0.000000  0.014635  0.000000  -0.000000  0.000000 )
( -0.025349  0.000000  0.014635  0.000000  0.000000  0.000000 )
( -0.000000  0.000000  -0.281011  0.000000  -0.000000  0.000000 )
(  0.243362  0.000000  0.140505  0.000000  -0.000000  0.000000 )
( -0.243362  0.000000  0.140505  0.000000  0.000000  0.000000 )
(  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 )
( -0.000000  0.000000  -0.362146  0.000000  -0.000000  0.000000 )
(  0.313628  0.000000  0.181073  0.000000  -0.000000  0.000000 )
( -0.313628  0.000000  0.181073  0.000000  0.000000  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  0.000000  0.000000 )
  freq ( 17) =  10.349574 [THz] =  345.224634 [cm-1]
(  0.257438  0.000000  0.000000  0.000000  0.020987  0.000000 )
( -0.128719  0.000000  0.222948  0.000000  0.020986  0.000000 )
( -0.128719  0.000000  -0.222948  0.000000  0.020986  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.038267  0.000000 )
( -0.000000  0.000000  0.000000  0.000000  -0.038267  0.000000 )
(  0.000000  0.000000  -0.000000  0.000000  -0.011218  0.000000 )
(  0.000000  0.000000  0.000000  0.000000  -0.011218  0.000000 )
(  0.000880  0.000000  -0.000000  0.000000  -0.031003  0.000000 )
( -0.000440  0.000000  0.000762  0.000000  -0.031003  0.000000 )
( -0.000440  0.000000  -0.000762  0.000000  -0.031003  0.000000 )
(  0.323926  0.000000  0.000000  0.000000  0.062432  0.000000 )
( -0.161963  0.000000  0.280528  0.000000  0.062432  0.000000 )
( -0.161963  0.000000  -0.280528  0.000000  0.062432  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.043590  0.000000 )
(  0.387510  0.000000  0.000000  0.000000  0.065048  0.000000 )
( -0.193755  0.000000  0.335594  0.000000  0.065047  0.000000 )
( -0.193755  0.000000  -0.335594  0.000000  0.065047  0.000000 )
( -0.000000  0.000000  0.000000  0.000000  -0.047166  0.000000 )
  freq ( 18) =  10.896221 [THz] =  363.458822 [cm-1]
( -0.000000  0.000000  0.104752  0.000000  0.000000  0.000000 )
(  0.122586  0.000000  -0.107574  0.000000  0.109653  0.000000 )
( -0.122586  0.000000  -0.107574  0.000000  -0.109653  0.000000 )
( -0.002082  0.000000  0.112303  0.000000  -0.000000  0.000000 )
(  0.002082  0.000000  0.112303  0.000000  0.000000  0.000000 )
(  0.030072  0.000000  0.293748  0.000000  -0.000000  0.000000 )
( -0.030072  0.000000  0.293748  0.000000  0.000000  0.000000 )
( -0.000000  0.000000  0.074758  0.000000  -0.000000  0.000000 )
(  0.197371  0.000000  -0.267099  0.000000  -0.031297  0.000000 )
( -0.197371  0.000000  -0.267099  0.000000  0.031297  0.000000 )
(  0.000000  0.000000  0.141880  0.000000  -0.000000  0.000000 )
(  0.054693  0.000000  0.047148  0.000000  -0.023265  0.000000 )
( -0.054693  0.000000  0.047148  0.000000  0.023265  0.000000 )
( -0.000000  0.000000  -0.589928  0.000000  -0.000000  0.000000 )
( -0.000000  0.000000  0.175591  0.000000  -0.000000  0.000000 )
(  0.088203  0.000000  0.022820  0.000000  -0.028107  0.000000 )
( -0.088203  0.000000  0.022820  0.000000  0.028107  0.000000 )
( -0.000000  0.000000  -0.235268  0.000000  -0.000000  0.000000 )
  freq ( 19) =  10.896221 [THz] =  363.458825 [cm-1]

```

```
( 0.178349 0.000000 0.000000 0.000000 -0.126617 0.000000 )
( -0.033976 0.000000 -0.122586 0.000000 0.063308 0.000000 )
( -0.033976 0.000000 0.122586 0.000000 0.063308 0.000000 )
( -0.112303 0.000000 -0.002082 0.000000 0.000000 0.000000 )
( -0.112303 0.000000 0.002082 0.000000 0.000000 0.000000 )
( -0.293748 0.000000 0.030072 0.000000 0.000000 0.000000 )
( -0.293748 0.000000 -0.030072 0.000000 0.000000 0.000000 )
( 0.381051 0.000000 0.000000 0.000000 0.036139 0.000000 )
( 0.039194 0.000000 -0.197371 0.000000 -0.018069 0.000000 )
( 0.039194 0.000000 0.197371 0.000000 -0.018069 0.000000 )
( -0.015571 0.000000 0.000000 0.000000 0.026865 0.000000 )
( -0.110303 0.000000 -0.054693 0.000000 -0.013432 0.000000 )
( -0.110303 0.000000 0.054693 0.000000 -0.013432 0.000000 )
( 0.589928 0.000000 -0.000000 0.000000 0.000000 0.000000 )
( 0.028105 0.000000 0.000000 0.000000 0.032455 0.000000 )
( -0.124667 0.000000 -0.088203 0.000000 -0.016228 0.000000 )
( -0.124667 0.000000 0.088203 0.000000 -0.016228 0.000000 )
( 0.235269 0.000000 -0.000000 0.000000 0.000000 0.000000 )
```

freq (20) = 11.252284 [THz] = 375.335789 [cm-1]

```
( -0.000000 0.000000 0.022461 0.000000 0.000000 0.000000 )
( -0.019452 0.000000 -0.011231 0.000000 0.000000 0.000000 )
( 0.019452 0.000000 -0.011231 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.407380 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.407380 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.401258 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.401258 0.000000 )
( -0.000000 0.000000 0.132591 0.000000 -0.000000 0.000000 )
( -0.114827 0.000000 -0.066295 0.000000 0.000000 0.000000 )
( 0.114827 0.000000 -0.066295 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 -0.273736 0.000000 0.000000 0.000000 )
( 0.237062 0.000000 0.136868 0.000000 0.000000 0.000000 )
( -0.237062 0.000000 0.136868 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 -0.149464 0.000000 0.000000 0.000000 )
( 0.129440 0.000000 0.074732 0.000000 0.000000 0.000000 )
( -0.129440 0.000000 0.074732 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
```

freq (21) = 11.460554 [THz] = 382.282936 [cm-1]

```
( -0.151914 0.000000 -0.000000 0.000000 0.119769 0.000000 )
( 0.075957 0.000000 -0.131561 0.000000 0.119769 0.000000 )
( 0.075957 0.000000 0.131561 0.000000 0.119769 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.025517 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.025517 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.003438 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.003438 0.000000 )
( 0.002036 0.000000 -0.000000 0.000000 -0.116250 0.000000 )
( -0.001018 0.000000 0.001763 0.000000 -0.116250 0.000000 )
( -0.001018 0.000000 -0.001763 0.000000 -0.116250 0.000000 )
( 0.088843 0.000000 0.000000 0.000000 0.150269 0.000000 )
( -0.044422 0.000000 0.076940 0.000000 0.150269 0.000000 )
```

