Innsbruckite, $Mn_{33}(Si_2O_5)_{14}(OH)_{38}$ – a new mineral from the Tyrol, Austria

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Files

- `innsbruckite.cif`: crystallographic information file, containing structural parameters, experimental details, and stucture factors.
- `innsbruckite.cgd`: systre (Delgado-Friedrichs & O'Keeffe, 2003; Delgado-Friedrichs, 2013) structure file (containing the definition of the 3-connected, 2-periodic innsbruckite net).
- `innsbruckite.arc`: systre archive file, containing the fingerprint of the innsbruckite net.

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A Supplementary material

Structural parameters

Table 1: Atomic parameters

Atom	x	y	z	U_{iso}
Mn1	-0.00007(5)	0	-0.00641(11)	0.01108(18)
Mn2	-0.00075(3)	0.091165(12)	-0.00791(9)	0.01243(14)
Mn3	-0.00492(3)	0.182345(12)	-0.02038(8)	0.01218(14)
Mn4	-0.50420(3)	0.224898(12)	-0.01923(7)	0.01110(13)
Mn5	-0.00418(3)	0.365769(13)	0.02053(8)	0.01213(14)
Mn6	-0.00187(3)	0.455546(12)	0.04824(8)	0.01168(15)
Mn7	-0.33416(3)	0.454773(12)	0.05570(8)	0.01212(15)
Mn8	-0.33838(3)	0.362738(13)	0.04441(8)	0.01144(14)
Mn9	-0.33658(3)	0.271428(14)	-0.02443(8)	0.01102(13)
Mn10	-0.33637(3)	0.178856(13)	-0.05503(7)	0.01121(14)
Mn11	-0.33534(3)	0.089416(13)	-0.02874(8)	0.01151(14)
Mn12	-0.33399(4)	0	-0.02555(11)	0.0127(2)
Mn13	-0.16928(4)	0.5	0.07795(10)	0.0126(2)
Mn14	-0.16961(3)	0.409540(13)	0.06113(8)	0.01208(15)
Mn15	-0.17083(3)	0.319539(15)	0.02426(8)	0.01155(14)
Mn16	-0.17120(3)	0.227531(13)	-0.04551(7)	0.01096(13)
Mn17	-0.16715(3)	0.135049(13)	-0.05803(8)	0.01211(15)
Mn18	-0.16700(3)	0.044561(13)	-0.04094(9)	0.01264(15)
Si1	-0.42383(5)	0.45743(2)	-0.37002(12)	0.0077(2)
Si2	-0.27431(5)	0.41440(2)	-0.32811(13)	0.0075(2)
Si3	-0.12420(5)	0.45781(2)	-0.31947(13)	0.0078(2)
Si4	0.02616(5)	0.41603(2)	-0.36719(12)	0.0079(2)
Si5	0.14143(5)	0.45772(2)	-0.62259(12)	0.0081(2)
Si6	-0.21439(5)	0.09021(2)	0.33938(12)	0.0075(2)
Si7	-0.56869(5)	0.45749(2)	-0.63457(13)	0.0078(2)
Si8	-0.40252(5)	0.29837(2)	-0.61783(12)	0.0076(2)
Si9	-0.27746(5)	0.33094(2)	-0.36509(12)	0.0074(2)
Si10	-0.12553(5)	0.29017(2)	-0.39472(12)	0.0077(2)
Si11	-0.47742(5)	0.16785(2)	-0.39876(12)	0.0078(2)
Si12	-0.36990(5)	0.21682(2)	0.34882(12)	0.0078(2)
Si13	-0.21783(5)	0.17444(2)	0.32723(12)	0.0079(2)
Si14	-0.07279(5)	0.22185(2)	0.35587(12)	0.0076(2)
O1	0.05729(15)	0.04508(5)	-0.1566(4)	0.0103(7)
O2	0.1029(2)	0	0.1696(5)	0.0137(10)
O3	-0.27795(20)	0.5	-0.0898(5)	0.0124(9)

