Supplement of Eur. J. Mineral., 38, 75–101, 2026
https://doi.org/10.5194/ejm-38-75-2026-supplement

European Journal of Mineralogy
Open Access

Supplement of

Crystal structure, chemical composition, and twinning of götzenite and wöhlerite from the Fohberg phonolite, Kaiserstuhl

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Supplements

Table S1: Weight fractions of trace elements related to the main elements by scaling Ca measured by LA-ICP-MS to Ca from EPMA. All values are given in wt%. UF = University of Freiburg, UB = University of Bremen.

	götzenite	wöhlerite			götzenite	wöhlerite		götzenite	wöhlerite
	UB	UF	UB		UB	UB		UB	UB
Ca	25.86(78)	22.04(38)	21.41(41)	Ca	25.86(78)	21.41(41)			
Na	4.30(16)	4.66(18)	4.63(14)	Rb	0.00003(2)	0.00008(8)	Dy	0.003(2)	0.0017(4)
Mn	0.10(3)	0.60(5)	0.62(4)	Y	0.019(8)	0.018(3)	Ho	0.0005(3)	0.00034(7)
Fe	0.18(8)	1.62(11)	1.60(13)	Ba	0.013(1)	0.0.0012(5)	Er	0.0012(7)	0.0012(2)
Si	13.99(22)	14.06(15)	13.79(12)	La	1.3(2)	0.07(2)	Tm	0.00016(8)	0.00023(4)
Zr	0.64(26)	7.08(43)	7.21(27)	Ce	2.0(4)	0.17(5)	Yb	0.0011(5)	0.0022(3)
Sr	1.44(33)	0.41(7)	0.38(8)	Pr	0.14(3)	0.016(5)	Lu	0.00015(6)	0.00039(6)
Ti	4.78(46)	1.22(22)	1.15(22)	Nd	0.30(3)	0.05(1)	Hf	0.0030(6)	0.048(0)
Nb	2.03(69)	8.86(25)	9.33(42)	Sm	0.017(3)	0.004(1)	Ta	0.04(2)	0.26(2)
O	32.39(55)	34.26(85)	33.89(27)	Eu	0.0031(9)	0.0009(3)	Pb	0.00071(7)	0.00039(4)
F	8.38(30)	2.80(15)	3.61(24)	Gd	0.006(3)	0.0023(6)	Th	0.20(7)	0.017(5)
				Tb	0.0006(3)	0.00028(7)	U	0.07(1)	0.043(2)

Table S2: Comparison of atomic parameters of götzenites with other triclinic minerals of the rinkite group, the separation sep representing the distance to the corresponding atom in this work, references (ref), and 'No.' referring to the entry number in Table 10.

site	*x*	*y*	*z*	U_{iso}/U_{eq} (Å^2)	mineral	sep (Å)	ref	No.
M^H	0.63090(4)	0.22767(7)	0.90948(12)	0.0100(1)	götzenite Fohberg		this work	2
Ca1	0.6389(7)	0.2115(11)	0.9097(8)	0.001(2)	götzenite Mt. Shaheru	0.131	(1)	5
M1	0.63094(5)	0.22638(8)	0.90950(5)	0.0110(1)	götzenite East Greenland	0.007	(2)	15
Ca1	0.6322(2)	0.2218(4)	0.9096(2)	0.013(1)	Zr-rich götzenite Umbria	0.038	(3)	17
M^H	0.63631(2)	0.22040(4)	0.90986(7)	0.00776(9)	fogoite-(Y)	0.072	(4)	23
M1	0.61214(5)	0.25871(6)	0.90480(5)	0.0156(1)	batievaite-(Y)	0.273	(5)	25
M1	0.63494(3)	0.22243(4)	0.91042(3)	0.01043(7)	hainite-(Y)	0.053	(6)	27
M^H	0.63264(4)	0.22434(7)	0.90910(5)	0.0159(1)	bortolanite Brazil	0.028	(7)	30
M^H	0.64043(6)	0.21591(11)	0.91081(8)	0.0113(2)	bortolanite Lovozero	0.122	(8)	31
A^P	0.63252(5)	0.22794(8)	0.40746(14)	0.0158(1)	götzenite Fohberg		this work	2
Ca3	0.6305(7)	0.2268(11)	0.4075(9)	0.002(2)	götzenite Mt. Shaheru	0.020	(1)	5
M3	0.63285(6)	0.2274(1)	0.40744(6)	0.0168(2)	götzenite East Greenland	0.005	(2)	15
Ca2	0.6345(2)	0.2194(4)	0.4078(3)	0.011(1)	Zr-rich götzenite Umbria	0.055	(3)	17
A^P	0.63726(6)	0.22484(10)	0.41070(16)	0.0159(2)	fogoite-(Y)	0.053	(4)	23
M3	0.61613(8)	0.2661(1)	0.40340(8)	0.0179(2)	batievaite-(Y)	0.291	(5)	25
M3	0.63580(5)	0.22290(8)	0.40921(6)	0.0168(1)	hainite-(Y)	0.046	(6)	27
A^P	0.63248(5)	0.23075(8)	0.40732(6)	0.0181(1)	bortolanite	0.016	(7)	30
A^P	0.63706(8)	0.21885(15)	0.40961(11)	0.0144(3)	bortolanite Lovozero	0.074	(8)	31
M^{o}1	-0.0131(3)	0.0240(5)	-0.0041(6)	0.0041(4)	götzenite Fohberg		this work	2
Ti	0	0	0	0.012(3)	götzenite Mt. Shaheru	0.201	(1)	5
M5	0	0	0	0.0243(3)	götzenite East Greenland	0.201	(2)	15
Ti5	0	0	0	0.018(1)	Zr-rich götzenite Umbria	0.201	(3)	17
M^{o}1	0.0117(4)	0.0221(6)	-0.0037(9)	0.0036(4)	fogoite-(Y)	0.240	(4)	23
M5	0	0	0	0.0208(2)	batievaite-(Y)	0.201	(5)	25
M5	0	0	0	0.0198(1)	hainite-(Y)	0.201	(6)	27
M^{o}1	-0.0131(3)	0.0233(5)	-0.0034(4)	0.0083(4)	bortolanite	0.006	(7)	30
M^{o}1	0	0	0	0.0167(4)	bortolanite Lovozero	0.201	(8)	31
M^{o}2	0	0	½	0.0180(5)	götzenite Fohberg		this work	2
Na	0	0	½	0.015(6)	götzenite Mt. Shaheru	0.000	(1)	5
M4	0	0	½	0.0153(4)	götzenite East Greenland	0.000	(2)	15