```

( -0.044422  0.000000  -0.076940  0.000000   0.150269  0.000000 )
(  0.000000  0.000000   0.000000  0.000000  -0.560264  0.000000 )
(  0.138158  0.000000   0.000000  0.000000   0.157283  0.000000 )
( -0.069079  0.000000   0.119648  0.000000   0.157283  0.000000 )
( -0.069079  0.000000  -0.119648  0.000000   0.157283  0.000000 )
( -0.000000  0.000000  -0.000000  0.000000  -0.555930  0.000000 )
freq ( 22) = 12.133654 [THz] = 404.735121 [cm-1]
(  0.175550  0.000000   0.000000  0.000000  -0.001784  0.000000 )
(  0.299353  0.000000   0.071477  0.000000   0.000892  0.000000 )
(  0.299353  0.000000  -0.071477  0.000000   0.000892  0.000000 )
( -0.030048  0.000000  -0.001004  0.000000   0.000000  0.000000 )
( -0.030048  0.000000   0.001004  0.000000   0.000000  0.000000 )
(  0.049063  0.000000   0.026724  0.000000   0.000000  0.000000 )
(  0.049063  0.000000  -0.026724  0.000000   0.000000  0.000000 )
(  0.062238  0.000000  -0.000000  0.000000   0.041822  0.000000 )
(  0.001173  0.000000  -0.035256  0.000000  -0.020911  0.000000 )
(  0.001173  0.000000   0.035256  0.000000  -0.020911  0.000000 )
( -0.240507  0.000000  -0.000000  0.000000   0.082918  0.000000 )
( -0.366315  0.000000  -0.072635  0.000000  -0.041459  0.000000 )
( -0.366315  0.000000   0.072635  0.000000  -0.041459  0.000000 )
( -0.188233  0.000000  -0.000000  0.000000  -0.000000  0.000000 )
( -0.153967  0.000000  -0.000000  0.000000   0.088395  0.000000 )
( -0.302461  0.000000  -0.085733  0.000000  -0.044197  0.000000 )
( -0.302461  0.000000   0.085733  0.000000  -0.044197  0.000000 )
( -0.383528  0.000000  -0.000000  0.000000  -0.000000  0.000000 )
freq ( 23) = 12.133654 [THz] = 404.735122 [cm-1]
(  0.000000  0.000000  -0.340620  0.000000  -0.000000  0.000000 )
( -0.071477  0.000000  -0.216818  0.000000   0.001545  0.000000 )
(  0.071477  0.000000  -0.216818  0.000000  -0.001545  0.000000 )
( -0.001004  0.000000   0.030048  0.000000  -0.000000  0.000000 )
(  0.001004  0.000000   0.030048  0.000000   0.000000  0.000000 )
(  0.026724  0.000000  -0.049063  0.000000  -0.000000  0.000000 )
( -0.026724  0.000000  -0.049063  0.000000   0.000000  0.000000 )
(  0.000000  0.000000   0.019182  0.000000   0.000000  0.000000 )
(  0.035256  0.000000  -0.041882  0.000000  -0.036219  0.000000 )
( -0.035256  0.000000  -0.041882  0.000000   0.036219  0.000000 )
( -0.000000  0.000000   0.408251  0.000000   0.000000  0.000000 )
(  0.072635  0.000000   0.282443  0.000000  -0.071809  0.000000 )
( -0.072635  0.000000   0.282443  0.000000   0.071809  0.000000 )
( -0.000000  0.000000   0.188233  0.000000  -0.000000  0.000000 )
( -0.000000  0.000000   0.351960  0.000000   0.000000  0.000000 )
(  0.085733  0.000000   0.203465  0.000000  -0.076552  0.000000 )
( -0.085733  0.000000   0.203465  0.000000   0.076552  0.000000 )
( -0.000000  0.000000   0.383526  0.000000  -0.000000  0.000000 )
freq ( 24) = 12.598436 [THz] = 420.238597 [cm-1]
(  0.071274  0.000000   0.000000  0.000000  -0.126249  0.000000 )
( -0.000844  0.000000  -0.041638  0.000000   0.063124  0.000000 )
( -0.000844  0.000000   0.041638  0.000000   0.063124  0.000000 )
(  0.168006  0.000000  -0.025462  0.000000  -0.000000  0.000000 )
(  0.168006  0.000000   0.025462  0.000000  -0.000000  0.000000 )

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(-0.193594	0.000000	-0.014810	0.000000	-0.000000	0.000000)
(-0.193594	0.000000	0.014810	0.000000	-0.000000	0.000000)
(-0.323281	0.000000	-0.000000	0.000000	0.038792	0.000000)
(-0.003856	0.000000	0.184420	0.000000	-0.019396	0.000000)
(-0.003856	0.000000	-0.184420	0.000000	-0.019396	0.000000)
(0.234290	0.000000	0.000000	0.000000	-0.000097	0.000000)
(-0.136142	0.000000	-0.213869	0.000000	0.000048	0.000000)
(-0.136142	0.000000	0.213869	0.000000	0.000048	0.000000)
(0.023213	0.000000	-0.000000	0.000000	-0.000000	0.000000)
(0.150200	0.000000	0.000000	0.000000	-0.007027	0.000000)
(-0.092907	0.000000	-0.140358	0.000000	0.003514	0.000000)
(-0.092907	0.000000	0.140358	0.000000	0.003514	0.000000)
(0.629525	0.000000	-0.000000	0.000000	-0.000000	0.000000)

freq (25) = 12.598436 [THz] = 420.238599 [cm-1]

(-0.000000	0.000000	0.024884	0.000000	0.000000	0.000000)
(0.041638	0.000000	-0.047234	0.000000	0.109335	0.000000)
(-0.041638	0.000000	-0.047234	0.000000	-0.109335	0.000000)
(-0.025462	0.000000	-0.168006	0.000000	-0.000000	0.000000)
(0.025462	0.000000	-0.168006	0.000000	0.000000	0.000000)
(-0.014810	0.000000	0.193593	0.000000	-0.000000	0.000000)
(0.014810	0.000000	0.193593	0.000000	0.000000	0.000000)
(0.000000	0.000000	-0.102620	0.000000	-0.000000	0.000000)
(-0.184420	0.000000	0.216806	0.000000	-0.033595	0.000000)
(0.184420	0.000000	0.216806	0.000000	0.033595	0.000000)
(-0.000000	0.000000	0.259620	0.000000	0.000000	0.000000)
(0.213870	0.000000	-0.110813	0.000000	0.000084	0.000000)
(-0.213870	0.000000	-0.110813	0.000000	-0.000084	0.000000)
(-0.000000	0.000000	-0.023213	0.000000	0.000000	0.000000)
(-0.000000	0.000000	0.173942	0.000000	0.000000	0.000000)
(0.140358	0.000000	-0.069165	0.000000	0.006086	0.000000)
(-0.140358	0.000000	-0.069165	0.000000	-0.006086	0.000000)
(-0.000000	0.000000	-0.629524	0.000000	0.000000	0.000000)

freq (26) = 12.941684 [THz] = 431.688113 [cm-1]

