Table 4a-4b-4c-4d (for deposit)

Table 4a. Atomic coordinates and U_{eq} (U_{iso}) (Å^2) values for veszelyite at -100 °C

Site	*Atom*	*Occ.*	*x*	*y*	*z*	U_{eq}/U_{iso}
Cu1	Cu	1	0.49198(5)	0.07238(3)	0.13093(4)	0.01162(11)
Cu2	Cu,Zn	1	0.46096(5)	0.25245(3)	0.35992(3)	0.01119(11)
Zn	Zn	1	0.06991(5)	0.07500(3)	0.21193(3)	0.01166(11)
P	P	1	0.06580(10)	0.29795(7)	0.41611(7)	0.01059(15)
O1	O	1	0.9742(3)	0.1587(2)	0.0333(2)	0.0143(4)
O2	O	1	0.9831(3)	0.1641(2)	0.3609(2)	0.0133(4)
O3	O	1	0.2755(3)	0.2848(2)	0.4716(2)	0.0128(4)
O4	O	1	0.0241(3)	0.3982(2)	0.2951(2)	0.0143(4)
OH1	O	1	0.3384(3)	0.0858(2)	0.2706(2)	0.0115(4)
H1	H	1	0.355(10)	0.025(5)	0.345(5)	0.080
OH2	O	1	0.6237(3)	0.2175(2)	0.2350(2)	0.0124(4)
H2	H	1	0.740(5)	0.183(6)	0.279(7)	0.080
OH3	O	1	0.6003(3)	0.40765(19)	0.4639(2)	0.0115(4)
H3	H	1	0.727(3)	0.387(7)	0.484(8)	0.080
H_2O1	O	1	0.6559(3)	0.3839(2)	0.0381(2)	0.0196(4)
H4	H	1	0.765(5)	0.374(7)	0.006(7)	0.080
H5	H	1	0.653(9)	0.324(5)	0.111(5)	0.080
H_2O2	O	1	0.3212(3)	0.4065(2)	0.1931(2)	0.0185(4)
H6	H	1	0.319(9)	0.365(6)	0.106(4)	0.080
H7	H	1	0.208(5)	0.398(7)	0.220(7)	0.080

Table 4b. Anisotropic displacement parameters (Å^2) for veszelyite at -100 °C.

Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	0.01277(18)	0.01137(18)	0.01161(18)	-0.00213(11)	0.00465(13)	-0.00168(11)
Cu2	0.01179(18)	0.01072(18)	0.01177(17)	-0.00159(12)	0.00416(12)	-0.00092(11)
Zn	0.01218(17)	0.01132(18)	0.01164(17)	-0.00062(11)	0.00304(12)	-0.00075(11)
P	0.0110(3)	0.0099(3)	0.0111(3)	-0.0007(2)	0.0029(2)	-0.0001(2)
O1	0.0130(9)	0.0163(10)	0.0141(9)	0.0031(8)	0.0039(7)	0.0004(8)
O2	0.0147(9)	0.0119(9)	0.0143(9)	-0.0022(7)	0.0049(7)	-0.0004(7)
O3	0.0118(9)	0.0153(10)	0.0120(9)	-0.0019(7)	0.0039(7)	-0.0010(7)
O4	0.0170(10)	0.0114(9)	0.0151(9)	0.0011(8)	0.0046(7)	0.0034(8)
OH1	0.0111(9)	0.0125(9)	0.0110(9)	-0.0001(7)	0.0028(7)	-0.0007(7)
OH2	0.0118(9)	0.0132(9)	0.0125(9)	-0.0016(7)	0.0032(7)	-0.0010(7)
OH3	0.0131(9)	0.0109(9)	0.0113(9)	0.0007(7)	0.0047(7)	-0.0004(7)
H_2O1	0.0232(11)	0.0181(10)	0.0177(10)	0.0011(8)	0.0051(8)	0.0002(9)
H_2O2	0.0152(10)	0.0229(11)	0.0180(10)	-0.0005(8)	0.0048(8)	-0.0013(8)

Table 4c. Hydrogen bond distances (Å) and O-H···O angles (°). H positions were determined with the restraint O-H is 0.95(1) Å and H-H = 1.59(5) Å. D: donor; A: acceptor.

