Supplementary Materials. Inorganic structures in space group *P*31*m*; coordinate analysis and systematic prediction of new ferroelectrics

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Abstract

The 62 entries listed in ICSD release 2009/1 under polar space group *P*31*m* correspond to 31 families of inorganic crystal structures, some with only one member. Coordinate analysis reveals, over a wide confidence range, 11 of these families as ferroelectric candidates. One includes the well-known improper ferroelectric GASH [$(C(NH_2)_3)Al(SO_4)_2(H_2O)_6$], another the previously-predicted ferroelectric $CsNO_3$ phase II. Those remaining include $K_3Nb_3B_2O_{12}$, the minerals schairerite, galeite and lizardite 1*T*, $LaNi_5D_6$ and γ-$CaNi_5D_{6.1}$, $Ca(OCl)_2Ca(OH)_2$, $(N(CH_3)_4)_2Mo_3S_{13}$, $Li_{17}Ag_3Sn_6$ and $Cs_3As_5O_9$. Candidate selection is based upon detecting an approach by the reported atomic arrangement to the symmetry of a corresponding nonpolar supergroup. A further 13 families are typified by their reduced predictive properties, with four others likely to remain polar at higher temperatures and the remaining three noted as having a unit cell larger than reported or a misassigned space group. The primary sources of uncertainty in structurally-based predictions of ferroelectricity are the reliability of the underlying structural determination and the upper limit assigned to the cationic displacement magnitudes required to achieve supergroup symmetry.

Table S1(*a*)

Modified atomic positions in $K_3B_2Nb_3O_{12}$ subcell (Choisnet *et al*., 1977) [968], with hypothetical $x'\,y'\,z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4 in paper).

a = 8.753(5), c = 3.966(1) Å, $z^* = z + 0.0086$.

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	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K	3(*c*)	3(*g*)	0.5964(9)	0.0	0.4989(22)	0.5075	0.5964	0.0	0.5	0.0	0.0	0.03	0.03	0.11
Nb	3(*c*)	3(*f*)	0.2463(3)	0.0	0.0	0.0086	0.2463	0.0	0.0	0.0	0.0	0.03	0.03	0.08
O1	3(*c*)	3(*f*)	0.8179(35)	0.0	-0.0076(75)	0.0010	0.8179	0.0	0.0	0.0	0.0	0.00	0.00	0.1
O2	3(*c*)	3(*g*)	0.2606(29)	0.0	0.493(12)	0.5016	0.2606	0.0	0.5	0.0	0.0	0.01	0.01	0.1
O3	6(*d*)	6(*j*)	0.503(28)	0.1854(20)	-0.0169(57)	-0.0083	0.503	0.1854	0.0	0.0	0.0	-0.03	0.03	0.12
B	2(*b*)	2(*d*)	0.3333	0.6667	-0.019(13)	-0.0104	0.3333	0.6667	0.0	0.0	0.0	-0.04	0.04	0.09

Table S1(*b*)

Modified atomic positions in $K_3B_2Nb_3O_{12}$ full cell (Choisnet *et al*., 1977) [969], with hypothetical $x'\,y'\,z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4 in paper).

a = 34.01, c = 3.966 Å; $z^* = z + 0.0402$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K1	3(*c*)	3(*g*)	0.1489(3)	0.0	0.4596(21)	0.4998	0.1489	0.0	½	0	0	-0.160	0.160	0.10
K4	3(*c*)	3(*g*)	0.8996(3)	0.0	0.4687(23)	0.5089	0.8996	0.0	½	0	0	0.035	0.035	0.11
K2	3(*c*)	3(*g*)	0.3983(3)	0.0	0.4585(20)	0.4987	0.3983	0.0	½	0	0	-0.005	0.005	0.09
K3	3(*c*)	3(*g*)	0.649(3)	0.0	0.4493(22)	0.4895	0.649	0.0	½	0	0	-0.042	0.042	0.12
K5	6(*d*)	6(*k*)	0.1482(2)	0.248(2)	0.4583(16)	0.4985	0.1482	0.248	½	0	0	-0.006	0.006	0.11
K7	6(*d*)	6(*k*)	0.1502(2)	0.7523(2)	0.4543(15)	0.4945	0.1502	0.7523	½	0	0	-0.022	0.022	0.10
K6	6(*d*)	6(*k*)	0.1492(2)	0.5(2)	0.4641(17)	0.5043	0.1492	0.5	½	0	0	0.017	0.017	0.11
K9	6(*d*)	6(*k*)	0.1003(2)	0.6009(2)	0.4583(16)	0.4985	0.1003	0.6009	½	0	0	-0.006	0.006	0.11
K8	6(*d*)	6(*k*)	0.1013(2)	0.35(2)	0.4523(16)	0.4925	0.1013	0.35	½	0	0	-0.030	0.030	0.11
K10	6(*d*)	6(*k*)	0.3523(2)	0.6007(2)	0.4723(16)	0.5125	0.3523	0.6007	½	0	0	0.050	0.050	0.11
Nb1	3(*c*)	3(*f*)	0.0617(1)	0.0	0.0	0.0402	0.0617	0.0	0	0	0	0.159	0.159	0.00
Nb2	3(*c*)	3(*f*)	0.311(1)	0.0	-0.0738(9)	-0.0336	0.311	0.0	0	0	0	-0.133	0.133	0.04
Nb3	3(*c*)	3(*f*)	0.5612(1)	0.0	-0.0664(11)	-0.0262	0.5612	0.0	0	0	0	-0.104	0.104	0.07
Nb4	3(*c*)	3(*f*)	0.8126(1)	0.0	-0.014(11)	0.0262	0.8126	0.0	0	0	0	0.104	0.104	0.09
Nb5	6(*d*)	6(*j*)	0.0609(1)	0.2498(1)	-0.0648(9)	-0.0246	0.0609	0.2498	0	0	0	-0.098	0.098	0.08
Nb7	6(*d*)	6(*j*)	0.0622(1)	0.7508(1)	-0.0733(8)	-0.0331	0.0622	0.7508	0	0	0	-0.131	0.131	0.05
Nb6	6(*d*)	6(*j*)	0.0611(1)	0.499(1)	-0.0277(9)	0.0125	0.0611	0.499	0	0	0	0.050	0.050	0.07
Nb9	6(*d*)	6(*j*)	0.1888(1)	0.6883(1)	-0.0204(10)	0.0198	0.1888	0.6883	0	0	0	0.079	0.079	0.08
Nb8	6(*d*)	6(*j*)	0.1873(1)	0.4381(1)	-0.0676(8)	-0.0274	0.1873	0.4381	0	0	0	-0.109	0.109	0.07
Nb10	6(*d*)	6(*j*)	0.4389(1)	0.6888(1)	0.0071(9)	0.0473	0.4389	0.6888	0	0	0	0.188	0.188	0.00