(0.205255	0.000000	-0.000000	0.000000	0.142130	0.000000)
(0.034417	0.000000	-0.098634	0.000000	-0.071065	0.000000)
(0.034417	0.000000	0.098634	0.000000	-0.071065	0.000000)
(0.097942	0.000000	0.006512	0.000000	-0.000000	0.000000)
(0.097942	0.000000	-0.006512	0.000000	-0.000000	0.000000)
(-0.188189	0.000000	-0.059305	0.000000	-0.000000	0.000000)
(-0.188189	0.000000	0.059305	0.000000	-0.000000	0.000000)
(-0.161263	0.000000	0.000000	0.000000	-0.103644	0.000000)
(0.005183	0.000000	0.096098	0.000000	0.051822	0.000000)
(0.005183	0.000000	-0.096098	0.000000	0.051822	0.000000)
(-0.389417	0.000000	0.000000	0.000000	-0.047599	0.000000)
(0.056956	0.000000	0.257713	0.000000	0.023799	0.000000)
(0.056956	0.000000	-0.257713	0.000000	0.023799	0.000000)
(0.038004	0.000000	0.000000	0.000000	0.000000	0.000000)
(-0.390713	0.000000	0.000000	0.000000	-0.046787	0.000000)
(0.016514	0.000000	0.235113	0.000000	0.023394	0.000000)
(0.016514	0.000000	-0.235113	0.000000	0.023394	0.000000)

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( 0.430250 0.000000 0.000000 0.000000 0.000000 0.000000 )
freq ( 27) = 12.941684 [THz] = 431.688127 [cm-1]
( -0.000000 0.000000 -0.022530 0.000000 -0.000000 0.000000 )
( -0.098634 0.000000 0.148309 0.000000 0.123088 0.000000 )
( 0.098634 0.000000 0.148309 0.000000 -0.123088 0.000000 )
( -0.006512 0.000000 0.097942 0.000000 0.000000 0.000000 )
( 0.006512 0.000000 0.097942 0.000000 -0.000000 0.000000 )
( 0.059305 0.000000 -0.188189 0.000000 0.000000 0.000000 )
( -0.059305 0.000000 -0.188189 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.060666 0.000000 0.000000 0.000000 )
( 0.096099 0.000000 -0.105782 0.000000 -0.089759 0.000000 )
( -0.096099 0.000000 -0.105782 0.000000 0.089759 0.000000 )
( 0.000000 0.000000 0.205746 0.000000 0.000000 0.000000 )
( 0.257713 0.000000 -0.240626 0.000000 -0.041222 0.000000 )
( -0.257713 0.000000 -0.240626 0.000000 0.041222 0.000000 )
( -0.000000 0.000000 0.038004 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.152256 0.000000 0.000000 0.000000 )
( 0.235113 0.000000 -0.254971 0.000000 -0.040519 0.000000 )
( -0.235113 0.000000 -0.254971 0.000000 0.040519 0.000000 )
( -0.000000 0.000000 0.430251 0.000000 -0.000000 0.000000 )
freq ( 28) = 13.586761 [THz] = 453.205566 [cm-1]
( -0.290129 0.000000 -0.000000 0.000000 0.006944 0.000000 )
( 0.099435 0.000000 0.224915 0.000000 -0.003472 0.000000 )
( 0.099435 0.000000 -0.224915 0.000000 -0.003472 0.000000 )
( 0.048900 0.000000 -0.012881 0.000000 -0.000000 0.000000 )
( 0.048900 0.000000 0.012881 0.000000 -0.000000 0.000000 )
( -0.140792 0.000000 0.124336 0.000000 -0.000000 0.000000 )
( -0.140792 0.000000 -0.124336 0.000000 -0.000000 0.000000 )
( -0.073128 0.000000 -0.000000 0.000000 0.129306 0.000000 )
( 0.002360 0.000000 0.043584 0.000000 -0.064653 0.000000 )
( 0.002360 0.000000 -0.043583 0.000000 -0.064653 0.000000 )
( -0.094988 0.000000 -0.000000 0.000000 0.378679 0.000000 )
( 0.071690 0.000000 0.096232 0.000000 -0.189339 0.000000 )
( 0.071690 0.000000 -0.096232 0.000000 -0.189339 0.000000 )
( 0.247879 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( -0.104267 0.000000 -0.000000 0.000000 0.375996 0.000000 )
( 0.036098 0.000000 0.081040 0.000000 -0.187998 0.000000 )
( 0.036098 0.000000 -0.081040 0.000000 -0.187998 0.000000 )
( 0.363116 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
freq ( 29) = 13.586761 [THz] = 453.205575 [cm-1]
( -0.000000 0.000000 0.229291 0.000000 0.000000 0.000000 )
( 0.224913 0.000000 -0.160275 0.000000 0.006014 0.000000 )
( -0.224913 0.000000 -0.160275 0.000000 -0.006014 0.000000 )
( 0.012881 0.000000 0.048900 0.000000 -0.000001 0.000000 )
( -0.012881 0.000000 0.048900 0.000000 0.000001 0.000000 )
( -0.124336 0.000000 -0.140792 0.000000 -0.000000 0.000000 )
( 0.124336 0.000000 -0.140792 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 0.027524 0.000000 0.000000 0.000000 )
( 0.043583 0.000000 -0.047966 0.000000 0.111982 0.000000 )
( -0.043583 0.000000 -0.047966 0.000000 -0.111982 0.000000 )