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Atom	x	y	z	U_{iso}
O4	-0.22433(16)	0.45386(6)	0.2054(4)	0.0135(7)
O5	-0.11769(14)	0.45679(5)	-0.0996(3)	0.0103(7)
O6	-0.0519(2)	0.5	0.2011(5)	0.0136(10)
O7	0.04732(19)	0.5	-0.1167(5)	0.0125(9)
O8	0.11718(15)	0.45404(6)	-0.8357(3)	0.0110(7)
O9	-0.28124(17)	0.04496(6)	-0.1663(4)	0.0126(7)
O10	-0.2203(2)	0	0.1172(5)	0.0129(10)
O11	-0.1067(2)	0	-0.1663(5)	0.0135(10)
O12	-0.55548(15)	0.45508(6)	-0.8508(4)	0.0105(7)
O13	0.05914(15)	0.13751(6)	-0.1359(4)	0.0122(7)
O14	0.10391(16)	0.09186(6)	0.1657(4)	0.0134(7)
O15	-0.27920(14)	0.41166(6)	-0.1091(3)	0.0101(7)
O16	-0.22710(16)	0.36196(7)	0.1797(3)	0.0141(7)
O17	-0.11890(15)	0.36717(6)	-0.1119(3)	0.0129(7)
O18	-0.05418(16)	0.40905(6)	0.1805(3)	0.0140(7)
O19	-0.45462(14)	0.08578(6)	-0.1521(3)	0.0105(7)
O20	-0.38643(15)	0.13469(6)	0.1195(3)	0.0123(7)
O21	-0.28260(16)	0.13327(6)	-0.1872(3)	0.0135(7)
O22	-0.21879(15)	0.08914(6)	0.1207(3)	0.0112(7)
O23	-0.10806(15)	0.08930(6)	-0.1715(3)	0.0122(7)
O24	-0.06020(15)	0.13716(6)	0.1227(4)	0.0134(7)
O25	-0.44999(14)	0.27043(6)	-0.1501(3)	0.0117(7)
O26	-0.39457(13)	0.31054(6)	0.1712(3)	0.0105(6)
O27	-0.28390(13)	0.32271(6)	-0.1491(3)	0.0095(6)
O28	-0.22644(14)	0.27007(7)	0.1216(3)	0.0126(7)
O29	-0.61896(14)	0.22299(6)	-0.1846(3)	0.0112(6)
O30	-0.55569(14)	0.18302(7)	0.1369(3)	0.0129(7)
O31	-0.45322(13)	0.17687(6)	-0.1898(3)	0.0103(6)
O32	-0.38695(13)	0.21999(6)	0.1309(3)	0.0099(6)
O33	-0.28398(15)	0.22726(6)	-0.1785(3)	0.0123(7)
O34	-0.22286(14)	0.17754(6)	0.1086(3)	0.0113(7)
O35	-0.11277(15)	0.18312(6)	-0.1796(3)	0.0124(7)
O36	-0.06488(13)	0.22836(6)	0.1390(3)	0.0101(6)
O37	-0.49440(13)	0.44523(6)	-0.5074(3)	0.0139(6)
O38	-0.35407(12)	0.42939(6)	-0.4248(3)	0.0110(6)
O39	-0.20847(12)	0.44370(6)	-0.3952(3)	0.0110(6)
O40	-0.06254(12)	0.42934(6)	-0.4107(3)	0.0119(6)
O41	0.07559(13)	0.44574(6)	-0.4801(3)	0.0149(6)
O42	-0.28470(12)	0.06805(6)	0.4329(3)	0.0137(6)
O43	-0.13618(12)	0.07128(6)	0.4264(3)	0.0121(6)