Na4	0	0	½	0.025(2)	Zr-rich götzenite Umbria	0.000	(3)	17
Mo2	0	0	½	0.0090(3)	fogoite-(Y)	0.000	(4)	23
M4	0	0	½	0.035(3)	batievaite-(Y)	0.000	(5)	25
M4	0	0	½	0.0217(5)	hainite-(Y)	0.000	(6)	27
Mo2	0	0	½	0.0150(4)	bortolanite	0.000	(7)	30
Mo2	0	0	½	0.0188(8)	bortolanite Lovozero	0.000	(8)	31
Mo3	0.99338(7)	0.49638(10)	0.24195(8)	0.0171(3)	götzenite Fohberg		this work	2
Ca2	0.9859(8)	0.4955(15)	0.2418(12)	0.007(2)	götzenite Mt. Shaheru	0.071	(1)	5
M2	0.99344(9)	0.4966(1)	0.24160(9)	0.0186(2)	götzenite East Greenland	0.003	(2)	15
Ca3	0.9935(4)	0.4960(6)	0.2421(4)	0.018(1)	Zr-rich götzenite Umbria	0.003	(3)	17
Mo3	0.99700(11)	0.49783(17)	0.24679(14)	0.0133(3)	fogoite-(Y)	0.044	(4)	23
M2	0.9994(2)	0.4970(3)	0.2520(2)	0.0279(5)	batievaite-(Y)	0.084	(5)	25
M2	0.99577(9)	0.4973(1)	0.2446(1)	0.0210(3)	hainite-(Y)	0.027	(6)	27
Mo3	0.99424(8)	0.49700(11)	0.24233(9)	0.0133(2)	bortolanite	0.008	(7)	30
Mo3	0.99473(11)	0.49734(19)	0.24513(14)	0.0175(5)	bortolanite Lovozero	0.025	(8)	31
Si1	0.71722(7)	0.75153(12)	0.65187(11)	0.0076(2)	götzenite Fohberg		this work	2
Si1	0.7197(6)	0.7475(11)	0.6460(14)	0.009(2)	götzenite Mt. Shaheru	0.059	(1)	5
Si1	0.71688(8)	0.7504(1)	0.6519(1)	0.0091(1)	götzenite East Greenland	0.007	(2)	15
Si1	0.7179(3)	0.7478(5)	0.6529(4)	0.012(1)	Zr-rich götzenite Umbria	0.024	(3)	17
Si1	0.71363(8)	0.74517(14)	0.65351(15)	0.0071(2)	fogoite-(Y)	0.049	(4)	23
Si1	0.7201(1)	0.7803(2)	0.6500(1)	0.0150(2)	batievaite-(Y)	0.163	(5)	25
Si1	0.71371(6)	0.7469(1)	0.65096(8)	0.0102(1)	hainite-(Y)	0.038	(6)	27
Si1	0.71686(7)	0.75021(11)	0.65134(8)	0.0107(1)	bortolanite	0.008	(7)	30
Si1	0.71409(11)	0.7423(2)	0.65579(16)	0.0112(3)	bortolanite Lovozero	0.065	(8)	31
Si2	0.72454(8)	0.75572(13)	0.21531(9)	0.0075(2)	götzenite Fohberg		this work	2
Si2	0.7210(6)	0.7471(10)	0.2100(12)	0.003(2)	götzenite Mt. Shaheru	0.063	(1)	5
Si2	0.72432(8)	0.7551(1)	0.2148(1)	0.0094(1)	götzenite East Greenland	0.005	(2)	15
Si2	0.7229(3)	0.7510(6)	0.2132(4)	0.016(1)	Zr-rich götzenite Umbria	0.031	(3)	17
Si2	0.72015(9)	0.74442(15)	0.21150(12)	0.0075(2)	fogoite-(Y)	0.073	(4)	23
Si2	0.7260(1)	0.7813(2)	0.2171(1)	0.0151(2)	batievaite-(Y)	0.145	(5)	25
Si2	0.72028(6)	0.7486(1)	0.21358(8)	0.0103(1)	hainite-(Y)	0.052	(6)	27
Si2	0.72274(7)	0.7545(1)	0.21326(8)	0.0110(1)	bortolanite	0.020	(7)	30
Si2	0.71794(12)	0.7430(2)	0.20724(17)	0.0131(3)	bortolanite Lovozero	0.099	(8)	31

O1	0.7590(2)	0.7867(4)	0.4441(3)	0.0230(4)	götzenite Fohberg		this work	2
O1	0.762(2)	0.784(4)	0.443(3)	0.030(4)	götzenite Mt. Shaheru	0.039	(1)	5
O1	0.7583(2)	0.7860(4)	0.4440(3)	0.0233(5)	götzenite East Greenland	0.007	(2)	15
O1	0.7592(8)	0.7899(13)	0.4424(10)	0.024(2)	Zr-rich götzenite Umbria	0.021	(3)	17
O1	0.7446(3)	0.7708(5)	0.4393(4)	0.0206(5)	fogoite-(Y)	0.149	(4)	23
O1	0.7566(4)	0.7803(8)	0.4419(4)	0.0401(9)	batievaite-(Y)	0.042	(5)	25
O1	0.7495(2)	0.7793(4)	0.4408(3)	0.0291(5)	hainite-(Y)	0.092	(6)	27
O1	0.7555(2)	0.7791(4)	0.4420(3)	0.0315(5)	bortolanite	0.051	(7)	30
O1	0.7437(4)	0.7728(10)	0.4387(5)	0.0505(13)	bortolanite Lovozero	0.152	(8)	31
O2	0.6160(2)	0.9413(3)	0.6684(6)	0.0142(5)	götzenite Fohberg		this work	2
O2	0.619(2)	0.927(3)	0.673(3)	0.000(4)	götzenite Mt. Shaheru	0.096	(1)	5
O2	0.6152(2)	0.9402(3)	0.6688(3)	0.0145(4)	götzenite East Greenland	0.010	(2)	15
O2	0.6147(8)	0.9339(13)	0.6689(9)	0.017(2)	Zr-rich götzenite Umbria	0.042	(3)	17
O2	0.6138(3)	0.9385(4)	0.6769(6)	0.0141(7)	fogoite-(Y)	0.071	(4)	23
O2	0.6209(3)	0.9963(5)	0.6647(4)	0.0220(5)	batievaite-(Y)	0.312	(5)	25
O2	0.6142(2)	0.9412(3)	0.6717(3)	0.0163(3)	hainite-(Y)	0.033	(6)	27
O2	0.6161(2)	0.9416(3)	0.6679(3)	0.0177(3)	bortolanite	0.004	(7)	30
O2	0.6140(3)	0.9341(6)	0.6714(5)	0.0203(7)	bortolanite Lovozero	0.049	(8)	31
O3	0.6189(2)	0.9360(3)	0.1423(6)	0.0157(5)	götzenite Fohberg		this work	2
O3	0.614(2)	0.925(4)	0.127(3)	0.018(5)	götzenite Mt. Shaheru	0.124	(1)	5
O3	0.6188(2)	0.9363(3)	0.1415(3)	0.0171(4)	götzenite East Greenland	0.004	(2)	15
O3	0.6181(8)	0.9314(13)	0.1407(9)	0.016(2)	Zr-rich götzenite Umbria	0.028	(3)	17
O3	0.6131(2)	0.9248(4)	0.1324(7)	0.0151(7)	fogoite-(Y)	0.098	(4)	23
O3	0.6236(3)	0.9924(5)	0.1478(4)	0.0231(5)	batievaite-(Y)	0.319	(5)	25
O3	0.6155(2)	0.9326(3)	0.1368(3)	0.0187(3)	hainite-(Y)	0.048	(6)	27
O3	0.6181(2)	0.9369(3)	0.1411(3)	0.0200(4)	bortolanite	0.012	(7)	30
O3	0.6127(4)	0.9233(6)	0.1353(5)	0.0254(8)	bortolanite Lovozero	0.094	(8)	31
O4	0.6450(3)	0.4796(4)	0.6657(7)	0.0237(5)	götzenite Fohberg		this work	2
O4	0.636(2)	0.472(4)	0.665(3)	0.026(5)	götzenite Mt. Shaheru	0.091	(1)	5
O4	0.6436(3)	0.4773(4)	0.6670(3)	0.0238(5)	götzenite East Greenland	0.023	(2)	15
O4	0.6467(8)	0.4764(14)	0.6648(10)	0.021(2)	Zr-rich götzenite Umbria	0.026	(3)	17
O4	0.6374(3)	0.4697(4)	0.6756(7)	0.0177(6)	fogoite-(Y)	0.122	(4)	23
O4	0.6247(3)	0.5248(5)	0.6681(4)	0.0227(5)	batievaite-(Y)	0.356	(5)	25
O4	0.6390(2)	0.4735(3)	0.6693(3)	0.0230(4)	hainite-(Y)	0.074	(6)	27
O4	0.6419(3)	0.4786(3)	0.6690(3)	0.0272(4)	bortolanite	0.044	(7)	30