Species	D-H	H…A	D…A	<(DHA)	Hydrogen bond
OH	0.945(10)	1.85(2)	2.776(3)	167(6)	OH1-H1···H2O1
OH	0.946(10)	1.83(2)	2.747(3)	164(6)	OH2-H2···O2
OH	0.947(10)	1.863(12)	2.808(3)	176(7)	OH3-H3···O1
H_2O	0.947(10)	2.43(2)	3.345(3)	163(6)	H2O1-H4···O2
H_2O	0.948(10)	1.675(13)	2.619(3)	174(6)	H2O1-H5···OH2
H_2O	0.947(10)	1.99(3)	2.878(3)	155(6)	H2O2-H6···O3
H_2O	0.948(10)	1.701(16)	2.638(3)	169(6)	H2O2-H7···O4

Table 4d. Interatomic distances (Å) and T-O-T angles (°) of veszelyite at -100 °C.

Cu1 coordination	-100 °C
Cu1-OH2	1.934(2)
Cu1-OH3(2×)	1.966(2)
	1.995(2)
Cu1-OH1	1.982(2)
Cu1-O3	2.455(2)
Cu1-H_2O2	2.586(2)
Mean	2.153
Cu2 coordination	-100 °C
Cu2-OH2	1.946(2)
Cu2-O3	1.981(2)
Cu2-OH3	2.035(2)
Cu2-OH1	2.031(2)
Cu2- H_2O2	2.334(2)
Cu2-H_2O1	2.438(2)
Mean	2.128
Zn coordination	-100 °C
Zn-O1	1.931(2)
Zn-O4	1.931(2)
Zn-O2	1.951(2)
Zn-OH1	1.964(2)
Mean	1.944
P coordination	-100 °C
P-O1	1.530(2)

P-O4	1.541(2)
P-O2	1.544(2)
P-O3	1.546(2)
Mean	1.540
T-O-T angles	-100 °C
P O1 Zn	132.03(13)
P O2 Zn	119.84(12)
P O4 Zn	130.86(13)
Mean T-O-T	127.58

Table 6: For deposit

Table 6. Interatomic distances (Å) and T-O-T angles (°) of veszelyite under ambient conditions and after partial dehydration at 200 °C.

Cu1 coordination	RT	200 °C
Cu1-OH2	1.9308(12)	1.940(8)
Cu1-OH3(2×)	1.9681(12)	1.981(7)
	1.9963(13)	1.986(8)
Cu1-OH1	1.9814(14)	1.962(9)
Cu1-O3	2.4541(12)	2.375(8)
Cu1-H_2O2	2.6164(16)	
Mean	2.158	2.049
Cu2 coordination	RT	200 °C
Cu2-OH2	1.9497(13)	1.954(9)
Cu2-O3	1.9862(13)	1.962(8)
Cu2-OH3	2.0419(12)	2.006(7)
Cu2-OH1	2.0455(12)	2.068(8)
Cu2- H_2O2	2.3385(17)	
Cu2-H_2O1	2.4441(16)	2.248(10)
Mean	2.134	2.048
Zn coordination	RT	200 °C
Zn-O1	1.9304(13)	1.941(8)
Zn-O4	1.9309(12)	1.926(9)
Zn-O2	1.9520(13)	1.905(8)
Zn-OH1	1.9670(13)	1.984(9)
Mean	1.945	1.939
P coordination	RT	200 °C
P-O1	1.5300(14)	1.525(9)
P-O4	1.5380(13)	1.491(9)
P-O2	1.5402(13)	1.524(9)
P-O3	1.5456(13)	1.554(9)
Mean	1.538	1.523
T-O-T angles	RT	200 °C
P O1 Zn	132.42(8)	135.6(5)
P O2 Zn	120.59(8)	123.1(5)
P O4 Zn	131.23(9)	127.5(6)
Mean T-O-T	128.08	128.73

Table7: For deposit

Table 7. Results of bond valence calculations for veszelyite RT (a) and 200 °C (b), parameters from Brown and Altermatt (1985).