O1	3(*c*)	3(*f*)	0.2053(7)	0.0	-0.0004(54)	0.0398	0.2053	0.0	0	0	0	0.158	0.158	0.00
O2	3(*c*)	3(*f*)	0.4537(7)	0.0	-0.0409(58)	-0.0007	0.4537	0.0	0	0	0	-0.028	0.028	0.04
O3	3(*c*)	3(*f*)	0.7067(7)	0.0	-0.0904(59)	-0.0502	0.7067	0.0	0	0	0	-0.199	0.199	0.05
O4	3(*c*)	3(*f*)	0.9546(8)	0.0	-0.063(62)	-0.0228	0.9546	0.0	0	0	0	-0.090	0.090	0.06
O5	6(*d*)	6(*j*)	0.2032(6)	0.2468(6)	0.0021(41)	0.0423	0.2032	0.2468	0	0	0	0.168	0.168	0.05
O6	6(*d*)	6(*j*)	0.2056(7)	0.4999(7)	-0.0313(50)	0.0089	0.2056	0.4999	0	0	0	0.035	0.035	0.09
O7	6(*d*)	6(*j*)	0.2039(6)	0.7501(7)	-0.0425(41)	-0.0023	0.2039	0.7501	0	0	0	-0.009	0.009	0.06
O8	6(*d*)	6(*j*)	0.0457(8)	0.2935(8)	-0.0372(56)	0.0030	0.0457	0.2935	0	0	0	0.012	0.012	0.12
O9	6(*d*)	6(*j*)	0.0461(8)	0.5471(8)	-0.0489(55)	-0.0087	0.0461	0.5471	0	0	0	-0.035	0.035	0.10
O10	6(*d*)	6(*j*)	0.2961(6)	0.5458(6)	-0.0668(40)	-0.0266	0.2961	0.5458	0	0	0	-0.105	0.105	0.05
O21	6(*d*)	6(*j*)	0.1255(7)	0.0465(7)	-0.0867(50)	-0.0669	0.1255	0.0465	0	0	0	-0.265	0.265	0.10
O22	6(*d*)	6(*j*)	0.1255(6)	0.296(6)	-0.0151(42)	0.0251	0.1255	0.296	0	0	0	0.100	0.100	0.05
O23	6(*d*)	6(*j*)	0.1251(7)	0.5465(7)	-0.0364(45)	0.0038	0.1251	0.5465	0	0	0	0.015	0.015	0.07
O24	6(*d*)	6(*j*)	0.1256(9)	0.7934(9)	-0.0691(61)	-0.0289	0.1256	0.7934	0	0	0	-0.115	0.115	0.13
O25	6(*d*)	6(*j*)	0.3771(8)	0.0489(8)	-0.0044(53)	0.0358	0.3771	0.0489	0	0	0	0.142	0.142	0.11
O26	6(*d*)	6(*j*)	0.3771(8)	0.2968(8)	0.0015(52)	0.0417	0.3771	0.2968	0	0	0	0.165	0.165	0.10
O27	6(*d*)	6(*j*)	0.3751(7)	0.5475(7)	-0.054(47)	-0.0138	0.3751	0.5475	0	0	0	-0.055	0.055	0.08
O28	6(*d*)	6(*j*)	0.376(1)	0.7952(10)	-0.0674(67)	-0.0272	0.376	0.7952	0	0	0	-0.108	0.108	0.14
O29	6(*d*)	6(*j*)	0.6277(7)	0.0473(7)	-0.0204(46)	0.0198	0.6277	0.0473	0	0	0	0.078	0.078	0.07
O30	6(*d*)	6(*j*)	0.6254(9)	0.2963(9)	-0.0015(56)	0.0387	0.6254	0.2963	0	0	0	0.153	0.153	0.12
O31	6(*d*)	6(*j*)	0.6244(9)	0.5461(9)	-0.0191(61)	0.0211	0.6244	0.5461	0	0	0	0.084	0.084	0.13