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( -0.000000  0.000000  0.127252  0.000000  0.000000  0.000000 )
(  0.096231  0.000000 -0.039430  0.000000  0.327945  0.000000 )
( -0.096231  0.000000 -0.039430  0.000000 -0.327945  0.000000 )
(  0.000000  0.000000  0.247879  0.000000  0.000000  0.000000 )
( -0.000000  0.000000  0.082889  0.000000  0.000000  0.000000 )
(  0.081038  0.000000 -0.057480  0.000000  0.325622  0.000000 )
( -0.081038  0.000000 -0.057480  0.000000 -0.325622  0.000000 )
(  0.000000  0.000000  0.363116  0.000000  0.000000  0.000000 )
freq ( 30) = 13.636366 [THz] = 454.860216 [cm-1]
(  0.000000  0.000000 -0.251510  0.000000 -0.000000  0.000000 )
(  0.217816  0.000000  0.125755  0.000000 -0.000000  0.000000 )
( -0.217816  0.000000  0.125755  0.000000  0.000000  0.000000 )
(  0.000000  0.000000  0.000000  0.000000  0.111622  0.000000 )
( -0.000000  0.000000  0.000000  0.000000 -0.111622  0.000000 )
( -0.000001  0.000000 -0.000001  0.000000  0.090713  0.000000 )
(  0.000001  0.000000 -0.000001  0.000000 -0.090713  0.000000 )
(  0.000000  0.000000 -0.046003  0.000000 -0.000000  0.000000 )
(  0.039840  0.000000  0.023001  0.000000  0.000001  0.000000 )
( -0.039840  0.000000  0.023001  0.000000 -0.000001  0.000000 )
(  0.000000  0.000000 -0.323384  0.000000 -0.000000  0.000000 )
(  0.280059  0.000000  0.161692  0.000000  0.000002  0.000000 )
( -0.280059  0.000000  0.161692  0.000000 -0.000002  0.000000 )
( -0.000000  0.000000  0.000001  0.000000 -0.000000  0.000000 )
(  0.000000  0.000000 -0.386768  0.000000 -0.000000  0.000000 )
(  0.334952  0.000000  0.193384  0.000000  0.000002  0.000000 )
( -0.334952  0.000000  0.193384  0.000000 -0.000002  0.000000 )
( -0.000000  0.000000  0.000002  0.000000 -0.000000  0.000000 )
freq ( 31) = 14.234017 [THz] = 474.795686 [cm-1]
(  0.230116  0.000000  0.000000  0.000000  0.000760  0.000000 )
( -0.115058  0.000000  0.199286  0.000000  0.000760  0.000000 )
( -0.115058  0.000000 -0.199286  0.000000  0.000760  0.000000 )
( -0.000000  0.000000 -0.000000  0.000000 -0.010125  0.000000 )
( -0.000000  0.000000  0.000000  0.000000 -0.010125  0.000000 )
(  0.000000  0.000000  0.000000  0.000000 -0.005150  0.000000 )
(  0.000000  0.000000 -0.000000  0.000000 -0.005150  0.000000 )
(  0.002177  0.000000  0.000000  0.000000  0.005234  0.000000 )
( -0.001088  0.000000  0.001885  0.000000  0.005234  0.000000 )
( -0.001088  0.000000 -0.001885  0.000000  0.005234  0.000000 )
( -0.294425  0.000000  0.000000  0.000000  0.115563  0.000000 )
(  0.147213  0.000000 -0.254980  0.000000  0.115563  0.000000 )
(  0.147213  0.000000  0.254980  0.000000  0.115563  0.000000 )
(  0.000000  0.000000  0.000000  0.000000 -0.320657  0.000000 )
( -0.312956  0.000000  0.000000  0.000000  0.114365  0.000000 )
(  0.156478  0.000000 -0.271028  0.000000  0.114365  0.000000 )
(  0.156478  0.000000  0.271028  0.000000  0.114365  0.000000 )
(  0.000000  0.000000  0.000000  0.000000 -0.323692  0.000000 )
freq ( 32) = 14.681404 [THz] = 489.718923 [cm-1]
(  0.085423  0.000000  0.000000  0.000000  0.024342  0.000000 )
( -0.031875  0.000000 -0.067722  0.000000 -0.012171  0.000000 )
( -0.031875  0.000000  0.067722  0.000000 -0.012171  0.000000 )

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( 0.012065 0.000000 -0.050054 0.000000 -0.000000 0.000000 )
( 0.012065 0.000000 0.050054 0.000000 -0.000000 0.000000 )
( 0.021260 0.000000 0.469207 0.000000 -0.000000 0.000000 )
( 0.021260 0.000000 -0.469207 0.000000 -0.000000 0.000000 )
( -0.041265 0.000000 -0.000000 0.000000 0.484565 0.000000 )
( -0.006538 0.000000 0.020049 0.000000 -0.242282 0.000000 )
( -0.006538 0.000000 -0.020049 0.000000 -0.242282 0.000000 )
( -0.076113 0.000000 -0.000000 0.000000 -0.212062 0.000000 )
( 0.028283 0.000000 0.060273 0.000000 0.106031 0.000000 )
( 0.028283 0.000000 -0.060273 0.000000 0.106031 0.000000 )
( -0.064065 0.000000 0.000000 0.000000 0.000000 0.000000 )
( 0.140936 0.000000 -0.000000 0.000000 -0.198979 0.000000 )
( 0.060556 0.000000 -0.046408 0.000000 0.099489 0.000000 )
( 0.060556 0.000000 0.046408 0.000000 0.099489 0.000000 )
( 0.046747 0.000000 -0.000000 0.000000 0.000000 0.000000 )
freq ( 33) = 14.681404 [THz] = 489.718925 [cm-1]
( 0.000000 0.000000 -0.070975 0.000000 0.000000 0.000000 )
( -0.067723 0.000000 0.046324 0.000000 0.021081 0.000000 )
( 0.067723 0.000000 0.046324 0.000000 -0.021081 0.000000 )
( 0.050054 0.000000 0.012065 0.000000 0.000000 0.000000 )
( -0.050054 0.000000 0.012065 0.000000 -0.000000 0.000000 )
( -0.469207 0.000000 0.021260 0.000000 0.000000 0.000000 )
( 0.469207 0.000000 0.021260 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 0.005037 0.000000 0.000000 0.000000 )
( 0.020049 0.000000 -0.029689 0.000000 0.419645 0.000000 )
( -0.020049 0.000000 -0.029689 0.000000 -0.419645 0.000000 )
( -0.000000 0.000000 0.063081 0.000000 -0.000000 0.000000 )
( 0.060273 0.000000 -0.041314 0.000000 -0.183652 0.000000 )
( -0.060273 0.000000 -0.041314 0.000000 0.183652 0.000000 )
( -0.000000 0.000000 -0.064065 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 0.033762 0.000000 -0.000000 0.000000 )
( -0.046408 0.000000 0.114142 0.000000 -0.172321 0.000000 )
( 0.046408 0.000000 0.114142 0.000000 0.172321 0.000000 )
( 0.000000 0.000000 0.046747 0.000000 0.000000 0.000000 )
freq ( 34) = 15.739777 [THz] = 525.022462 [cm-1]
( 0.069050 0.000000 0.000000 0.000000 0.240230 0.000000 )
( -0.034525 0.000000 0.059799 0.000000 0.240230 0.000000 )
( -0.034525 0.000000 -0.059799 0.000000 0.240230 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.105451 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.105451 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.090861 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.090861 0.000000 )
( 0.004900 0.000000 -0.000000 0.000000 -0.151532 0.000000 )
( -0.002450 0.000000 0.004243 0.000000 -0.151532 0.000000 )
( -0.002450 0.000000 -0.004243 0.000000 -0.151532 0.000000 )
( -0.036544 0.000000 -0.000000 0.000000 -0.347395 0.000000 )
( 0.018272 0.000000 -0.031648 0.000000 -0.347395 0.000000 )
( 0.018272 0.000000 0.031648 0.000000 -0.347395 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.082631 0.000000 )
( -0.015167 0.000000 0.000000 0.000000 -0.328956 0.000000 )