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Atom	x	y	z	U_{iso}
O44	-0.25247(12)	0.37369(5)	-0.4112(3)	0.0106(6)
O45	-0.46102(12)	0.12483(5)	-0.4581(3)	0.0106(6)
O46	-0.22031(13)	0.13275(5)	0.4126(3)	0.0119(6)
O47	0.00772(12)	0.20532(6)	0.4445(3)	0.0141(6)
O48	-0.36028(11)	0.32681(5)	-0.4740(3)	0.0105(6)
O49	-0.21318(12)	0.30361(6)	-0.4543(3)	0.0109(6)
O50	-0.56998(12)	0.17408(6)	-0.4340(3)	0.0115(6)
O51	-0.43645(13)	0.19411(6)	0.4524(3)	0.0150(6)
O52	-0.28956(12)	0.19726(6)	0.4137(3)	0.0133(6)
O53	-0.13776(12)	0.19154(6)	0.4095(3)	0.0135(6)
O54	-0.36350(12)	0.25836(5)	0.4321(3)	0.0124(6)
O55	-0.09811(12)	0.25905(6)	-0.5391(3)	0.0157(6)
O56	-0.39973(17)	0.5	-0.4260(4)	0.0118(8)
O57	-0.11105(16)	0.5	-0.3993(4)	0.0105(8)
O58	0.16517(16)	0.5	-0.5677(4)	0.0111(8)
O59	-0.59232(17)	0.5	-0.5730(4)	0.0112(8)
H2	0.101(3)	0	0.2831(15)	0.016457
H3	-0.273(3)	0.5	-0.2024(17)	0.014894
H4	-0.220(2)	0.4510(9)	0.3174(15)	0.016158
H6	-0.044(3)	0.5	0.3134(18)	0.016291
H7	0.033(3)	0.5	-0.225(2)	0.014977
H9	-0.286(2)	0.0491(9)	-0.2771(17)	0.015153
H10	-0.207(3)	0	0.227(2)	0.01543
H11	-0.106(3)	0	-0.2800(15)	0.016205
H13	0.0740(19)	0.1410(10)	-0.240(2)	0.014652
H14	0.110(2)	0.0877(10)	0.2761(17)	0.016044
H16	-0.230(2)	0.3643(10)	0.2922(15)	0.016926
H17	-0.124(2)	0.3651(10)	-0.2249(15)	0.015509
H18	-0.061(2)	0.4090(10)	0.2924(16)	0.01684
H20	-0.3597(18)	0.1298(9)	0.211(3)	0.014776
H21	-0.287(2)	0.1326(10)	-0.3006(15)	0.016232
H23	-0.112(2)	0.0958(9)	-0.2798(19)	0.014648
H24	-0.064(2)	0.1332(10)	0.2348(17)	0.016134
H25	-0.4608(19)	0.2703(10)	-0.2597(17)	0.014074
H28	-0.218(2)	0.2693(10)	0.2329(16)	0.015111
H30	-0.550(2)	0.1869(10)	0.2471(17)	0.015436
H33	-0.283(2)	0.2310(10)	-0.2910(16)	0.014805
H35	-0.107(2)	0.1863(10)	-0.2908(17)	0.014916