O4	0.6416(4)	0.4694(6)	0.6724(5)	0.0255(8)	bortolanite Lovozero	0.083	(8)	31
O5	0.6674(3)	0.4807(4)	0.1612(7)	0.0271(5)	götzenite Fohberg		this work	2
O5	0.676(2)	0.465(3)	0.162(3)	0.014(4)	götzenite Mt. Shaheru	0.132	(1)	5
O5	0.6660(3)	0.4790(4)	0.1607(3)	0.0288(5)	götzenite East Greenland	0.017	(2)	15
O5	0.6706(9)	0.4755(15)	0.1664(10)	0.027(2)	Zr-rich götzenite Umbria	0.057	(3)	17
O5	0.6552(3)	0.4686(4)	0.1488(7)	0.0183(6)	fogoite-(Y)	0.142	(4)	23
O5	0.6316(4)	0.5282(5)	0.1461(4)	0.0275(6)	batievaite-(Y)	0.474	(5)	25
O5	0.6567(3)	0.4734(3)	0.1553(3)	0.0257(4)	hainite-(Y)	0.106	(6)	27
O5	0.6613(3)	0.4794(4)	0.1558(3)	0.0341(5)	bortolanite	0.065	(7)	30
O5	0.6585(4)	0.4664(6)	0.1529(5)	0.0258(8)	bortolanite Lovozero	0.115	(8)	31
O6	0.8760(2)	0.8134(4)	0.7858(3)	0.0175(4)	götzenite Fohberg		this work	2
O6	0.879(2)	0.819(3)	0.778(3)	0.022(4)	götzenite Mt. Shaheru	0.075	(1)	5
O6	0.8757(2)	0.8129(3)	0.7855(3)	0.0170(4)	götzenite East Greenland	0.005	(2)	15
O6	0.8791(8)	0.8184(13)	0.7806(9)	0.022(2)	Zr-rich götzenite Umbria	0.058	(3)	17
O6	0.8746(3)	0.8111(4)	0.7826(3)	0.0144(5)	fogoite-(Y)	0.028	(4)	23
O6	0.8778(3)	0.8118(6)	0.7870(4)	0.0296(7)	batievaite-(Y)	0.021	(5)	25
O6	0.8743(2)	0.8111(4)	0.7818(3)	0.0219(4)	hainite-(Y)	0.034	(6)	27
O6	0.8763(2)	0.8138(3)	0.7835(3)	0.0198(4)	bortolanite	0.019	(7)	30
O6	0.8765(3)	0.8114(6)	0.7764(5)	0.0261(8)	bortolanite Lovozero	0.071	(8)	31
O7	0.8861(2)	0.8361(3)	0.1719(3)	0.0163(4)	götzenite Fohberg		this work	2
O7	0.881(2)	0.830(3)	0.171(3)	0.019(4)	götzenite Mt. Shaheru	0.054	(1)	5
O7	0.8856(2)	0.8355(3)	0.1717(3)	0.0165(4)	götzenite East Greenland	0.006	(2)	15
O7	0.8848(8)	0.8307(13)	0.1722(9)	0.023(2)	Zr-rich götzenite Umbria	0.030	(3)	17
O7	0.8824(2)	0.8285(5)	0.1703(3)	0.0142(5)	fogoite-(Y)	0.050	(4)	23
O7	0.8846(3)	0.8218(6)	0.1659(4)	0.0299(7)	batievaite-(Y)	0.089	(5)	25
O7	0.8826(2)	0.8290(4)	0.1718(3)	0.0219(4)	hainite-(Y)	0.047	(6)	27
O7	0.8842(2)	0.8329(3)	0.1699(3)	0.0193(4)	bortolanite	0.025	(7)	30
O7	0.8806(3)	0.8274(6)	0.1740(5)	0.0254(8)	bortolanite Lovozero	0.070	(8)	31
X^{o}_{M}	0.8856(2)	0.2602(3)	0.9677(5)	0.0143(5)	götzenite Fohberg		this work	2
O8	0.884(2)	0.256(3)	0.969(3)	0.004(4)	götzenite Mt. Shaheru	0.030	(1)	5
X8	0.8852(2)	0.2592(3)	0.9675(2)	0.0216(4)	götzenite East Greenland	0.007	(2)	15
F2	0.8856(7)	0.2635(12)	0.9688(9)	0.028(2)	Zr-rich götzenite Umbria	0.021	(3)	17
X^{o}_{M}	0.8787(2)	0.2498(4)	0.9673(6)	0.0163(4)	fogoite-(Y)	0.081	(4)	23

X8	0.8702(4)	0.2748(8)	0.9674(5)	0.0300(7)	batievaite-(Y)	0.183	(5)	25
X8	0.8813(2)	0.2583(3)	0.9671(2)	0.0207(4)	hainite-(Y)	0.041	(6)	27
X^{o}_{M}	0.8841(2)	0.2569(3)	0.9671(2)	0.0182(3)	bortolanite	0.022	(7)	30
X^{o}_{M}	0.8810(3)	0.2568(6)	0.9660(4)	0.0206(10)	bortolanite Lovozero	0.044	(8)	31
X^{o}_{A}	0.8869(2)	0.3062(3)	0.4761(5)	0.0189(4)	götzenite Fohberg		this work	2
O9,F	0.890(2)	0.313(3)	0.475(3)	0.007(4)	götzenite Mt. Shaheru	0.045	(1)	5
F9	0.8856(2)	0.3062(3)	0.4759(2)	0.0187(4)	götzenite East Greenland	0.012	(2)	15
F1	0.8888(6)	0.3059(11)	0.4757(8)	0.019(1)	Zr-rich götzenite Umbria	0.019	(3)	17
X^{o}_{A}	0.8806(2)	0.2988(4)	0.4721(7)	0.0221(4)	fogoite-(Y)	0.069	(4)	23
X9	0.8803(4)	0.3013(8)	0.4721(7)	0.048(1)	batievaite-(Y)	0.065	(5)	25
F9	0.8820(2)	0.3019(3)	0.4739(3)	0.0280(4)	hainite-(Y)	0.049	(6)	27
X^{o}_{A}	0.8842(2)	0.3044(3)	0.4744(2)	0.0217(3)	bortolanite	0.026	(7)	30
X^{o}_{A}	0.8834(3)	0.2978(5)	0.4746(4)	0.0231(6)	bortolanite Lovozero	0.053	(8)	31