O32	6(*d*)	6(*j*)	0.6262(7)	0.7974(7)	-0.0847(47)	-0.0445	0.6262	0.7974	0	0	0	-0.176	0.176	0.09
O33	6(*d*)	6(*j*)	0.8771(7)	0.047(7)	-0.0385(47)	0.0017	0.8771	0.047	0	0	0	0.007	0.007	0.08
O34	6(*d*)	6(*j*)	0.8763(7)	0.2959(7)	-0.0374(46)	0.0028	0.8763	0.2959	0	0	0	0.011	0.011	0.07
O35	6(*d*)	6(*j*)	0.875(7)	0.5466(7)	-0.0568(45)	-0.0166	0.875	0.5466	0	0	0	-0.066	0.066	0.08
O36	6(*d*)	6(*j*)	0.2015(8)	0.0784(8)	-0.0725(55)	-0.0323	0.2015	0.0784	0	0	0	-0.128	0.128	0.11
O11	3(c)	6(*j*)	0.0606(7)	0.0	0.4316(54)	0.4718	0.0606	0.0	½	0	0	-0.112	0.112	0.00
O12	3(c)	3(*g*)	0.31(8)	0.0	0.4544(82)	0.4946	0.31	0.0	½	0	0	-0.021	0.021	0.09
O13	3(c)	3(*g*)	0.5673(7)	0.0	0.4816(62)	0.5218	0.5673	0.0	½	0	0	0.086	0.086	0.05
O14	3(c)	3(*g*)	0.8166(7)	0.0	0.4672(53)	0.5074	0.8166	0.0	½	0	0	0.029	0.029	0.06
O15	6(*d*)	6(*k*)	0.061(6)	0.2439(6)	0.4667(42)	0.5069	0.061	0.2439	½	0	0	0.027	0.027	0.05
O16	6(*d*)	6(*k*)	0.0644(7)	0.497(8)	0.4528(48)	0.4930	0.0644	0.497	½	0	0	-0.028	0.028	0.08
O17	6(*d*)	6(*k*)	0.0644(7)	0.7541(8)	0.4809(71)	0.5211	0.0644	0.7541	½	0	0	0.084	0.084	0.12
O18	6(*d*)	6(*k*)	0.1848(5)	0.4305(6)	0.4519(41)	0.4912	0.1848	0.4305	½	0	0	-0.035	0.035	0.11
O19	6(*d*)	6(*k*)	0.1839(8)	0.6827(7)	0.4512(54)	0.4914	0.1839	0.6827	½	0	0	-0.034	0.034	0.09
O20	6(*d*)	6(*k*)	0.4341(9)	0.6811(10)	0.4512(56)	0.4914	0.4341	0.6811	½	0	0	-0.034	0.034	0.13
B1	2(*b*)	2(*c*)	0.3333	0.6667	-0.014(16)	0.0262	0.3333	0.6667	0	0	0	0.104	0.104	0.13
B2	6(*d*)	6(*j*)	0.0831(10)	0.1673(10)	-0.0496(70)	-0.0094	0.0821	0.1673	0	0	0	-0.037	0.037	0.09
B3	6(*d*)	6(*j*)	0.0821(9)	0.4166(9)	-0.0269(63)	0.0161	0.0831	0.4166	0	0	0	0.064	0.064	0.07
B4	6(*d*)	6(*j*)	0.1678(9)	0.3359(9)	-0.0386(58)	0.0016	0.0428	0.3359	0	0	0	0.006	0.006	0.05
B6	6(*d*)	6(*j*)	0.0822(11)	0.6654(11)	-0.0115(71)	0.0287	-0.0428	0.6654	0	0	0	0.114	0.114	0.10
B5	6(*d*)	6(*j*)	0.1674(8)	0.5845(8)	-0.054(54)	-0.0138	0.0	0.5845	0	0	0	-0.055	0.055	0.00