Table 2: Anisotropic displacement parameters

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn1	0.0105(3)	0.0085(3)	0.0142(3)	0	0.0009(3)	0
Mn2	0.0098(3)	0.0089(2)	0.0186(3)	-0.00013(18)	0.00039(19)	-0.00043(18)
Mn3	0.0099(3)	0.0083(2)	0.0184(3)	-0.00019(18)	0.00060(19)	-0.00028(20)
Mn4	0.0090(3)	0.0089(2)	0.0153(2)	-0.00115(18)	-0.00052(18)	0.0003(2)
Mn5	0.0093(3)	0.0094(2)	0.0176(3)	-0.00024(16)	-0.0006(2)	-0.00015(17)
Mn6	0.0103(3)	0.0094(2)	0.0153(3)	-0.00036(16)	-0.0008(2)	-0.00041(17)
Mn7	0.0101(3)	0.0096(2)	0.0167(3)	-0.00007(16)	0.0004(2)	-0.00057(17)
Mn8	0.0086(3)	0.0098(2)	0.0159(3)	0.00100(16)	-0.0003(2)	-0.00112(18)
Mn9	0.0079(3)	0.0094(2)	0.0157(2)	0.00007(17)	-0.00064(18)	0.00021(18)
Mn10	0.0100(3)	0.0086(2)	0.0150(3)	0.00038(17)	-0.0004(2)	-0.00065(17)
Mn11	0.0097(3)	0.0089(2)	0.0158(2)	0.00027(16)	-0.00099(19)	0.00025(18)
Mn12	0.0094(4)	0.0096(3)	0.0190(4)	0	-0.0004(3)	0
Mn13	0.0107(4)	0.0103(3)	0.0168(4)	0	0.0008(3)	0
Mn14	0.0099(3)	0.0103(2)	0.0160(3)	0.00023(17)	-0.0001(2)	-0.00018(18)
Mn15	0.0092(2)	0.0090(2)	0.0164(2)	-0.00037(16)	-0.00032(19)	0.00001(17)
Mn16	0.0090(2)	0.0091(2)	0.0147(2)	0.00002(17)	-0.00105(18)	0.00004(18)
Mn17	0.0106(3)	0.0087(2)	0.0171(3)	0.00027(17)	0.0006(2)	0.00001(17)
Mn18	0.0115(3)	0.0096(2)	0.0168(3)	0.00066(17)	0.0002(2)	-0.00035(17)
Si1	0.0059(4)	0.0069(3)	0.0102(4)	0.0005(3)	-0.0014(3)	-0.0008(3)
Si2	0.0068(4)	0.0061(3)	0.0095(4)	0.0001(3)	-0.0003(3)	-0.0003(3)
Si3	0.0070(5)	0.0064(3)	0.0099(4)	-0.0004(3)	-0.0006(3)	-0.0002(3)
Si4	0.0075(5)	0.0060(3)	0.0104(4)	-0.0003(3)	0.0008(3)	0.0007(3)
Si5	0.0071(5)	0.0058(3)	0.0113(4)	0.0008(3)	0.0006(3)	0.0009(3)
Si6	0.0065(4)	0.0061(3)	0.0097(4)	0.0000(3)	-0.0007(3)	-0.0002(3)
Si7	0.0064(5)	0.0070(3)	0.0100(4)	-0.0009(3)	-0.0020(3)	0.0000(3)
Si8	0.0051(4)	0.0074(3)	0.0103(4)	-0.0007(3)	-0.0016(3)	-0.0004(3)
Si9	0.0065(4)	0.0057(3)	0.0100(4)	0.0001(3)	-0.0007(3)	-0.0004(3)
Si10	0.0061(4)	0.0068(3)	0.0102(4)	0.0002(3)	-0.0008(3)	-0.0009(3)
Si11	0.0057(4)	0.0075(3)	0.0101(4)	-0.0004(3)	-0.0007(3)	0.0004(3)
Si12	0.0067(4)	0.0058(3)	0.0108(3)	0.0008(3)	-0.0001(3)	0.0009(3)
Si13	0.0060(4)	0.0067(3)	0.0109(4)	0.0004(3)	-0.0006(3)	-0.0002(3)
Si14	0.0054(4)	0.0073(3)	0.0101(4)	0.0004(3)	-0.0007(3)	-0.0013(3)
O1	0.0113(14)	0.0091(11)	0.0104(12)	0.0001(7)	0.0016(10)	0.0004(7)
O2	0.0159(19)	0.0136(16)	0.0117(16)	0	0.0009(14)	0
O3	0.0141(18)	0.0121(15)	0.0111(15)	0	-0.0003(13)	0
O4	0.0144(14)	0.0157(12)	0.0103(12)	0.0003(8)	-0.0008(11)	0.0000(8)
O5	0.0116(14)	0.0095(10)	0.0095(11)	0.0001(7)	-0.0020(9)	-0.0008(7)
O6	0.0159(19)	0.0125(15)	0.0123(16)	0	-0.0010(14)	0
O7	0.0121(18)	0.0126(14)	0.0129(16)	0	0.0014(13)	0