(1) Cannillo et al. (1972); (2) Christiansen et al. (2003a); (3) Bellezza et al. (2004b), transformed according to left-hand transformation **a**, **c**, **b**; (4) Cámara et al. (2017); (5) Lyalina et al. (2016); (6) Lyalina et al. (2015); (7) Day et al. (2022); (8) Selivanova et al. (2024)

Table S3: Anisotropic displacement parameters (Å^2) of götzenite

site	Wyck. pos.	$U11$	$U22$	$U33$	$U23$	$U13$	$U12$	U_{eq}
M^H	2i	0.0124(2)	0.0100(2)	0.0058(2)	-0.0009(4)	0.0016(4)	-0.0025(2)	0.0100(1)
A^P	2i	0.0134(2)	0.0217(3)	0.0092(3)	-0.0026(5)	0.0033(4)	-0.0059(2)	0.0158(1)
M°1	2i	0.0043(10)	0.0042(11)	0.0044(5)	0.0009(8)	0.0003(8)	0.0026(5)	0.0041(4)
M°2	1b	0.0116(7)	0.0176(7)	0.0235(8)	-0.0029(12)	-0.0004(11)	0.0030(5)	0.0180(5)
M°3	2i	0.0324(5)	0.0114(4)	0.0107(4)	0.0014(6)	0.0057(6)	0.0108(3)	0.0171(3)
Si1	2i	0.0074(3)	0.0079(3)	0.0077(5)	-0.0002(2)	0.0013(2)	0.0024(2)	0.0076(2)
Si2	2i	0.0077(3)	0.0082(3)	0.0075(5)	0.0010(2)	0.0024(2)	0.0027(2)	0.0075(2)
O1	2i	0.0226(10)	0.0367(12)	0.0084(8)	0.0003(9)	0.0063(9)	-0.0010(9)	0.0230(4)
O2	2i	0.0114(9)	0.0152(9)	0.0174(12)	-0.0031(11)	0.0019(10)	0.0070(7)	0.0142(5)
O3	2i	0.0119(9)	0.0171(9)	0.0209(13)	0.0058(12)	0.0047(11)	0.0085(7)	0.0157(5)
O4	2i	0.0357(12)	0.0124(9)	0.0188(10)	0.0028(13)	0.0045(14)	-0.0056(8)	0.0237(5)
O5	2i	0.0465(14)	0.0129(9)	0.0200(11)	-0.0021(14)	0.0106(16)	-0.0041(9)	0.0271(5)
O6	2i	0.0139(10)	0.0199(11)	0.0165(9)	-0.0066(8)	-0.0054(7)	0.0064(8)	0.0175(4)
O7	2i	0.0128(9)	0.0202(10)	0.0187(10)	0.0070(7)	0.0085(7)	0.0052(8)	0.0163(4)
X^o_M	2i	0.0107(8)	0.0164(9)	0.0156(9)	-0.0002(10)	0.0018(10)	0.0032(6)	0.0143(5)
X^o_A	2i	0.0155(8)	0.0182(8)	0.0235(9)	0.0009(10)	0.0039(10)	0.0042(6)	0.0189(4)

The isotropic displacement parameter U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor. Coefficients Uij of the anisotropic displacement factor tensor of the atoms are defined by: $-2\pi^2[(ha^*)^2U_{11} + \cdots + 2hka^*b^*U_{12} + \cdots]$.

Table S4: Comparison of atomic parameters of wöhlerites, listing the separation sep representing the distance to the corresponding atom in this work, references (ref), and 'No.' referring to the entry number in Table 16.

site	*x*	*y*	*z*	U_{iso}/U_{eq} (Å^2)	locality	sep (Å)	ref	No.
X1	0.34094(3)	0.24269(3)	0.05379(5)	0.0071(1)	Fohberg		this work	2
Ca_1	0.345	0.248	0.031		Langesundsfjord Norway	0.193	(1)	6
Zr_1	0.343	0.247	0.053		Barkevik Norway	0.051	(2)	8
Zr	0.34201(3)	0.24330(7)	0.05379(4)	0.0053	Brevik Norway	0.013	(3)	10
M2	0.3413(1)	0.2446(1)	0.0535(1)	0.0093(2)	Prairie Lake Ontario	0.020	(4)	18
Zr1	0.34331	0.24260	0.05357	0.00842	Los Archipelago	0.026	(5)	22
Zr	0.3427(1)	0.2432(1)	0.0535(2)	0.012(3)	Monte Somma, Italy	0.021	(6)	23
X2	0.34498(6)	0.25512(8)	0.55269(11)	0.0129(2)	Fohberg		this work	2
$(Zr,Nb)_1$	0.345	0.248	0.548		Langesundsfjord Norway	0.081	(1)	6
Ca_1	0.347	0.257	0.552		Barkevik Norway	0.031	(2)	8
Ca(1)	0.34605(7)	0.25395(13)	0.55184(10)	0.0099	Brevik Norway	0.019	(3)	10
Ca4	0.3463(2)	0.2556(2)	0.5522(3)	0.0154(3)	Prairie Lake Ontario	0.017	(4)	18
Ca1	0.34587	0.25271	0.55109	0.01293	Los Archipelago	0.030	(5)	22
Ca(1)	0.3469(3)	0.2529(4)	0.5526(4)	0.019(1)	Monte Somma, Italy	0.031	(6)	23
X3	0.63036(10)	0.36900(13)	0.44481(20)	0.0151(5)	Fohberg		this work	2
Ca_3	0.631	0.373	0.437		Langesundsfjord Norway	0.072	(1)	6
Na_2	0.636	0.369	0.454		Barkevik Norway	0.074	(2)	8
Na(2)	0.63327(16)	0.37013(20)	0.44880(23)	0.0134	Brevik Norway	0.037	(3)	10
Na1	0.6306(3)	0.3685(4)	0.4467(6)	0.0135(7)	Prairie Lake Ontario	0.014	(4)	18
Na2	0.6339	0.37054	0.44905	0.0161	Los Archipelago	0.043	(5)	22
Na(2)	0.6319(4)	0.3706(5)	0.4486(8)	0.020(2)	Monte Somma, Italy	0.032	(6)	23
X4	0.36944(6)	0.86545(8)	0.05333(11)	0.0116(2)	Fohberg		this work	2
Na_2	0.369	0.867	0.055		Langesundsfjord Norway	0.021	(1)	6
Ca_3	0.365	0.871	0.052		Barkevik Norway	0.073	(2)	8
Ca(3)	0.36750(8)	0.86642(10)	0.05383(11)	0.0092	Brevik Norway	0.025	(3)	10
Ca2	0.3684(1)	0.8662(2)	0.0537(3)	0.0138(3)	Prairie Lake Ontario	0.015	(4)	18
Ca3	0.36868	0.86617	0.05497	0.01136	Los Archipelago	0.018	(5)	22
Ca(3)	0.3693(2)	0.8668(3)	0.0554(5)	0.017(1)	Monte Somma, Italy	0.021	(6)	23