Table S2.

Modified atomic positions for the mineral schairerite $Na_{21}(SO_4)_7F_6Cl$, based on Fanfani *et al.* (1975*a*) [4289], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 12.197(4), c = 19.359(11) Å; z^* = z - 0.0078.

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Na1	3(*c*)	3(*g*)	0.5152(4)	0.0	0.5166(4)	0.5088	0.5	0.0	0.5	0.19	0.0	0.17	0.25	0.14
Na11	3(*c*)		0.4879(5)	0.0	0.7928(5)	0.785	0.4849	0.0	0.7785	0.04	0.0	0.13	0.14	0.12
		6(*k*)												
Na13	3(*c*)		0.518(5)	0.0	0.2357(5)	0.2279	0.5151	0.0	0.2215	0.04	0.0	0.12	0.14	0.14
Na2	6(*d*)	6(*j*)	0.1591(4)	0.334(5)	0.5147(4)	0.5069	0.1643	0.3287	0.5	-0.06	0.0	0.13	0.14	0.13
Na8	6(*d*)		0.8448(3)	0.3337(4)	0.6527(4)	0.6449	0.8491	0.3327	0.6341	-0.05	-0.0	0.21	0.22	0.13
		12(*l*)												
Na4	6(*d*)		0.4788(3)	0.3318(4)	0.3846(4)	0.3768	0.4783	0.3327	0.3659	0.01	0.01	0.21	0.21	0.13
Na3	3(*c*)		0.8128(4)	0.0	0.3789(4)	0.3711	0.8184	0.0	0.3661	-0.07	0.0	0.10	0.12	0.12
		6(*k*)												
Na7	3(*c*)		0.1759(4)	0.0	0.6468(4)	0.639	0.1816	0.0	0.6339	-0.07	0.0	0.10	0.12	0.12
Na5	3(*c*)		0.1892(4)	0.0	0.9294(5)	0.9216	0.1828	0.0	0.9169	0.08	0.0	0.09	0.12	0.12
		6(*k*)												
Na9	3(*c*)		0.8236(5)	0.0	0.0957(5)	0.0879	0.8172	0.0	0.0831	0.08	0.0	0.09	0.12	0.15
Na6	6(*d*)		0.847(3)	0.3359(4)	0.9339(4)	0.9261	0.8511	0.3335	0.9152	-0.05	0.03	0.21	0.22	0.12
		12(*l*)												
Na10	6(*d*))		0.4783(4)	0.3312(4)	0.1034(4)	0.0956	0.4824	0.3335	0.0848	-0.05	-0.01	0.21	0.22	0.15
Na14	6(*d*)		0.1811(4)	0.3334(5)	0.2391(4)	0.2313	0.1818	0.3340	0.2225	-0.01	-0.01	0.17	0.17	0.14
		12(*l*)												
Na12	6(*d*))		0.1515(3)	0.3345(4)	0.7941(4)	0.7863	0.1522	0.3340	0.7775	-0.01	0.01	0.17	0.17	0.11
Cl1	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.0078	0.0	0.0	0.0	0.0	0.0	-0.15	0.15	0.1
Cl2	2(*b*)	2(*c*)	0.6667	0.3333	0.0296(2)	0.0218	0.6667	0.3333	0.0	0.0	0.0	0.42	0.42	0.15
S1	1(*a*)		0.0	0.0	0.2376(4)	0.2298	0.0	0.0	0.2297	0.0	0.0	0.00	0.00	0.12
		2(*e*)												
S3	1(*a*)		0.0	0.0	0.7782(5)	0.7704	0.0	0.0	0.7703	0.0	0.0	0.00	0.00	0.11
S5	1(*a*)	1(*b*)	0.0	0.0	0.5074(4)	0.4996	0.0	0.0	0.5	0.0	0.0	-0.01	0.01	0.11
S2	2(*b*)		0.6667	0.3333	0.2532(4)	0.2454	0.6667	0.3333	0.2291	0.0	0.0	0.32	0.32	0.11
		4(*h*)												
S4	2(*b*)		0.6667	0.3333	0.795(4)	0.7872	0.6667	0.3333	0.7709	0.0	0.0	0.32	0.32	0.1
S6	2(*b*)	2(*d*)	0.6667	0.3333	0.5266(4)	0.5188	0.6667	0.3333	0.5	0.0	0.0	0.36	0.36	0.1
S7	3(*c*)		0.6699(3)	0.0	0.6659(4)	0.6581	0.6667	0.0	0.6493	0.04	0.0	0.17	0.17	0.1
		6(*k*)												
S9	3(*c*)		0.3366(3)	0.0	0.3673(4)	0.3595	0.3333	0.0	0.3507	0.04	0.0	0.17	0.17	0.1
S8	3(*c*)		0.6672(3)	0.0	0.9387(4)	0.9309	0.6664	0.0	0.9227	0.01	0.0	0.16	0/16	0.11
		6(*k*)												
S10	3(*c*)		0.3344(3)	0.0	0.0933(4)	0.0855	0.3336	0.0	0.0773	0.01	0.0	0.16	0.16	0.09
F1	3(*c*)		0.6858(5)	0.0	0.4658(5)	0.6686	0.6686	0.0	0.4492	0.21	0.0	0.17	0.27	0.13
		6(*k*)												
F3	3(*c*)		0.3486(5)	0.0	0.5674(5)	0.3314	0.3314	0.0	0.5508	0.21	0.0	0.17	0.27	0.11
F2	3(*c*)		0.3396(6)	0.0	0.8636(5)	0.8558	0.3322	0.0	0.8485	0.09	0.0	0.14	0.17	0.1
		6(*k*)												
F5	3(*c*)		0.6753(6)	0.0	0.1666(5)	0.1588	0.6678	0.0	0.1515	0.09	0.0	0.14	0.17	0.12