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( 0.007583 0.000000 -0.013135 0.000000 -0.328956 0.000000 )
( 0.007583 0.000000 0.013135 0.000000 -0.328956 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.081509 0.000000 )
freq ( 35) = 19.187373 [THz] = 640.021864 [cm-1]
( 0.002173 0.000000 -0.000000 0.000000 -0.016898 0.000000 )
( 0.000200 0.000000 -0.001139 0.000000 0.008449 0.000000 )
( 0.000200 0.000000 0.001139 0.000000 0.008449 0.000000 )
( -0.012810 0.000000 0.019562 0.000000 -0.000000 0.000000 )
( -0.012810 0.000000 -0.019562 0.000000 -0.000000 0.000000 )
( 0.010393 0.000000 -0.008543 0.000000 -0.000000 0.000000 )
( 0.010393 0.000000 0.008543 0.000000 -0.000000 0.000000 )
( 0.017830 0.000000 -0.000000 0.000000 0.002680 0.000000 )
( -0.003253 0.000000 -0.012172 0.000000 -0.001340 0.000000 )
( -0.003253 0.000000 0.012172 0.000000 -0.001340 0.000000 )
( -0.035371 0.000000 -0.000000 0.000000 0.010774 0.000000 )
( -0.018196 0.000000 0.009916 0.000000 -0.005387 0.000000 )
( -0.018196 0.000000 -0.009916 0.000000 -0.005387 0.000000 )
( -0.041557 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.524299 0.000000 0.000000 0.000000 0.043427 0.000000 )
( 0.395441 0.000000 -0.074396 0.000000 -0.021714 0.000000 )
( 0.395441 0.000000 0.074396 0.000000 -0.021714 0.000000 )
( 0.626033 0.000000 0.000000 0.000000 -0.000000 0.000000 )
freq ( 36) = 19.187374 [THz] = 640.021920 [cm-1]
( -0.000000 0.000000 -0.000457 0.000000 0.000000 0.000000 )
( -0.001139 0.000000 0.001515 0.000000 -0.014634 0.000000 )
( 0.001139 0.000000 0.001515 0.000000 0.014634 0.000000 )
( -0.019562 0.000000 -0.012810 0.000000 -0.000000 0.000000 )
( 0.019562 0.000000 -0.012810 0.000000 0.000000 0.000000 )
( 0.008543 0.000000 0.010392 0.000000 -0.000000 0.000000 )
( -0.008543 0.000000 0.010392 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 -0.010281 0.000000 -0.000000 0.000000 )
( -0.012172 0.000000 0.010802 0.000000 0.002321 0.000000 )
( 0.012172 0.000000 0.010802 0.000000 -0.002321 0.000000 )
( 0.000000 0.000000 -0.012471 0.000000 -0.000000 0.000000 )
( 0.009916 0.000000 -0.029646 0.000000 0.009330 0.000000 )
( -0.009916 0.000000 -0.029646 0.000000 -0.009330 0.000000 )
( 0.000000 0.000000 -0.041556 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 0.352492 0.000000 -0.000000 0.000000 )
( -0.074397 0.000000 0.481351 0.000000 0.037609 0.000000 )
( 0.074397 0.000000 0.481351 0.000000 -0.037609 0.000000 )
( -0.000000 0.000000 0.626023 0.000000 0.000000 0.000000 )
freq ( 37) = 19.620747 [THz] = 654.477680 [cm-1]
( 0.000188 0.000000 -0.000000 0.000000 0.007370 0.000000 )
( -0.000521 0.000000 -0.000410 0.000000 -0.003685 0.000000 )
( -0.000521 0.000000 0.000410 0.000000 -0.003685 0.000000 )
( 0.011970 0.000000 0.008301 0.000000 -0.000000 0.000000 )
( 0.011970 0.000000 -0.008301 0.000000 -0.000000 0.000000 )
( -0.020761 0.000000 -0.003052 0.000000 -0.000000 0.000000 )
( -0.020761 0.000000 0.003052 0.000000 -0.000000 0.000000 )
( -0.028806 0.000000 0.000000 0.000000 -0.001226 0.000000 )

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( 0.004748 0.000000 0.019373 0.000000 0.000613 0.000000 )
( 0.004748 0.000000 -0.019373 0.000000 0.000613 0.000000 )
( -0.016728 0.000000 -0.000000 0.000000 -0.004122 0.000000 )
( -0.014979 0.000000 0.001010 0.000000 0.002061 0.000000 )
( -0.014979 0.000000 -0.001010 0.000000 0.002061 0.000000 )
( 0.042813 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( 0.414546 0.000000 0.000000 0.000000 0.020891 0.000000 )
( 0.358275 0.000000 -0.032488 0.000000 -0.010446 0.000000 )
( 0.358275 0.000000 0.032488 0.000000 -0.010446 0.000000 )
( -0.750373 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
freq ( 38) = 19.620754 [THz] = 654.477918 [cm-1]
( -0.000000 0.000000 -0.000758 0.000000 -0.000000 0.000000 )
( -0.000410 0.000000 -0.000048 0.000000 0.006382 0.000000 )
( 0.000410 0.000000 -0.000048 0.000000 -0.006382 0.000000 )
( -0.008301 0.000000 0.011970 0.000000 -0.000000 0.000000 )
( 0.008301 0.000000 0.011970 0.000000 0.000000 0.000000 )
( 0.003052 0.000000 -0.020761 0.000000 -0.000000 0.000000 )
( -0.003052 0.000000 -0.020761 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 0.015933 0.000000 0.000000 0.000000 )
( 0.019373 0.000000 -0.017621 0.000000 -0.001062 0.000000 )
( -0.019373 0.000000 -0.017621 0.000000 0.001062 0.000000 )
( 0.000000 0.000000 -0.014395 0.000000 0.000000 0.000000 )
( 0.001010 0.000000 -0.016145 0.000000 -0.003570 0.000000 )
( -0.001010 0.000000 -0.016145 0.000000 0.003570 0.000000 )
( -0.000000 0.000000 0.042814 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 0.339514 0.000000 -0.000000 0.000000 )
( -0.032487 0.000000 0.395783 0.000000 0.018092 0.000000 )
( 0.032487 0.000000 0.395783 0.000000 -0.018092 0.000000 )
( 0.000000 0.000000 -0.750381 0.000000 0.000000 0.000000 )
freq ( 39) = 19.988149 [THz] = 666.732880 [cm-1]
( -0.007793 0.000000 -0.000000 0.000000 0.155061 0.000000 )
( 0.003896 0.000000 -0.006749 0.000000 0.155061 0.000000 )
( 0.003896 0.000000 0.006749 0.000000 0.155061 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.206718 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.206718 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.297359 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.297359 0.000000 )
( -0.012876 0.000000 0.000000 0.000000 0.348363 0.000000 )
( 0.006438 0.000000 -0.011151 0.000000 0.348363 0.000000 )
( 0.006438 0.000000 0.011151 0.000000 0.348363 0.000000 )
( -0.012740 0.000000 -0.000000 0.000000 -0.102940 0.000000 )
( 0.006370 0.000000 -0.011033 0.000000 -0.102940 0.000000 )
( 0.006370 0.000000 0.011033 0.000000 -0.102940 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.101440 0.000000 )
( 0.276762 0.000000 0.000000 0.000000 -0.081547 0.000000 )
( -0.138384 0.000000 0.239685 0.000000 -0.081547 0.000000 )
( -0.138384 0.000000 -0.239685 0.000000 -0.081547 0.000000 )
( 0.000001 0.000000 -0.000000 0.000000 -0.092179 0.000000 )
freq ( 40) = 20.987619 [THz] = 700.071628 [cm-1]
( -0.006016 0.000000 -0.000000 0.000000 0.024826 0.000000 )