X5	0.87654(14)	0.52373(15)	0.30968(24)	0.0187(5)	Fohberg		this work	2
Na_1	0.872	0.507	0.318		Langesundsfjord Norway	0.193	(1)	6
Na_1	0.885	0.525	0.318		Barkevik Norway	0.092	(2)	8
Na(1)	0.87790(18)	0.52249(21)	0.31346(24)	0.0158	Brevik Norway	0.029	(3)	10
Na2	0.8757(3)	0.5231(3)	0.3088(5)	0.0145(7)	Prairie Lake Ontario	0.011	(4)	18
Na1	0.87929	0.52275	0.31198	0.0185	Los Archipelago	0.031	(5)	22
Na(1)	0.8784(4)	0.5239(6)	0.3091(7)	0.021(2)	Monte Somma, Italy	0.022	(6)	23
X6	0.13331(3)	0.00691(3)	0.19442(5)	0.00791(8)	Fohberg		this work	2
$(Zr,Nb)_2$	0.128	0.007	0.193		Langesundsfjord Norway	0.055	(1)	6
$(Nb,Zr)_2$[a]	0.131	0.010	0.192		Barkevik Norway	0.041	(2)	8
Nb	0.13104(4)	0.00601(6)	0.19173(5)	0.0094	Brevik Norway	0.027	(3)	10
M1	0.1339(1)	0.0065(1)	0.1955(1)	0.0067(1)	Prairie Lake Ontario	0.009	(4)	18
Nb1	0.12664	0.00854	0.18665	0.01356	Los Archipelago	0.077	(5)	22
Nb	0.1299(1)	0.0085(1)	0.1897(2)	0.014(1)	Monte Somma, Italy	0.044	(6)	23
X7	0.84623(6)	0.13562(6)	0.30041(10)	0.0104(1)	Fohberg		this work	2
Ca_4	0.848	0.138	0.310		Langesundsfjord Norway	0.070	(1)	6
Ca_4	0.847	0.141	0.300		Barkevik Norway	0.056	(2)	8
Ca(4)	0.84655(7)	0.13718(10)	0.30017(10)	0.0079	Brevik Norway	0.017	(3)	10
Ca3	0.8449(1)	0.1362(2)	0.2994(2)	0.0129(3)	Prairie Lake Ontario	0.015	(4)	18
Ca4	0.84744	0.13700	0.30036	0.01144	Los Archipelago	0.019	(5)	22
Ca(4)	0.8469(2)	0.1367(3)	0.3005(4)	0.014(1)	Monte Somma, Italy	0.013	(6)	23
X8	0.14704(6)	0.63424(6)	0.19874(10)	0.0090(1)	Fohberg		this work	2
Ca_2	0.152	0.638	0.200		Langesundsfjord Norway	0.064	(1)	6
Ca_2	0.147	0.641	0.199		Barkevik Norway	0.069	(2)	8
Ca(2)	0.14570(6)	0.63508(10)	0.19979(9)	0.0071	Brevik Norway	0.020	(3)	10
Ca1	0.1470(2)	0.6340(2)	0.1997(2)	0.0117(3)	Prairie Lake Ontario	0.008	(4)	18
Ca2	0.1453	0.63869	0.19921	0.01093	Los Archipelago	0.050	(5)	22
Ca(2)	0.1460(2)	0.6381(2)	0.1986(4)	0.012(1)	Monte Somma, Italy	0.041	(6)	23
Si1	0.08090(8)	0.32657(9)	0.19685(12)	0.0075(2)	Fohberg		this work	2
Si_1[l]	0.063	0.326	0.185		Langesundsfjord Norway	0.185	(1)	6
Si_2[l]	0.082	0.329	0.200		Barkevik Norway	0.033	(2)	8
Si(1)	0.07971(9)	0.32701(10)	0.19740(14)	0.0053	Brevik Norway	0.015	(3)	10

Si2	0.0796(2)	0.3271(2)	0.1962(3)	0.0088(4)	Prairie Lake Ontario	0.014	(4)	18
Si1	0.08083	0.32710	0.19737	0.00813	Los Archipelago	0.007	(5)	22
Si(1)	0.0808(3)	0.3277(3)	0.1980(5)	0.012(1)	Monte Somma, Italy	0.015	(6)	23
Si2	0.07360(8)	0.31850(9)	0.63767(14)	0.0078(2)	Fohberg		this work	2
Si_2^I	0.083	0.317	0.630		Langesundsfjord Norway	0.132	(1)	6
Si_1^I	0.073	0.321	0.637		Barkevik Norway	0.026	(2)	8
Si(2)	0.07238(10)	0.31851(11)	0.63666(14)	0.0056	Brevik Norway	0.013	(3)	10
Si1	0.0721(2)	0.3187(2)	0.6359(3)	0.0083(4)	Prairie Lake Ontario	0.017	(4)	18
Si2	0.07316	0.31925	0.63719	0.00815	Los Archipelago	0.009	(5)	22
Si(2)	0.0724(3)	0.3196(3)	0.6358(6)	0.012(1)	Monte Somma, Italy	0.019	(6)	23
Si3	0.55874(9)	0.06903(9)	0.43635(12)	0.0080(2)	Fohberg		this work	2
Si_3^{II}	0.567	0.060	0.385		Langesundsfjord Norway	1.019	(1)	6
Si_4^{II}	0.562	0.070	0.437		Barkevik Norway	0.035	(2)	8
Si(3)	0.56059(10)	0.06691(11)	0.43688(14)	0.0062	Brevik Norway	0.029	(3)	10
Si4	0.5597(2)	0.0681(2)	0.4365(3)	0.0105(4)	Prairie Lake Ontario	0.014	(4)	18
Si3	0.56274	0.06715	0.43813	0.00839	Los Archipelago	0.045	(5)	22
Si(3)	0.5626(3)	0.0676(4)	0.4375(5)	0.012(1)	Monte Somma, Italy	0.042	(6)	23
Si4	0.43497(8)	0.56557(9)	0.12171(13)	0.0079(2)	Fohberg		this work	2
Si_4^{II}	0.433	0.581	0.059		Langesundsfjord Norway	0.476	(1)	6
Si_3^{II}	0.433	0.567	0.124		Barkevik Norway	0.034	(2)	8
Si(4)	0.43303(10)	0.56618(10)	0.12460(14)	0.0056	Brevik Norway	0.035	(3)	10
Si3	0.4345(2)	0.5664(2)	0.1238(3)	0.0084(4)	Prairie Lake Ontario	0.020	(4)	18
Si4	0.43164	0.56666	0.12396	0.00783	Los Archipelago	0.046	(5)	22
Si(4)	0.4319(3)	0.5671(4)	0.1231(6)	0.012(1)	Monte Somma, Italy	0.041	(6)	23
O1	0.0086(2)	0.1891(2)	0.1215(4)	0.0116(4)	Fohberg		this work	2
O_3^I	0.005	0.194	0.089		Langesundsfjord Norway	0.232	(1)	6
O_4^I	0.008	0.191	0.116		Barkevik Norway	0.043	(2)	8
O(1)	0.0095(3)	0.1900(3)	0.1200(4)	0.0104	Brevik Norway	0.019	(3)	10
O5	0.0090(5)	0.1897(5)	0.1209(9)	0.0122(9)	Prairie Lake Ontario	0.009	(4)	18
O1	0.00622	0.19243	0.1161	0.0141	Los Archipelago	0.052	(5)	22
O(1)	0.0065(9)	0.1924(9)	0.1164(15)	0.019(2)	Monte Somma, Italy	0.046	(6)	23