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Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O8	0.0135(14)	0.0121(11)	0.0071(11)	0.0012(8)	-0.0015(9)	-0.0017(8)
O9	0.0152(14)	0.0125(11)	0.0101(12)	0.0006(8)	-0.0010(10)	0.0017(8)
O10	0.0115(18)	0.0146(15)	0.0124(16)	0	-0.0010(14)	0
O11	0.0155(19)	0.0122(15)	0.0129(16)	0	0.0012(14)	0
O12	0.0137(14)	0.0097(11)	0.0082(11)	-0.0004(8)	0.0020(10)	0.0003(7)
O13	0.0118(13)	0.0121(11)	0.0129(12)	-0.0008(8)	0.0024(10)	0.0016(8)
O14	0.0161(14)	0.0153(12)	0.0087(11)	-0.0015(8)	0.0007(10)	0.0009(9)
O15	0.0091(13)	0.0116(10)	0.0096(11)	0.0016(8)	-0.0017(9)	0.0001(8)
O16	0.0159(14)	0.0148(12)	0.0116(12)	0.0007(9)	-0.0008(10)	0.0036(9)
O17	0.0154(14)	0.0107(10)	0.0126(11)	-0.0001(8)	-0.0009(10)	-0.0019(8)
O18	0.0159(14)	0.0141(12)	0.0120(12)	0.0000(8)	-0.0025(10)	0.0005(9)
O19	0.0104(13)	0.0111(10)	0.0099(10)	-0.0011(8)	-0.0023(9)	-0.0007(8)
O20	0.0127(14)	0.0117(11)	0.0124(12)	0.0001(8)	-0.0022(10)	-0.0011(8)
O21	0.0178(15)	0.0118(11)	0.0109(12)	0.0007(8)	0.0000(10)	0.0019(8)
O22	0.0106(14)	0.0120(11)	0.0110(11)	-0.0004(8)	-0.0004(9)	0.0000(8)
O23	0.0133(15)	0.0131(11)	0.0102(11)	0.0008(8)	0.0001(10)	-0.0002(8)
O24	0.0139(14)	0.0108(11)	0.0157(12)	0.0010(8)	0.0010(10)	0.0002(9)
O25	0.0111(13)	0.0130(11)	0.0110(11)	-0.0007(8)	-0.0012(9)	0.0011(9)
O26	0.0105(12)	0.0113(10)	0.0097(10)	0.0010(8)	0.0004(8)	0.0011(8)
O27	0.0092(12)	0.0091(10)	0.0100(10)	-0.0001(8)	-0.0018(8)	0.0009(8)
O28	0.0123(13)	0.0134(11)	0.0120(11)	-0.0002(8)	-0.0027(9)	0.0022(9)
O29	0.0130(13)	0.0101(10)	0.0105(10)	0.0001(8)	0.0004(9)	-0.0018(8)
O30	0.0154(14)	0.0129(11)	0.0102(11)	-0.0002(8)	-0.0009(9)	-0.0008(9)
O31	0.0103(13)	0.0119(10)	0.0088(10)	-0.0005(8)	-0.0005(9)	-0.0014(8)
O32	0.0079(12)	0.0114(10)	0.0103(10)	0.0004(8)	-0.0012(8)	0.0008(8)
O33	0.0116(13)	0.0123(11)	0.0131(11)	-0.0020(8)	0.0003(10)	0.0003(9)
O34	0.0135(13)	0.0097(10)	0.0107(11)	0.0010(8)	0.0016(9)	0.0009(8)
O35	0.0122(13)	0.0117(11)	0.0134(12)	0.0009(8)	0.0010(10)	0.0009(9)
O36	0.0112(13)	0.0098(10)	0.0093(10)	0.0000(8)	-0.0010(9)	0.0010(8)
O37	0.0077(11)	0.0146(10)	0.0190(11)	0.0002(9)	-0.0060(8)	0.0006(9)
O38	0.0085(11)	0.0124(10)	0.0119(10)	0.0022(8)	-0.0027(8)	-0.0020(8)
O39	0.0089(11)	0.0096(10)	0.0145(10)	-0.0024(8)	-0.0008(8)	0.0013(8)
O40	0.0091(11)	0.0122(10)	0.0142(10)	0.0027(8)	-0.0004(8)	-0.0017(8)
O41	0.0129(12)	0.0121(10)	0.0200(11)	-0.0013(8)	0.0052(9)	0.0018(9)
O42	0.0121(11)	0.0145(10)	0.0144(10)	-0.0055(8)	-0.0015(8)	0.0009(8)
O43	0.0095(11)	0.0126(10)	0.0141(10)	0.0034(8)	-0.0036(8)	-0.0017(8)
O44	0.0109(11)	0.0066(9)	0.0144(10)	-0.0013(7)	0.0021(8)	-0.0014(7)
O45	0.0106(11)	0.0067(9)	0.0146(10)	0.0001(7)	0.0001(8)	0.0001(7)
O46	0.0159(12)	0.0049(9)	0.0149(11)	-0.0004(8)	0.0000(9)	0.0015(7)
O47	0.0078(11)	0.0203(11)	0.0142(11)	0.0030(8)	-0.0001(8)	0.0023(8)