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( 0.005156 0.000000 0.006450 0.000000 -0.012413 0.000000 )
( 0.005156 0.000000 -0.006450 0.000000 -0.012413 0.000000 )
( -0.016437 0.000000 -0.294919 0.000000 -0.000000 0.000000 )
( -0.016437 0.000000 0.294919 0.000000 -0.000000 0.000000 )
( -0.000337 0.000000 0.066450 0.000000 0.000000 0.000000 )
( -0.000337 0.000000 -0.066450 0.000000 0.000000 0.000000 )
( 0.023527 0.000000 -0.000000 0.000000 -0.148540 0.000000 )
( 0.007739 0.000000 -0.009116 0.000000 0.074270 0.000000 )
( 0.007739 0.000000 0.009116 0.000000 0.074270 0.000000 )
( 0.015067 0.000000 0.000000 0.000000 -0.004933 0.000000 )
( -0.027483 0.000000 -0.024567 0.000000 0.002466 0.000000 )
( -0.027483 0.000000 0.024567 0.000000 0.002466 0.000000 )
( -0.007980 0.000000 0.000000 0.000000 -0.000000 0.000000 )
( -0.148232 0.000000 -0.000000 0.000000 -0.004092 0.000000 )
( 0.484453 0.000000 0.365282 0.000000 0.002046 0.000000 )
( 0.484453 0.000000 -0.365282 0.000000 0.002046 0.000000 )
( 0.142641 0.000000 -0.000000 0.000000 0.000000 0.000000 )
freq ( 41) = 20.987620 [THz] = 700.071649 [cm-1]
( 0.000000 0.000000 -0.008879 0.000000 -0.000000 0.000000 )
( -0.006450 0.000000 0.002292 0.000000 -0.021500 0.000000 )
( 0.006450 0.000000 0.002292 0.000000 0.021500 0.000000 )
( -0.294920 0.000000 0.016437 0.000000 -0.000000 0.000000 )
( 0.294920 0.000000 0.016437 0.000000 0.000000 0.000000 )
( 0.066450 0.000000 0.000337 0.000000 -0.000000 0.000000 )
( -0.066450 0.000000 0.000337 0.000000 0.000000 0.000000 )
( -0.000000 0.000000 -0.002476 0.000000 0.000000 0.000000 )
( 0.009116 0.000000 -0.018264 0.000000 0.128639 0.000000 )
( -0.009116 0.000000 -0.018264 0.000000 -0.128639 0.000000 )
( -0.000000 0.000000 0.041667 0.000000 0.000000 0.000000 )
( 0.024566 0.000000 -0.000883 0.000000 0.004272 0.000000 )
( -0.024566 0.000000 -0.000883 0.000000 -0.004272 0.000000 )
( 0.000000 0.000000 0.007981 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 -0.695349 0.000000 0.000000 0.000000 )
( -0.365281 0.000000 -0.062663 0.000000 0.003543 0.000000 )
( 0.365281 0.000000 -0.062663 0.000000 -0.003543 0.000000 )
( -0.000000 0.000000 -0.142641 0.000000 0.000000 0.000000 )
freq ( 42) = 21.783777 [THz] = 726.628594 [cm-1]
( 0.000707 0.000000 -0.000000 0.000000 0.005020 0.000000 )
( -0.000354 0.000000 0.000612 0.000000 0.005020 0.000000 )
( -0.000354 0.000000 -0.000612 0.000000 0.005020 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.001411 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.001411 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.019054 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.019054 0.000000 )
( 0.001049 0.000000 -0.000000 0.000000 0.014159 0.000000 )
( -0.000525 0.000000 0.000909 0.000000 0.014159 0.000000 )
( -0.000525 0.000000 -0.000909 0.000000 0.014159 0.000000 )
( 0.043352 0.000000 0.000000 0.000000 -0.002898 0.000000 )
( -0.021676 0.000000 0.037544 0.000000 -0.002898 0.000000 )
( -0.021676 0.000000 -0.037544 0.000000 -0.002898 0.000000 )

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( -0.000000  0.000000  -0.000000  0.000000  -0.014850  0.000000  )
( -0.573851  0.000000  -0.000000  0.000000  -0.039034  0.000000  )
(  0.286925  0.000000  -0.496971  0.000000  -0.039034  0.000000  )
(  0.286925  0.000000   0.496971  0.000000  -0.039034  0.000000  )
(  0.000000  0.000000   0.000000  0.000000  -0.014714  0.000000  )
  freq ( 43) =  23.320224 [THz] =  777.878953 [cm-1]
(  0.001504  0.000000   0.000000  0.000000   0.020436  0.000000  )
(  0.000744  0.000000  -0.000439  0.000000  -0.010218  0.000000  )
(  0.000744  0.000000   0.000439  0.000000  -0.010218  0.000000  )
( -0.008961  0.000000   0.045824  0.000000  -0.000000  0.000000  )
( -0.008961  0.000000  -0.045824  0.000000  -0.000000  0.000000  )
( -0.003481  0.000000  -0.002927  0.000000  -0.000000  0.000000  )
( -0.003481  0.000000   0.002927  0.000000  -0.000000  0.000000  )
(  0.004267  0.000000   0.000000  0.000000   0.029804  0.000000  )
(  0.011155  0.000000   0.003977  0.000000  -0.014902  0.000000  )
(  0.011155  0.000000  -0.003977  0.000000  -0.014902  0.000000  )
(  0.033070  0.000000  -0.000000  0.000000  -0.000161  0.000000  )
( -0.021997  0.000000  -0.031793  0.000000   0.000081  0.000000  )
( -0.021997  0.000000   0.031793  0.000000   0.000081  0.000000  )
(  0.002069  0.000000   0.000000  0.000000  -0.000000  0.000000  )
( -0.500645  0.000000   0.000000  0.000000  -0.033941  0.000000  )
(  0.352683  0.000000   0.492667  0.000000   0.016970  0.000000  )
(  0.352683  0.000000  -0.492667  0.000000   0.016970  0.000000  )
(  0.051611  0.000000   0.000000  0.000000  -0.000000  0.000000  )
  freq ( 44) =  23.320225 [THz] =  777.878981 [cm-1]
( -0.000000  0.000000   0.000491  0.000000  -0.000000  0.000000  )
( -0.000439  0.000000   0.001251  0.000000   0.017698  0.000000  )
(  0.000439  0.000000   0.001251  0.000000  -0.017698  0.000000  )
( -0.045824  0.000000  -0.008961  0.000000  -0.000000  0.000000  )
(  0.045824  0.000000  -0.008961  0.000000   0.000000  0.000000  )
(  0.002927  0.000000  -0.003481  0.000000   0.000000  0.000000  )
( -0.002927  0.000000  -0.003481  0.000000  -0.000000  0.000000  )
( -0.000000  0.000000   0.013451  0.000000  -0.000000  0.000000  )
(  0.003977  0.000000   0.006563  0.000000   0.025811  0.000000  )
( -0.003977  0.000000   0.006563  0.000000  -0.025811  0.000000  )
( -0.000000  0.000000  -0.040353  0.000000   0.000000  0.000000  )
( -0.031793  0.000000   0.014714  0.000000  -0.000140  0.000000  )
(  0.031793  0.000000   0.014714  0.000000   0.000140  0.000000  )
( -0.000000  0.000000   0.002069  0.000000   0.000000  0.000000  )
(  0.000000  0.000000   0.637126  0.000000   0.000000  0.000000  )
(  0.492667  0.000000  -0.216202  0.000000  -0.029394  0.000000  )
( -0.492667  0.000000  -0.216202  0.000000   0.029394  0.000000  )
( -0.000000  0.000000   0.051611  0.000000   0.000000  0.000000  )
  freq ( 45) =  23.556256 [THz] =  785.752138 [cm-1]
( -0.000000  0.000000   0.001114  0.000000  -0.000000  0.000000  )
( -0.000965  0.000000  -0.000557  0.000000  -0.000000  0.000000  )
(  0.000965  0.000000  -0.000557  0.000000   0.000000  0.000000  )
(  0.000000  0.000000   0.000000  0.000000  -0.005943  0.000000  )
( -0.000000  0.000000   0.000000  0.000000   0.005943  0.000000  )
( -0.000000  0.000000   0.000000  0.000000   0.040623  0.000000  )