O2		-0.0191(2)	0.1941(2)	0.6163(4)	0.0113(4)	Fohberg		this work	2
	O_4^I	0.001	0.199	0.645		Langesundsfjord Norway	0.252	(1)	6
	O_3^I	-0.023	0.196	0.617		Barkevik Norway	0.048	(2)	8
	O(2)	-0.0197(3)	0.1949(3)	0.6175(4)	0.0104	Brevik Norway	0.015	(3)	10
	O1	-0.0207(5)	0.1945(4)	0.6178(9)	0.0116(9)	Prairie Lake Ontario	0.024	(4)	18
	O2	-0.01991	0.19577	0.6198	0.0131	Los Archipelago	0.034	(5)	22
	O(2)	-0.0181(8)	0.1950(8)	0.6213(15)	0.016(2)	Monte Somma, Italy	0.036	(6)	23
O3		0.0049(2)	0.4538(2)	0.0855(4)	0.0140(5)	Fohberg		this work	2
	O_5^I	0.005	0.454	0.086		Langesundsfjord Norway	0.004	(1)	6
	O_6^I	0.004	0.454	0.078		Barkevik Norway	0.052	(2)	8
	O(3)	0.0056(3)	0.4553(3)	0.0851(4)	0.0120	Brevik Norway	0.018	(3)	10
	O4	0.0051(5)	0.4525(5)	0.0822(8)	0.0138(11)	Prairie Lake Ontario	0.028	(4)	18
	O3	0.00954	0.45748	0.0921	0.0177	Los Archipelago	0.068	(5)	22
	O(3)	0.0078(9)	0.4562(10)	0.0912(15)	0.024(2)	Monte Somma, Italy	0.049	(6)	23
O4		0.0180(2)	0.4526(2)	0.6968(4)	0.0155(5)	Fohberg		this work	2
	O_6^I	0.000	0.454	0.650		Langesundsfjord Norway	0.332	(1)	6
	O_5^I	0.017	0.455	0.700		Barkevik Norway	0.038	(2)	8
	O(4)	0.0185(3)	0.4530(3)	0.6986(4)	0.0118	Brevik Norway	0.013	(3)	10
	O3	0.0183(5)	0.4524(5)	0.6990(9)	0.0188(12)	Prairie Lake Ontario	0.015	(4)	18
	O4	0.0186	0.45445	0.6918	0.0186	Los Archipelago	0.043	(5)	22
	O(4)	0.0169(9)	0.4533(10)	0.6944(14)	0.022(2)	Monte Somma, Italy	0.019	(6)	23
O5		0.2320(2)	0.3284(3)	0.2038(4)	0.0146(5)	Fohberg		this work	2
	O_7^I	0.233	0.327	0.250		Langesundsfjord Norway	0.333	(1)	6
	O_8^I	0.238	0.329	0.213		Barkevik Norway	0.077	(2)	8
	O(5)	0.2322(3)	0.3290(3)	0.2078(4)	0.0120	Brevik Norway	0.029	(3)	10
	O8	0.2329(5)	0.3299(5)	0.2088(9)	0.0151(11)	Prairie Lake Ontario	0.038	(4)	18
	O5	0.23359	0.32461	0.2074	0.0157	Los Archipelago	0.047	(5)	22
	O(5)	0.2324(8)	0.3263(9)	0.2070(15)	0.020(2)	Monte Somma, Italy	0.031	(6)	23
O6		0.2223(2)	0.2900(3)	0.7786(4)	0.0152(5)	Fohberg		this work	2
	O_8^I	0.227	0.325	0.696		Langesundsfjord Norway	0.715	(1)	6
	O_7^I	0.225	0.287	0.778		Barkevik Norway	0.044	(2)	8
	O(6)	0.2209(3)	0.2899(3)	0.7744(4)	0.0125	Brevik Norway	0.029	(3)	10
	O7	0.2237(4)	0.2899(6)	0.7729(9)	0.0160(12)	Prairie Lake Ontario	0.049	(4)	18