F6	3(*c*)		0.3262(6)	0.0	0.7175(5)	0.7097	0.3321	0.0	0.7022	-0.07	0.0	0.15	0.17	0.1
		6(*k*)												
F4	3(*c*)		0.662(7)	0.0	0.3131(6)	0.3053	0.6679	0.0	0.2978	-0.07	0.0	0.15	0.17	0.14
O1	1(*a*)†		0.0	0.0	0.1631(12)	0.1553	0.0	0.0	0.2302	0.0	0.0	*-1.45*	*1.45*	0.2
		2(*e*)												
O5	1(*a*)†		0.0	0.0	0.7026(10)	0.6948	0.0	0.0	0.7698	0.0	0.0	*-1.45*	*1.45*	0.15
O9	1(*a*)†	1(*b*)	0.0	0.0	0.4317(9)	0.4239	0.0	0.0	0.5	0.0	0.0	*-1.47*	*1.47*	0.12
O2	3(*c*)		0.8884(7)	0.0	0.2636(5)	0.2558	0.8872	0.0	0.2286	0.01	0.0	0.53	0.53	0.12
		6(*k*)												
O6	3(*c*)		0.114(7)	0.0	0.8064(6)	0.7986	0.1128	0.0	0.7714	0.01	0.0	0.53	0.53	0.12
O16	3(*c*)		0.6678(8)	0.0	0.0146(6)	0.0068	0.6660	0.0	-0.0011	0.02	0.0	0.15	0.15	0.11
		6(*k*)												
O22	3(*c*)		0.3358(9)	0.0	0.0167(6)	0.0089	0.3340	0.0	0.0011	0.02	0.0	0.15	0.15	0.14
O3	2(*b*)		0.6667	0.3333	0.3301(8)	0.3223	0.6667	0.3333	0.3629	0.0	0.0	-0.79	0.79	0.15
		4(*h*)												
O11	2(*b*)	2(*d*)	0.6667	0.3333	0.6043(7)	0.5965	0.6667	0.3333	0.6371	0.0	-0.0	-0.79	0.79	0.12
O7	2(*b*)†	2(*c*)	0.6667	0.3333	-0.1283(6)	-0.1361	0.6667	0.3333	0.0	0.0	0.0	*-2.63*	*2.63*	0.1
O4	6(*d*)		0.6683(5)	0.2201(7)	0.2318(5)	0.2240	0.6680	0.2180	0.2309	0.0	0.03	-0.13	0.13	0.16
		12(*l*)												
O8	6(*d*)		0.5502(7)	0.2158(7)	0.7701(5)	0.7623	0.5500	0.2180	0.7691	0.0	-0.03	-0.13	0.13	0.16
O24	6(*d*)		0.3342(9)	0.1123(7)	0.1204(5)	0.1126	0.3361	0.1138	0.1036	-0.03	-0.02	0.18	0.18	0.15
		12(*l*)												
O18	6(*d*)		0.7808(6)	0.1154(6)	0.9133(5)	0.9055	0.7777	0.1138	0.8964	-0.03	-0.02	0.18	0.18	0.12
O12	6(*d*)	6(*i*)	0.672(5)	0.2209(6)	0.5021(5)	0.4946	0.6310	0.2619	0.5	0.50	-0.50	-0.11	0.51	0.15
O13	3(*c*)		0.6771(8)	0.0	0.7416(6)	0.7338	0.6694	0.0	0.7259	0.09	0.0	0.15	0.17	0.12
		6(*k*)												
O19	3(*c*)		0.3384(8)	0.0	0.2897(6)	0.2819	0.3306	0.0	0.2741	0.10	0.0	0.15	0.18	0.13
O21	6(*d*)		0.3356(8)	0.1125(6)	0.3934(5)	0.3856	0.3334	0.1146	0.3766	0.03	-0.03	0.17	0.17	0.14
		12(*l*)												
O15	6(*d*)		0.7834(6)	0.1167(6)	0.6403(5)	0.6325	0.7812	0.1146	0.6234	0.03	0.03	0.18	0.18	0.13
O10	3(*c*)†	6(*k*)	0.113(7)	0.0	0.532(5)	0.5242	0.113	0.0	0.5	-0.01	0.0	*0.47*	*0.47*	0.12
O14	3(*c*)		0.5517(7)	0.0	0.646(6)	0.6382	0.5521	0.0	0.6244	0.01	0.0	0.27	0.27	0.12
		6(*k*))												
O20	3(*c*)		0.4475(7)	0.0	0.3971(6)	0.3893	0.4479	0.0	0.3756	0.01	0.0	0.27	0.27	0.14
O17	3(*c*)		0.5527(7)	0.0	0.9142(7)	0.9064	0.5533	0.0	0.8969	-0.01	0.0	0.18	0.18	0.13
		6(*k*)												
O23	3(*c*)		0.4461(8)	0.0	0.1203(7)	0.1125	0.4467	0.0	0.1031	-0.01	0.0	0.18	0.18	0.15

† Possible mislocation of one O atom and overlook of three others at (0, 0, ~0.57), (⅔, ⅓, ~0.13) and (~0.89, 0, ~0.47) by Fanfani *et al*. (1975) would result in a structural approach to $P\bar{3}1m$ symmetry.