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(0.000000	0.000000	0.000000	0.000000	-0.040623	0.000000)
(-0.000000	0.000000	0.015251	0.000000	-0.000000	0.000000)
(-0.013208	0.000000	-0.007626	0.000000	-0.000000	0.000000)
(0.013208	0.000000	-0.007626	0.000000	0.000000	0.000000)
(-0.000000	0.000000	-0.041591	0.000000	-0.000000	0.000000)
(0.036019	0.000000	0.020796	0.000000	0.000000	0.000000)
(-0.036019	0.000000	0.020796	0.000000	-0.000000	0.000000)
(-0.000000	0.000000	-0.000000	0.000000	-0.000000	0.000000)
(0.000000	0.000000	0.574669	0.000000	0.000000	0.000000)
(-0.497680	0.000000	-0.287334	0.000000	0.000000	0.000000)
(0.497680	0.000000	-0.287334	0.000000	-0.000000	0.000000)
(-0.000000	0.000000	-0.000000	0.000000	-0.000000	0.000000)

freq (46) = 26.289018 [THz] = 876.907247 [cm-1]

(0.000000	0.000000	-0.001488	0.000000	-0.000000	0.000000)
(-0.000617	0.000000	-0.000420	0.000000	0.007313	0.000000)
(0.000617	0.000000	-0.000420	0.000000	-0.007313	0.000000)
(-0.001832	0.000000	0.258117	0.000000	-0.000000	0.000000)
(0.001832	0.000000	0.258117	0.000000	0.000000	0.000000)
(0.003245	0.000000	0.021622	0.000000	0.000000	0.000000)
(-0.003245	0.000000	0.021622	0.000000	-0.000000	0.000000)
(-0.000000	0.000000	-0.699855	0.000000	-0.000000	0.000000)
(-0.331640	0.000000	-0.125438	0.000000	0.004160	0.000000)
(0.331640	0.000000	-0.125438	0.000000	-0.004160	0.000000)
(-0.000000	0.000000	-0.013241	0.000000	-0.000000	0.000000)
(-0.008862	0.000000	0.002108	0.000000	0.000151	0.000000)
(0.008862	0.000000	0.002108	0.000000	-0.000151	0.000000)
(-0.000000	0.000000	0.006309	0.000000	-0.000000	0.000000)
(0.000000	0.000000	0.253818	0.000000	0.000000	0.000000)
(0.154900	0.000000	-0.014476	0.000000	-0.005698	0.000000)
(-0.154900	0.000000	-0.014476	0.000000	0.005698	0.000000)
(0.000000	0.000000	-0.105499	0.000000	-0.000000	0.000000)

freq (47) = 26.289018 [THz] = 876.907248 [cm-1]

(-0.000064	0.000000	-0.000000	0.000000	0.008445	0.000000)
(-0.001132	0.000000	-0.000617	0.000000	-0.004222	0.000000)
(-0.001132	0.000000	0.000617	0.000000	-0.004222	0.000000)
(0.258117	0.000000	0.001832	0.000000	-0.000000	0.000000)
(0.258117	0.000000	-0.001832	0.000000	-0.000000	0.000000)
(0.021622	0.000000	-0.003245	0.000000	0.000000	0.000000)
(0.021622	0.000000	0.003245	0.000000	0.000000	0.000000)
(0.066034	0.000000	-0.000000	0.000000	0.004804	0.000000)
(-0.508383	0.000000	-0.331640	0.000000	-0.002402	0.000000)
(-0.508383	0.000000	0.331640	0.000000	-0.002402	0.000000)
(0.007224	0.000000	-0.000000	0.000000	0.000174	0.000000)
(-0.008125	0.000000	-0.008862	0.000000	-0.000087	0.000000)
(-0.008125	0.000000	0.008862	0.000000	-0.000087	0.000000)
(0.006309	0.000000	0.000000	0.000000	-0.000000	0.000000)
(-0.103908	0.000000	0.000000	0.000000	-0.006580	0.000000)
(0.164387	0.000000	0.154900	0.000000	0.003290	0.000000)
(0.164387	0.000000	-0.154900	0.000000	0.003290	0.000000)
(-0.105499	0.000000	-0.000000	0.000000	-0.000000	0.000000)

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freq ( 48) = 27.588039 [THz] = 920.237910 [cm-1]
( 0.000000 0.000000 0.006411 0.000000 -0.000000 0.000000 )
( -0.005552 0.000000 -0.003205 0.000000 0.000000 0.000000 )
( 0.005552 0.000000 -0.003205 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.192665 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.192665 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.424654 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.424654 0.000000 )
( -0.000000 0.000000 0.142714 0.000000 0.000000 0.000000 )
( -0.123594 0.000000 -0.071357 0.000000 -0.000000 0.000000 )
( 0.123594 0.000000 -0.071357 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 0.004590 0.000000 0.000000 0.000000 )
( -0.003975 0.000000 -0.002295 0.000000 0.000000 0.000000 )
( 0.003975 0.000000 -0.002295 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.409801 0.000000 0.000000 0.000000 )
( 0.354898 0.000000 0.204900 0.000000 -0.000000 0.000000 )
( -0.354898 0.000000 0.204900 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000 )
freq ( 49) = 29.803404 [THz] = 994.134559 [cm-1]
( -0.005610 0.000000 0.000000 0.000000 0.013668 0.000000 )
( 0.002805 0.000000 -0.004858 0.000000 0.013668 0.000000 )
( 0.002805 0.000000 0.004858 0.000000 0.013668 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.352551 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 -0.352551 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.557783 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.557783 0.000000 )
( -0.000177 0.000000 -0.000000 0.000000 0.060442 0.000000 )
( 0.000089 0.000000 -0.000154 0.000000 0.060442 0.000000 )
( 0.000089 0.000000 0.000154 0.000000 0.060442 0.000000 )
( -0.002827 0.000000 -0.000000 0.000000 -0.037001 0.000000 )
( 0.001413 0.000000 -0.002448 0.000000 -0.037001 0.000000 )
( 0.001413 0.000000 0.002448 0.000000 -0.037001 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.001902 0.000000 )
( -0.181820 0.000000 0.000000 0.000000 -0.068603 0.000000 )
( 0.090910 0.000000 -0.157461 0.000000 -0.068603 0.000000 )
( 0.090910 0.000000 0.157461 0.000000 -0.068603 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.011316 0.000000 )
freq ( 50) = 29.811633 [THz] = 994.409045 [cm-1]
( 0.000000 0.000000 0.018234 0.000000 -0.000000 0.000000 )
( -0.015791 0.000000 -0.009117 0.000000 0.000000 0.000000 )
( 0.015791 0.000000 -0.009117 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 -0.206057 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.206057 0.000000 )
( -0.000000 0.000000 0.000000 0.000000 0.114052 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.114052 0.000000 )
( -0.000000 0.000000 -0.537213 0.000000 -0.000000 0.000000 )
( 0.465240 0.000000 0.268607 0.000000 0.000000 0.000000 )
( -0.465240 0.000000 0.268607 0.000000 -0.000000 0.000000 )
( -0.000000 0.000000 -0.013443 0.000000 0.000000 0.000000 )