O6	0.22203	0.28936	0.7763	0.017	Los Archipelago	0.017	(5)	22
O(6)	0.2211(8)	0.2887(9)	0.7754(13)	0.017(2)	Monte Somma, Italy	0.026	(6)	23
O7	0.5097(2)	-0.0737(2)	0.3511(4)	0.0143(5)	Fohberg		this work	2
O_3^{II}	0.539	-0.078	0.375		Langesundsfjord Norway	0.311	(1)	6
O_4^{II}	0.509	-0.075	0.350		Barkevik Norway	0.016	(2)	8
O(7)	0.5108(3)	-0.0744(3)	0.3495(4)	0.0129	Brevik Norway	0.021	(3)	10
O2	0.5104(5)	-0.0745(6)	0.3495(9)	0.0170(12)	Prairie Lake Ontario	0.018	(4)	18
O7	0.5128	-0.07463	0.3509	0.0146	Los Archipelago	0.035	(5)	22
O(7)	0.5129(9)	-0.0746(9)	0.3514(14)	0.019(2)	Monte Somma, Italy	0.035	(6)	23
O8	0.4599(2)	0.4152(2)	0.0763(4)	0.0150(5)	Fohberg		this work	2
O_4^{II}	0.460	0.422	0.117		Langesundsfjord Norway	0.304	(1)	6
O_3^{II}	0.460	0.418	0.071		Barkevik Norway	0.048	(2)	8
O(8)	0.4573(3)	0.4180(3)	0.0718(4)	0.0115	Brevik Norway	0.046	(3)	10
O10	0.4603(5)	0.4170(6)	0.0741(8)	0.0148(11)	Prairie Lake Ontario	0.026	(4)	18
O8	0.45854	0.41877	0.0736	0.0146	Los Archipelago	0.042	(5)	22
O(8)	0.4607(9)	0.4167(9)	0.0772(15)	0.019(2)	Monte Somma, Italy	0.018	(6)	23
O9	0.4717(2)	0.1920(2)	0.3189(4)	0.0133(5)	Fohberg		this work	2
O_5^{II}	0.469	0.186	0.392		Langesundsfjord Norway	0.545	(1)	6
O_6^{II}	0.474	0.187	0.318		Barkevik Norway	0.058	(2)	8
O(9)	0.4746(3)	0.1895(3)	0.3195(4)	0.0110	Brevik Norway	0.040	(3)	10
O6	0.4724(5)	0.1910(5)	0.3210(8)	0.0164(12)	Prairie Lake Ontario	0.018	(4)	18
O9	0.47547	0.18955	0.319	0.0134	Los Archipelago	0.048	(5)	22
O(9)	0.4744(8)	0.1905(9)	0.3201(14)	0.016(2)	Monte Somma, Italy	0.032	(6)	23
O10	0.5392(2)	0.6679(3)	0.0851(4)	0.0174(5)	Fohberg		this work	2
O_6^{II}	0.543	0.682	0.204		Langesundsfjord Norway	0.864	(1)	6
O_5^{II}	0.542	0.669	0.093		Barkevik Norway	0.056	(2)	8
O(10)	0.5370(3)	0.6701(3)	0.0880(4)	0.0142	Brevik Norway	0.041	(3)	10
O11	0.5390(5)	0.6685(6)	0.0875(9)	0.0192(12)	Prairie Lake Ontario	0.019	(4)	18
O10	0.53299	0.67273	0.0875	0.0165	Los Archipelago	0.090	(5)	22
O(10)	0.5336(9)	0.6712(9)	0.0852(13)	0.018(2)	Monte Somma, Italy	0.070	(6)	23

O11	0.7105(2)	0.0968(3)	0.4817(4)	0.0184(5)	Fohberg		this work	2
O_7^{II}	0.710	0.109	0.500		Langesundsfjord Norway	0.184	(1)	6
O_8^{II}	0.713	0.096	0.484		Barkevik Norway	0.028	(2)	8
O(11)	0.7135(3)	0.0934(3)	0.4846(4)	0.0157	Brevik Norway	0.048	(3)	10
O9	0.7062(6)	0.0939(7)	0.4793(11)	0.0227(13)	Prairie Lake Ontario	0.053	(4)	18
O11	0.7149	0.09460	0.4873	0.0199	Los Archipelago	0.056	(5)	22
O(11)	0.7148(8)	0.0935(10)	0.4844(15)	0.023(2)	Monte Somma, Italy	0.056	(6)	23
O12	0.2912(2)	0.6230(2)	0.0205(4)	0.0135(4)	Fohberg		this work	2
O_8^{II}	0.290	0.609	0.043		Langesundsfjord Norway	0.221	(1)	6
O_7^{II}	0.300	0.627	0.027		Barkevik Norway	0.100	(2)	8
O(12)	0.2888(3)	0.6236(3)	0.0234(4)	0.0128	Brevik Norway	0.039	(3)	10
O15	0.2928(5)	0.6234(5)	0.0224(10)	0.0154(10)	Prairie Lake Ontario	0.019	(4)	18
O12	0.28695	0.62222	0.0247	0.0163	Los Archipelago	0.064	(5)	22
O(12)	0.2855(8)	0.6233(9)	0.0197(15)	0.019(2)	Monte Somma, Italy	0.060	(6)	23
W1,O13	0.2445(2)	0.0729(3)	0.0438(4)	0.0152(5)	Fohberg		this work	2
O_9	0.225	0.092	-0.025		Langesundsfjord Norway	0.513	(1)	6
O_{10}	0.224	0.070	0.045		Barkevik Norway	0.227	(2)	8
O(13)	0.2449(3)	0.0709(3)	0.0435(4)	0.0117	Brevik Norway	0.021	(3)	10
O12	0.2460(5)	0.0701(6)	0.0463(8)	0.0157(11)	Prairie Lake Ontario	0.035	(4)	18
O13,F1	0.2487	0.06911	0.0376	0.0236	Los Archipelago	0.083	(5)	22
O(13)	0.2461(8)	0.0696(9)	0.0365(15)	0.023(2)	Monte Somma, Italy	0.070	(6)	23
W2,O14	0.2253(2)	0.0704(2)	0.4405(4)	0.0158(7)	Fohberg		this work	2
O_{10}	0.250	0.042	0.467		Langesundsfjord Norway	0.399	(1)	6
$(F,O)_9^a$	0.221	0.074	0.428		Barkevik Norway	0.095	(2)	8
O(14)	0.2236(3)	0.0719(3)	0.4363(3)	0.0098	Brevik Norway	0.034	(3)	10
O17	0.2252(5)	0.0713(5)	0.4365(8)	0.0131(10)	Prairie Lake Ontario	0.030	(4)	18
O14,F2	0.22732	0.06889	0.4465	0.0214	Los Archipelago	0.045	(5)	22
O(14)	0.2283(9)	0.0699(9)	0.4503(16)	0.025(2)	Monte Somma, Italy	0.070	(6)	23
W4,O15	0.2164(2)	0.8459(2)	0.2267(4)	0.0142(6)	Fohberg		this work	2
O_{12}	0.229	0.836	0.241		Langesundsfjord Norway	0.174	(1)	6
O_{11}	0.217	0.847	0.225		Barkevik Norway	0.019	(2)	8
O(16)	0.2136(3)	0.8463(3)	0.2241(4)	0.0098	Brevik Norway	0.030	(3)	10
O16	0.2147(4)	0.8465(5)	0.2246(10)	0.0137(10)	Prairie Lake Ontario	0.021	(4)	18