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Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O48	0.0065(11)	0.0095(9)	0.0153(10)	0.0005(8)	-0.0024(8)	-0.0030(8)
O49	0.0090(11)	0.0110(10)	0.0126(10)	0.0020(8)	-0.0022(8)	-0.0009(8)
O50	0.0077(11)	0.0103(9)	0.0165(11)	0.0001(8)	-0.0014(8)	-0.0004(8)
O51	0.0124(12)	0.0151(10)	0.0174(11)	-0.0036(8)	0.0005(9)	0.0033(9)
O52	0.0101(12)	0.0169(11)	0.0129(10)	0.0065(8)	-0.0011(8)	-0.0009(8)
O53	0.0109(11)	0.0165(11)	0.0131(10)	-0.0045(8)	-0.0016(8)	0.0020(8)
O54	0.0121(11)	0.0080(9)	0.0169(10)	0.0005(8)	-0.0043(8)	-0.0004(8)
O55	0.0170(12)	0.0120(10)	0.0181(11)	0.0042(8)	0.0010(9)	-0.0043(8)
O56	0.0146(17)	0.0083(13)	0.0124(14)	0	0.0000(12)	0
O57	0.0122(16)	0.0084(13)	0.0109(14)	0	0.0002(12)	0
O58	0.0109(16)	0.0066(13)	0.0157(14)	0	-0.0005(12)	0
O59	0.0119(16)	0.0102(14)	0.0115(14)	0	-0.0009(12)	0

Distortion parameters

Table 3: Polyhedra: DV = Distance Variation, QE = Quadratic Elongation AV = Angle Variance (Robinson *et al.*, 1971)

Atom	Vol	DV	QE	AV
Mn1	13.785	0.00023	1.00877	28.69
Mn2	13.726	0.00037	1.01996	63.55
Mn3	13.898	0.00313	1.02601	79.70
Mn4	14.439	0.00441	1.02184	60.53
Mn5	13.849	0.00421	1.03058	92.29
Mn6	13.657	0.00108	1.02013	63.90
Mn7	13.685	0.00435	1.02913	85.99
Mn8	13.982	0.00372	1.02843	82.43
Mn9	14.016	0.00290	1.02552	75.88
Mn10	13.720	0.00115	1.02318	72.31
Mn11	13.751	0.00184	1.02095	64.80
Mn12	13.736	0.00398	1.03017	92.60
Mn13	13.416	0.00076	1.02540	79.96
Mn14	13.424	0.00105	1.02724	84.65
Mn15	13.740	0.00376	1.03204	96.66
Mn16	13.977	0.00195	1.02279	69.33
Mn17	13.525	0.00177	1.03092	94.32
Mn18	13.451	0.00286	1.02798	85.88
Si1	2.168	0.00024	1.00356	14.98
Si2	2.178	0.00017	1.00255	10.75
Si3	2.189	0.00021	1.00191	7.70

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Atom	Vol	DV	QE	AV
Si4	2.139	0.00022	1.00443	18.45
Si5	2.142	0.00007	1.00435	18.98
Si6	2.146	0.00019	1.00294	12.55
Si7	2.183	0.00029	1.00341	13.95
Si8	2.166	0.00010	1.00506	22.14
Si9	2.178	0.00012	1.00366	15.01
Si10	2.172	0.00021	1.00345	14.79
Si11	2.158	0.00017	1.00375	16.28
Si12	2.130	0.00001	1.00566	22.88
Si13	2.142	0.00015	1.00425	17.99
Si14	2.143	0.00011	1.00412	16.68

Coordination sequences of the Vertices

Table 4: Coordination sequences for all vertices. The vertex numbers correspond to the $c2mm$ embedding, as defined in the provided `innsbruckite.cgd` file. TD10 = 167

Vertex	Coordination sequence									
1	3	5	8	12	16	18	20	24	28	30
2	3	6	9	12	14	19	21	24	27	30
3	3	6	10	11	15	18	22	23	26	32
4	3	6	9	12	15	17	22	26	28	30
5	3	6	8	13	15	18	20	25	28	29
6	3	6	9	13	15	18	20	24	28	29
7	3	6	9	11	14	20	22	24	28	32
8	3	6	8	11	17	18	22	24	28	32

Calculated powder pattern

Table 5: Calculated powder diffraction pattern of innsbruckite for $CuK_{\alpha 1}$, using Xpow (Downs *et al.*, 1993).