Table S3

Modified atomic positions for $Na_{15}(SO_4)_5F_4Cl$ (Galeite), based on Fanfani *et al.* (1975*b*) [4290], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 12.197(4), c = 13.955(10) Å; $z^* = z - 0.0203$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Na1	3(*c*)		0.5118(5)	0.0	0.7167(7)	0.6964	0.5164	0.0	0.6947	-0.06	0.0	0.02	0.06	0.12
		6(*i*)												
Na9	3(*c*)		0.521(5)	0.0	0.3274(7)	0.3071	0.5164	0.0	0.3053	0.06	0.0	0.03	0.07	0.12
Na3	3(*c*)	3(*g*)	0.8161(5)	0.0	0.5253(7)	0.5050	0.8161	0.0	0.5	0.0	0.0	0.07	0.07	0.13
Na2	6(*d*)		0.1588(5)	0.3342(6)	0.7141(7)	0.6938	0.1694	0.3332	0.6915	-0.13	0.01	0.03	0.13	0.12
		12(*l*)												
Na10	6(*d*)		0.1799(4)	0.3322(5)	0.3312(6)	0.3109	0.1694	0.3332	0.3085	0.13	0.01	0.03	0.14	0.12
Na4	6(*d*)	6(*k*)	0.4852(4)	0.3326(4)	0.5310(6)	0.5107	0.4852	0.3326	0.5	0.0	0.0	0.10	0.10	0.13
Na5	3(*c*)		0.1914(6)	0.0	0.1046(7)	-0.1249	0.0082	0.0	-0.1185	-0.06	0.0	-0.09	0.24	0.12
		6(*i*)												
Na7	3(*c*)		-0.1749(5)	0.0	0.1324(7)	0.1121	0.0082	0.0	0.1185	-0.22	0.0	-0.09	0.24	0.12
Na6	6(*d*)		0.8465(5)	0.3357(5)	0.9072(6)	0.8869	0.7582	0.3247	0.8829	-0.08	0.07	0.06	0.10	0.12
		12(*l*)												
Na8	6(*d*)		0.4782(5)	0.3300(5)	0.1414(6)	0.1211	0.1535	0.2418	0.4892	-0.27	0.07	0.11	0.27	-0.27
Cl1	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.020	0.0	0.0	0.0	0.0	0.0	-0.28	0.28	0.12
Cl2	2(*b*)	2(*c*)	0.6667	0.3333	0.0447(5)	0.0244	0.6667	0.3333	0.0	0.0	0.0	0.34	0.34	0.12
S1	1(*a*)		0.0	0.0	0.3243(7)	0.3040	0.0	0.0	0.3143	0.0	0.0	0.14	0.14	0.09
		2(*e*)												
S3	1(*a*)		0.0	0.0	0.6957(7)	0.6754	0.0	0.0	0.6857	0.0	0.0	-0.14	0.14	0.08
S2	2(*b*)		0.6667	0.3333	0.3440(7)	0.3237	0.6667	0.3333	0.3120	0.0	0.0	0.16	0.16	0.09
		4(*h*)												
S4	2(*b*)		0.6667	0.3333	0.7200(6)	0.6997	0.6667	0.3333	0.6880	0.0	0.0	0.16	0.16	0.08
S5	3(*c*)		0.67(3)	0.0	0.9216(6)	0.9013	0.6680	0.0	0.8952	0.02	0.0	0.09	0.09	0.08
		6(*i*)												
S7	3(*c*)		0.3339(5)	0.0	0.1311(6)	0.1108	0.3320	0.0	0.1048	0.02	0.0	-0.08	0.08	0.09
S6	3(*c*)	3(*g*)	0.3365(3)	0.0	0.5092(6)	0.4889	0.3365	0.0	0.5	0.0	0.0	-0.15	0.15	0.08
F1	3(*c*)		0.6795(7)	0.0	0.6394(8)	0.6191	0.6694	0.0	0.6039	0.12	0.08	0.21	0.27	0.1
		6(*i*)												
F3	3(*c*)		0.6592(8)	0.0	0.4316(9)	0.4113	0.6694	0.0	0.3961	-0.12	0.08	0.21	0.24	0.14
F2	3(*c*)		0.6754(7)	0.0	0.2389(8)	0.2186	0.6630	0.0	0.2214	0.17	0.0	-0.04	0.17	0.09
		6(*i*)												
F4	3(*c*)		0.3494(9)	0.0	0.7962(9)	0.7759	0.3370	0.0	0.7786	0.17	0.0	-0.04	0.17	0.17
O1	1(*a*)†		0.0	0.0	0.2243(17)	0.2040	0.0	0.0	0.3178	0.0	0.0	-1.59	1.59	0.15
		2(*e*)												
O5	1(*a*)†		0.0	0.0	0.5887(13)	-0.4316	0.0	0.0	-0.3178	0.0	0.0	-1.59	1.59	0.09
O2	3(*c*)		0.8848(9)	0.0	0.3651(10)	0.3448	0.8853	0.0	0.3153	0.01	0.0	0.41	0.41	0.13
		6(*i*)												
O6	3(*c*)		0.1142(10)	0.0	0.7345(10)	0.7142	0.1147	0.0	0.6847	0.01	0.0	0.41	0.41	0.14
O3	2(*b*)†		0.6667	0.3333	0.4441(13)	0.4238	0.6667	0.3333	0.3086	0.0	0.0	1.61	1.61	0.15
		4(*h*)												
O7	2(*b*)†		0.6667	0.3333	0.827(10)	0.8067	0.6667	0.3333	0.6914	0.0	0.0	1.61	1.61	0.09