(a)

Site	O1	O2	O3	O4	OH1	OH2	OH3	H_2O1	H_2O2	Bvs[#]
Cu1			0.12		0.44	0.51	0.44 $2\times\rightarrow\downarrow$		0.08	2.03
Cu2			0.44		0.37	0.48	0.38	0.13	0.17	1.97
Zn	0.54	0.51		0.54	0.49					2.08
P	1.27	1.23	1.21	1.24						4.95
H1					0.81			0.19		1
H2		0.20				0.80				1
H3	0.19						0.81			1
H4		0.09						0.91		1
H5						0.24		0.76		1
H6			0.15						0.85	1
H7				0.23					0.77	1
Bvs[#] without H	1.81	1.74	1.77	1.78	1.30	0.99	1.26	0.13	0.25	
Bvs[#] with H	2.00	2.03	1.92	2.01	2.11	2.03	2.07	1.99	1.87	

(b)

Site	O1	O2	O3	O4	OH1	OH2	OH3	H_2O1	Bvs[#]
Cu1			0.15		0.47	0.49	0.44 $2\times\rightarrow\downarrow$		1.99
Cu2			0.47		0.35	0.48	0.41	0.22	1.93
Zn	0.53	0.58		0.55	0.47				2.13
P	1.28	1.29	1.19	1.41					5.17
H1					0.86	0.14			1
H2		0.16				0.84			1
H3	0.18						0.82		1
H4			0.18					0.82	1
H5		0.16						0.84	1
Bvs[#] without H	1.81	1.87	1.81	1.96	1.29	0.97	1.29	0.22	
Bvs[#] with H	1.99	2.19	1.99	1.96	2.15	1.95	2.11	1.88	

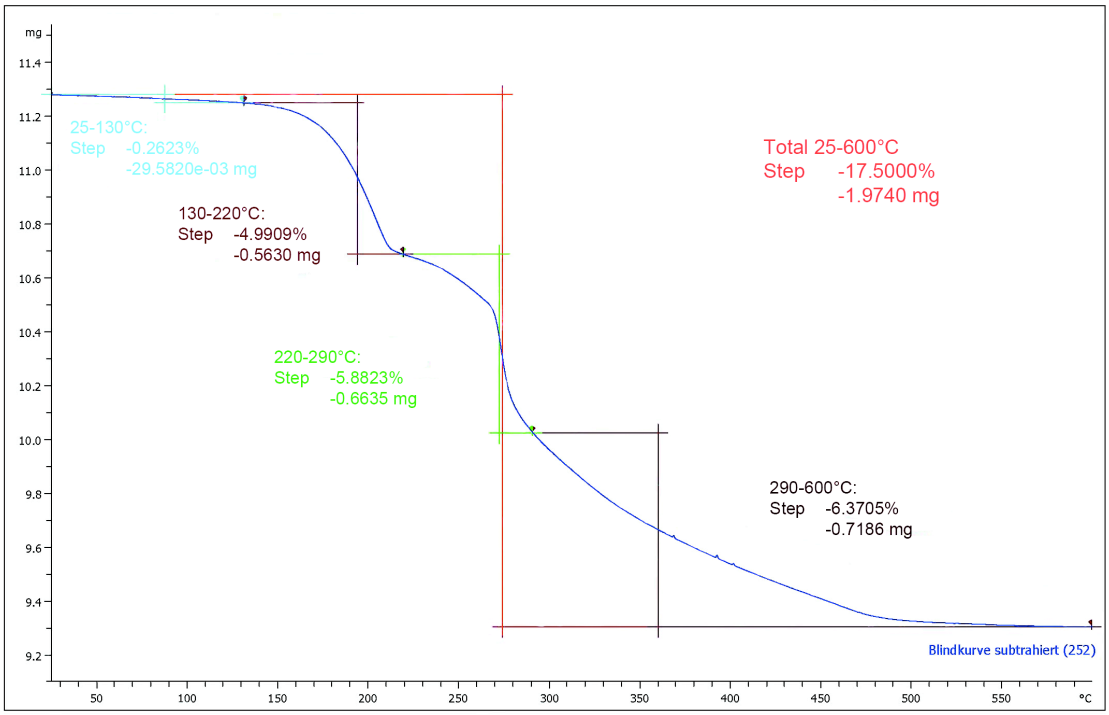
[#] bond valence sum (Brown and Altermatt 1985)

Note: $2\times\rightarrow\downarrow$ indicates that the bv value of 0.44 should be considered twice horizontally and vertically.

Table 9: For deposit

Table 9. The ratios L/S of the longest to the shortest cross-sections of eight-membered rings of veszelyite at different temperature.

	RT	200 °C
Tetrahedral sheet	2.16	2.27
Octahedral sheet	1.28	1.57



Deposit Figure 9: Weight curve and calculated mass loss of veszelyite.