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( 0.011642 0.000000 0.006722 0.000000 -0.000000 0.000000 )
( -0.011642 0.000000 0.006722 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 0.085111 0.000000 0.000000 0.000000 )
( -0.073708 0.000000 -0.042555 0.000000 -0.000000 0.000000 )
( 0.073708 0.000000 -0.042555 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000 )
freq ( 51) = 109.899985 [THz] = 3665.868919 [cm-1]
( -0.000017 0.000000 -0.000000 0.000000 0.000048 0.000000 )
( 0.000035 0.000000 0.000030 0.000000 -0.000024 0.000000 )
( 0.000035 0.000000 -0.000030 0.000000 -0.000024 0.000000 )
( -0.000063 0.000000 -0.000701 0.000000 0.000000 0.000000 )
( -0.000063 0.000000 0.000701 0.000000 0.000000 0.000000 )
( -0.000061 0.000000 0.000082 0.000000 -0.000000 0.000000 )
( -0.000061 0.000000 -0.000082 0.000000 -0.000000 0.000000 )
( 0.000263 0.000000 0.000000 0.000000 -0.000379 0.000000 )
( 0.000035 0.000000 -0.000132 0.000000 0.000189 0.000000 )
( 0.000035 0.000000 0.000132 0.000000 0.000189 0.000000 )
( -0.003161 0.000000 -0.000000 0.000000 0.050894 0.000000 )
( -0.000788 0.000000 0.001370 0.000000 -0.025447 0.000000 )
( -0.000788 0.000000 -0.001370 0.000000 -0.025447 0.000000 )
( 0.000101 0.000000 -0.000000 0.000000 -0.000000 0.000000 )
( 0.048416 0.000000 0.000000 0.000000 -0.813463 0.000000 )
( 0.011785 0.000000 -0.021149 0.000000 0.406731 0.000000 )
( 0.011785 0.000000 0.021149 0.000000 0.406731 0.000000 )
( 0.000294 0.000000 -0.000000 0.000000 0.000000 0.000000 )
freq ( 52) = 109.899985 [THz] = 3665.868921 [cm-1]
( -0.000000 0.000000 0.000053 0.000000 0.000000 0.000000 )
( 0.000030 0.000000 0.000000 0.000000 0.000042 0.000000 )
( -0.000030 0.000000 0.000000 0.000000 -0.000042 0.000000 )
( 0.000701 0.000000 -0.000063 0.000000 -0.000000 0.000000 )
( -0.000701 0.000000 -0.000063 0.000000 0.000000 0.000000 )
( -0.000082 0.000000 -0.000061 0.000000 -0.000000 0.000000 )
( 0.000082 0.000000 -0.000061 0.000000 0.000000 0.000000 )
( 0.000000 0.000000 -0.000041 0.000000 -0.000000 0.000000 )
( -0.000132 0.000000 0.000187 0.000000 -0.000328 0.000000 )
( 0.000132 0.000000 0.000187 0.000000 0.000328 0.000000 )
( -0.000000 0.000000 0.000003 0.000000 0.000000 0.000000 )
( 0.001370 0.000000 -0.002370 0.000000 0.044075 0.000000 )
( -0.001370 0.000000 -0.002370 0.000000 -0.044076 0.000000 )
( 0.000000 0.000000 0.000101 0.000000 -0.000000 0.000000 )
( 0.000000 0.000000 -0.000426 0.000000 -0.000000 0.000000 )
( -0.021149 0.000000 0.036206 0.000000 -0.704479 0.000000 )
( 0.021149 0.000000 0.036206 0.000000 0.704479 0.000000 )
( 0.000000 0.000000 0.000294 0.000000 0.000000 0.000000 )
freq ( 53) = 110.327993 [THz] = 3680.145717 [cm-1]
( 0.000013 0.000000 -0.000000 0.000000 0.000722 0.000000 )
( -0.000006 0.000000 0.000011 0.000000 0.000722 0.000000 )
( -0.000006 0.000000 -0.000011 0.000000 0.000722 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.000837 0.000000 )

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( 0.000000 0.000000 -0.000000 0.000000 0.000837 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.001161 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.001161 0.000000 )
( 0.000115 0.000000 0.000000 0.000000 -0.000396 0.000000 )
( -0.000057 0.000000 0.000099 0.000000 -0.000396 0.000000 )
( -0.000057 0.000000 -0.000099 0.000000 -0.000396 0.000000 )
( -0.002208 0.000000 -0.000000 0.000000 0.035535 0.000000 )
( 0.001104 0.000000 -0.001912 0.000000 0.035535 0.000000 )
( 0.001104 0.000000 0.001912 0.000000 0.035535 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000709 0.000000 )
( 0.034162 0.000000 0.000000 0.000000 -0.575235 0.000000 )
( -0.017081 0.000000 0.029585 0.000000 -0.575235 0.000000 )
( -0.017081 0.000000 -0.029585 0.000000 -0.575235 0.000000 )
( -0.000000 0.000000 -0.000000 0.000000 0.001724 0.000000 )
freq ( 54) = 111.207771 [THz] = 3709.491940 [cm-1]
( 0.000218 0.000000 0.000000 0.000000 -0.000188 0.000000 )
( -0.000109 0.000000 0.000189 0.000000 -0.000188 0.000000 )
( -0.000109 0.000000 -0.000189 0.000000 -0.000188 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 0.000326 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.000326 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.000105 0.000000 )
( 0.000000 0.000000 0.000000 0.000000 -0.000105 0.000000 )
( 0.000007 0.000000 -0.000000 0.000000 -0.000204 0.000000 )
( -0.000003 0.000000 0.000006 0.000000 -0.000204 0.000000 )
( -0.000003 0.000000 -0.000006 0.000000 -0.000204 0.000000 )
( 0.000005 0.000000 -0.000000 0.000000 0.000021 0.000000 )
( -0.000002 0.000000 0.000004 0.000000 0.000021 0.000000 )
( -0.000002 0.000000 -0.000004 0.000000 0.000021 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 -0.062680 0.000000 )
( -0.000102 0.000000 -0.000000 0.000000 0.001428 0.000000 )
( 0.000051 0.000000 -0.000089 0.000000 0.001428 0.000000 )
( 0.000051 0.000000 0.000089 0.000000 0.001428 0.000000 )
( 0.000000 0.000000 -0.000000 0.000000 0.998030 0.000000 )
*****

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