O4	6(*d*)		0.6704(7)	0.2209(8)	0.3098(8)	0.2895	0.6691	0.2205	0.3113	0.02	-0.44	-0.30	0.52	0.13
		12(*l*)												
O8	6(*d*)		0.6677(7)	0.2202(8)	0.6872(8)	0.6669	0.6691	0.2205	0.6887	-0.02	-0.44	-0.30	0.54	0.14
O9	3(*c*)	3(*f*)	0.6693(9)	0.0	0.0231(8)	0.0028	0.6693	0.0	0.0000	0.0	0.0	0.04	0.04	0.06
O10			0.5536(9)	0.0	0.8853(9)	0.8650	0.5525	0.0	0.8646	0.01	0.0	0.01	0.01	0.09
	3(*c*)	6(*i*)												
O16	3(*c*)		0.4487(10)	0.0	0.1561(10)	0.1358	0.4476	0.0	0.1354	0.01	0.0	0.01	0.01	0.12
O12	3(*c*)[††]	3(*g*)	0.3476(10)	0.0	0.3967(11)	0.3764	0.3767	0.0	0.5	0.0	0.0	1.72	1.72	0.15
O11	6(*d*)		0.7814(8)	0.1146(8)	-0.1214(8)	-0.1292	-0.1417	0.1412	-0.1406	-0.64	-0.32	0.16	0.86	0.12
		12(*l*)												
O17	6(*d*)		0.3341(10)	0.1141(9)	0.1599(8)	0.1519	0.1396	0.1664	0.1406	-0.69	0.64	0.16	0.89	0.14
O13	3(*c*)	3(*g*)	0.4506(9)	0.0	0.5484(9)	0.5404	0.5281	0.0	0.5	0.0	0.0	0.56	0.56	0.13
O14	6(*d*)	6(*k*)	0.8843(8)	0.2179(9)	0.5412(8)	0.5332	0.5129	0.2179	0.5	0.0	0.0	0.46	0.46	0.15
O15	3(*c*)	3(*f*)	0.3393(15)	0.0	0.023(1)	0.0027	0.3393	0.0	0.0000	0.0	0.0	0.04	0.04	0.2

[†] One or both *z*-values may be inappropriate.
[††] A 6(*k*)-symmetry related O atom may also be missing, *cf*. footnote to Table S2.

Table S4

Atomic coordinates from each of 13 Lizardite 1*T* structural determinations, see §2.4, with average *x*,*y*,*z* values.

ICSD	Mg1/2	Si	O1	O2	O3	O4	H1	H2
x								
17046	0.3327(5)	⅓	⅓	0.5087(1)	0.6654(10)	0	0.655(5)	0
67332	0.334(2)	⅓	⅓	0.505(5)	0.666(4)	0	0.58	0
67333	0.337(5)	⅓	⅓	0.513(9)	0.668(12)	0	0.64	0
75933	0.3326(2)	⅓	⅓	0.5071(5)	0.6662(4)	0	0.66	0
75934	0.3324(1)	⅓	⅓	0.5067(4)	0.6658(3)	0	0.66	0
81102†	0.334(7)/ 0.351(7)	⅓	⅓	0.521(11)	0.673(26)/ 0.307(14)	0.0/ 0.307(14)	n/d‡‡	n/d
82411	0.324(2)	⅓	⅓	0.507(2)	0.665(2)	0	0.646(3)	-0.046(6)
87436	0.3318(90	⅓	⅓	0.507(2)	0.664(2)	0	0.583	0
87437	0.3327(9)	⅓	⅓	0.501(2)	0.662(2)	0	n/d	n/d
87438	0.3321(8)	⅓	⅓	0.5(2)	0.664(2)	0	0.572	0
87506‡	0.3322(3)	⅔	⅔	0.4931(5)	0.6658(5)‡	0	0.663(4)	0
202358	0.3322(5)	⅓	⅓	0.4955(11)	0.6655(12)‡	0	0.58(7)	0
245887	0.3333	⅓	⅓	0.5000	0.6666	0	0.6666	0
⟨average⟩	0.3325	⅓	⅓	0.5054	0.6655	0	0.6278	-0.0042
	Mg1/2	Si	O1	O2	O3	O4	H1	H2
y								
17046	0	⅔	⅔	0	0	0	0	0
67332	0	⅔	⅔	0	0	0	0	0
67333	0	⅔	⅔	0	0	0	0	0
75933	0	⅔	⅔	0	0	0	0	0
75934	0	⅔	⅔	0	0	0	0	0
81102	0	⅔	⅔	0	0	0	n/d	n/d
82411	0	⅔	⅔	0	0	0	0	0
87436	0	⅔	⅔	0	0	0	0	0
87437	0	⅔	⅔	0	0	0	n/d	n/d
87438	0	⅔	⅔	0	0	0	0	0
87506‡	0	⅓	⅓	0	0	0	0	0
202358	0	⅔	⅔	0	0	0	0	0
245887	0	⅔	⅔	0	0	0	0	0
⟨average⟩	0	⅔	⅔	0	0	0	0	0