O15,F4	0.21728	0.84485	0.2255	0.0177	Los Archipelago	0.018	(5)	22
O(16)	0.2178(8)	0.8444(9)	0.2273(15)	0.018(2)	Monte Somma, Italy	0.021	(6)	23
O16	0.0913(3)	0.3489(2)	0.4251(4)	0.0213(5)	Fohberg		this work	2
O I	0.033	0.319	0.386		Langesundsfjord Norway	0.675	(1)	6
O_1	0.089	0.350	0.425		Barkevik Norway	0.027	(2)	8
O(17)	0.0867(3)	0.3486(3)	0.4228(4)	0.0176	Brevik Norway	0.047	(3)	10
O14	0.0878(6)	0.3494(5)	0.4213(8)	0.0220(11)	Prairie Lake Ontario	0.039	(4)	18
O16	0.08994	0.34326	0.4246	0.0256	Los Archipelago	0.059	(5)	22
O(17)	0.0865(9)	0.3450(9)	0.4241(15)	0.028(2)	Monte Somma, Italy	0.064	(6)	23
O17	0.5229(2)	0.0798(2)	0.6407(4)	0.0157(4)	Fohberg		this work	2
O II	0.567	0.066	0.152		Langesundsfjord Norway	3.589	(1)	6
O_2	0.527	0.080	0.645		Barkevik Norway	0.045	(2)	8
O(18)	0.5230(3)	0.0776(3)	0.6400(4)	0.0139	Brevik Norway	0.023	(3)	10
O13	0.5223(5)	0.0795(5)	0.6374(9)	0.0175(10)	Prairie Lake Ontario	0.023	(4)	18
O17	0.52382	0.07783	0.6391	0.0175	Los Archipelago	0.027	(5)	22
O(18)	0.5268(8)	0.0778(9)	0.6404(15)	0.022(2)	Monte Somma, Italy	0.048	(6)	23
W3,F	0.7617(2)	0.3434(2)	0.2579(3)	0.0131(4)	Fohberg		this work	2
O_{11}	0.777	0.336	0.279		Langesundsfjord Norway	0.200	(1)	6
F_{12}	0.760	0.344	0.255		Barkevik Norway	0.024	(2)	8
F(15)	0.7607(2)	0.3427(2)	0.2565(3)	0.0115	Brevik Norway	0.014	(3)	10
F	0.7598(4)	0.3435(4)	0.2536(8)	0.0091(8)	Prairie Lake Ontario	0.031	(4)	18
F3	0.76137	0.34272	0.25659	0.0141	Los Archipelago	0.011	(5)	22
F(15)	0.7618(7)	0.3430(7)	0.2555(12)	0.018(2)	Monte Somma, Italy	0.020	(6)	23

Note origin shifts: No. 2: (0, 0, 0,); No. 6: (0, 0.0578, 0); No. 8: (0, 0.0502, 0.5); No. 10: (0, 0.04642, 0); No. 18: (0.5, 0.2128, 0); No. 22: (0, 0.04585, 0); No. 23: (0, 0.0436, 0)

[a] the O:F ratio in the W2 site depends on the Nb:Zr ratio in the X6 site. Here, ideal composition is assumed yielding full occupancies by Nb and O, respectively.

[b] (1) Shibaeva and Belov (1962); (2) Golyshev et al. (1973); (3) Mellini and Merlino (1979); (4) Chakhmouradian et al. (2008); (5) Biagioni et al. (2012); ICSD 187604; (6) Bellezza et al. (2012)

Table S5: Anisotropic displacement parameters (Å^2) of wöhlerite

site	U11	U22	U33	U23	U13	U12	Ueq
X1	0.0060(2)	0.0084(2)	0.0065(2)	0.0001(2)	0.0015(1)	0.0010(1)	0.0071(1)
X2	0.0108(2)	0.0118(4)	0.0152(3)	-0.0020(3)	0.0033(3)	-0.0029(2)	0.0129(2)
X3	0.0148(6)	0.0157(7)	0.0155(7)	-0.0006(5)	0.0060(5)	-0.0015(4)	0.0151(5)
X4	0.0106(4)	0.0138(4)	0.0099(4)	-0.0008(3)	0.0026(3)	-0.0010(2)	0.0116(2)
X5	0.0191(7)	0.0149(9)	0.0227(8)	-0.0054(6)	0.0078(6)	-0.0074(5)	0.0187(5)
X6	0.0091(1)	0.0061(1)	0.0087(2)	-0.0005(1)	0.0031(1)	-0.0009(1)	0.0079(1)
X7	0.0097(3)	0.0113(3)	0.0095(3)	-0.0001(2)	0.0024(3)	0.0013(2)	0.0104(1)
X8	0.0085(2)	0.0097(3)	0.0085(3)	-0.0007(2)	0.0023(3)	-0.0020(2)	0.0090(1)
Si1	0.0076(3)	0.0066(3)	0.0078(4)	0.0007(3)	0.0019(3)	0.0005(3)	0.0075(2)
Si2	0.0075(3)	0.0064(3)	0.0096(4)	-0.0004(3)	0.0028(3)	-0.00004(29)	0.0078(2)
Si3	0.0078(4)	0.0078(4)	0.0080(4)	0.0000(3)	0.0019(3)	-0.0004(3)	0.0080(2)
Si4	0.0086(3)	0.0065(4)	0.0081(4)	0.0007(3)	0.0019(3)	0.0006(3)	0.0079(2)
O1	0.0115(9)	0.0086(9)	0.0130(11)	-0.0003(9)	0.0018(10)	-0.0015(7)	0.0116(4)
O2	0.0107(9)	0.0089(9)	0.0130(10)	-0.0015(9)	0.0021(10)	-0.0023(7)	0.0113(4)
O3	0.0149(10)	0.0073(9)	0.0171(12)	0.0022(9)	0.0015(9)	0.0009(8)	0.0140(5)
O4	0.0131(10)	0.0094(10)	0.0256(13)	-0.0041(9)	0.0085(9)	-0.0008(8)	0.0155(5)
O5	0.0097(9)	0.0147(11)	0.0192(12)	0.0002(9)	0.0047(8)	-0.0007(9)	0.0146(5)
O6	0.0099(9)	0.0178(12)	0.0152(11)	0.0025(9)	0.0004(8)	0.0026(8)	0.0152(5)
O7	0.0143(10)	0.0101(10)	0.0145(12)	-0.0017(9)	-0.0006(9)	0.0012(8)	0.0143(5)
O8	0.0162(10)	0.0093(11)	0.0227(14)	-0.0012(9)	0.0109(10)	0.0009(9)	0.0150(5)
O9	0.0135(10)	0.0111(10)	0.0127(11)	0.0018(8)	0.0009(9)	0.0010(8)	0.0133(5)
O10	0.0167(11)	0.0177(12)	0.0191(11)	0.0028(9)	0.0077(9)	-0.0056(9)	0.0174(5)
O11	0.0099(9)	0.0304(15)	0.0137(12)	-0.0007(12)	0.0025(10)	-0.0045(9)	0.0184(5)
O12	0.0082(9)	0.0160(10)	0.0139(11)	0.0015(10)	0.0004(10)	0.0029(8)	0.0135(4)
W1,O13	0.0170(11)	0.0106(11)	0.0159(11)	0.0007(9)	0.0026(9)	-0.0023(9)	0.0152(5)
W2,O14	0.0149(12)	0.0137(12)	0.0193(13)	-0.0045(9)	0.0063(9)	-0.0041(9)	0.0158(7)
W4,O15	0.0171(10)	0.0100(10)	0.0163(12)	0.0005(10)	0.0065(10)	-0.0024(8)	0.0142(6)
O16	0.0330(12)	0.0211(12)	0.0116(11)	-0.0017(10)	0.0099(11)	-0.0072(10)	0.0213(5)
W3,F	0.0138(8)	0.0114(9)	0.0129(9)	0.0004(8)	0.0026(8)	0.0004(7)	0.0131(4)

The isotropic displacement parameter U_{eq} is defined as one third of the trace of the orthogonalized *U*ij tensor. Coefficients *U*ij of the anisotropic displacement factor tensor of the atoms are defined by: $-2\pi^2[(ha^*)^2U_{11} + \cdots + 2hka^*b^*U_{12} + \cdots]$.