2Θ [°]	rel. Int. [%]	d_{hkl} [Å]	h	k	l
5.68	1.1	15.568	1	1	0
8.98	1.4	9.847	1	3	0
9.84	1.4	8.989	0	4	0
12.20	100.0	7.254	0	0	1
13.36	1.4	6.630	-1	1	1
13.58	3.0	6.522	1	1	1
14.22	2.7	6.228	2	4	0
15.07	1.5	5.878	-1	3	1
15.27	1.4	5.803	1	3	1
15.70	1.9	5.645	0	4	1
17.09	3.3	5.189	3	3	0
18.94	3.0	4.686	2	4	1
19.75	6.6	4.495	0	8	0
19.75	2.0	4.494	3	5	0
20.83	5.8	4.264	-3	3	1
21.75	1.6	4.087	-1	7	1
21.89	1.0	4.061	1	7	1
22.85	5.6	3.892	4	4	0

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2Θ	rel. int.	d_{hkl}	h	k	l
23.09	3.1	3.853	-3	5	1
23.28	5.5	3.821	0	8	1
24.54	29.1	3.627	0	0	2
25.05	4.2	3.555	0	2	2
25.09	14.9	3.549	-1	1	2
25.33	15.6	3.516	1	1	2
26.07	2.3	3.419	-1	3	2
26.21	5.1	3.400	4	4	1
26.30	1.3	3.389	1	3	2
26.50	1.6	3.364	0	4	2
28.26	1.2	3.158	-2	4	2
29.75	1.3	3.003	-3	3	2
30.37	1.0	2.944	3	3	2
30.51	1.1	2.930	-1	7	2
31.07	6.9	2.879	6	0	0
31.47	8.8	2.843	3	11	0
33.21	1.2	2.698	-6	0	1
33.73	77.1	2.657	-3	11	1
33.77	41.2	2.654	6	0	1
33.90	3.0	2.644	-2	12	1
34.01	4.2	2.636	3	11	1
34.09	1.6	2.630	2	12	1
34.15	1.2	2.626	6	2	1
34.56	1.8	2.595	-4	10	1
36.43	1.5	2.466	5	1	2
36.53	1.6	2.460	-2	10	2
36.68	1.0	2.450	-3	9	2
37.18	3.0	2.418	0	0	3
38.04	1.4	2.365	-3	13	1
38.46	1.4	2.341	-4	12	1
38.79	1.1	2.322	4	12	1
39.50	5.9	2.281	-6	0	2
40.07	32.1	2.250	-3	11	2
40.47	14.0	2.229	6	0	2
40.55	10.4	2.225	3	11	2
40.75	1.2	2.214	-4	10	2
46.42	1.8	1.956	5	1	3
48.60	2.5	1.874	-6	0	3
49.18	8.0	1.853	-3	11	3
49.38	3.3	1.846	-2	12	3

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2Θ	rel. int.	d_{hkl}	h	k	l
49.73	2.3	1.834	-4	10	3
49.79	4.8	1.831	3	11	3
49.82	4.6	1.830	6	0	3
50.10	1.3	1.821	6	2	3
52.45	1.0	1.745	-3	13	3
52.70	3.5	1.737	-4	12	3
53.77	2.8	1.705	7	1	3
55.53	18.8	1.655	9	11	0
56.29	8.2	1.634	0	22	0
56.81	8.9	1.621	-9	11	1
57.36	6.6	1.606	9	11	1
57.83	7.7	1.594	0	22	1
58.06	1.1	1.589	5	1	4
58.19	1.6	1.585	2	10	4
59.61	1.5	1.551	-6	0	4
60.21	3.5	1.537	-3	11	4
60.88	1.1	1.522	2	12	4
60.92	3.2	1.521	3	11	4
61.03	1.5	1.518	6	0	4
61.07	1.7	1.517	-9	11	2
62.13	2.0	1.494	9	11	2
62.31	1.6	1.490	0	22	2
62.93	2.0	1.477	-7	1	4
64.20	2.3	1.451	4	12	4
65.70	1.7	1.421	6	22	0
65.86	2.9	1.418	-12	0	1
67.28	5.9	1.392	6	22	1
67.99	1.0	1.379	-9	11	3
69.72	2.1	1.349	-12	0	2
70.94	1.5	1.329	-6	22	2
71.59	3.2	1.318	6	22	2
73.66	1.7	1.286	3	11	5
78.45	1.7	1.219	6	22	3

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