z	Mg1/2	Si	O1	O2	O3	O4	H1	H2
17046	0.4596(7)	0.0766(7)	0.3	-0.0036(9)	0.5935(7)	0.3088(14	0.709(5)	0.199(5)
67332	0.443(5)	0.067	0.291(3)	-0.016(4)	0.585(4)	0.272(7)	0.69	0.12
67333	0.457(9)	0.067	0.291(4)	-0.017(5)	0.587(7)	0.27(16)	0.71	0.11
75933	0.4513(5)	0.0699(5)	0.292	-0.0099(6)	0.5869(4)	0.299(6)	0.71	0.2
75934	0.4516(3)	0.0704(3)	0.292	-0.0111(4)	0.5862(4)	0.299(4)	0.71	0.2
81102[†]	0.449(4)/ 0.453(4)	0.054(2)	0.264(4)	-0.021(6)	0.546(13)/ 0.649(6)	0.291(11)	n/d	n/d
82411	0.447(2)	0.07(1)	0.292	-0.014(2)	0.587(1)	0.291(3)	0.715(2)	0.172(4)
87436	0.455(1)	0.074(1)	0.2911	-0.008(1)	0.588(1)	0.304(2)	0.732	0.197
87437	0.456(1)	0.077(1)	0.2918	-0.007(2)	0.592(2)	0.303(2)	n/d	n/d
87438	0.457(1)	0.078(1)	0.2914	-0.005(1)	0.592(1)	0.306(2)	0.73	0.19
87506[‡]	0.4466(3)	0.0667(3)	0.2879	-0.0135(4)	0.5839(4)	0.2941(6)	0.714(4)	0.160(3)
202358	0.4557(12)	0.0748(13)	0.292	-0.0082(16)	0.5899(15)	0.308(17)	0.738(7)	0.2(7)
245887	0.447	0.070	0.292	-0.014	0.587	0.291	0.715	0.172
⟨average⟩	0.4520	0.0704	0.2901	-0.0114	0.5850	0.2951	0.716	0.175

[†] Disordered over two sites.

[‡] An electron diffraction study with the published coodinates replaced above by 1-*x*, 1-*y*, 1-*z*+0.4374 allows a match to the values in other studies.

[‡‡] Not determined or reported.

Table S5

Six independent determinations of the $LaNi_5H/D_{5.6}$ structure, see §2.4 and Table 3. [38402 *et alii*]

Typical cell dimensions a = 5.411(5), c = 4.293(5) Å (Furrer *et al*. 1978), a = 5.336(1), c = 4.259(1) Å (Noreus *et al*. 1983).

ICSD#	La	Ni1	Ni2	H/D1	H/D2
	x	*x*	*x*	*x*	*x*
20188	0.0	0.473	0.3333	0.528	0.186
38402	0.0	0.499(1)	0.3333	0.470(1)	0.189(2)
87127†	0.0	0.5	0.3333	0.5	0.25
200242†	0.0	0.48(2)	0.3333	0.471(3)	0.176(4)
638253†	0.0	0.529	0.3333	0.536	0.203
638254†	0.0	0.482	0.3333	0.474	0.181
	y	*y*	*y*	*y*	*y*
20188	0.0	0.0	0.6667	0.0	0.347
38402	0.0	0.0	0.6667	0.0	0.864(3)
87127	0.0	0.0	0.6667	0.0	0.86
200242	0.0	0.0	0.6667	0.0	0.828(4)
638253	0.0	0.0	0.6667	0.0	0.869
638254	0.0	0.0	0.6667	0.0	0.831
	z	*z*	*z*	*z*	*z*
20188‡	0.0	0.513	0.033	0.107	0.623
38402	0.0	0.496(5)	0.98(5)	0.092(5)	0.493(4)
87127	0.0	0.48	0.95	0.08	0.58
200242	0.0	0.93(1)	0.479(8)	0.076(7)	0.55(2)
638253	0.0	0.459	0.96	0.065	0.514
638254	0.0	0.916	0.444	0.046	0.490

† Ni1 and Ni2 labels interchanged.

‡ All *z*-coordinates tend toward 0 or ½ as expected in supergroup $P\bar{6}\,2m$.

Table S6

Modified atomic positions for $(C(NH_2)_3)Al(SO_4)_2(H_2O)_6$, (GASH), based on Schein *et al*. (1967) [30566] with hypothetical x' y' z' coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 11.738(2), c = 8.951(2) Å; z^* = z - 0.0370.

	Wyckoff	Position												
	*P*31*m*	*P* $\bar{6}$ 2*m*†	*x*	*y*	*z*	*z**	*x′*	*y′*	*z′*	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{33}
N1	6(*d*)	6(*k*)	0.5595(5)	0.343(6)	0.5606(8)	0.5236	0.5595	0.343	0.5	0.0	0.0	0.21	0.21	0.22
O1	6(*d*)		0.8805(3)	0.2241(3)	0.8005(6)	0.7635	0.8355	0.1701	0.7778	0.52	0.63	-0.13	1.01	0.23
		12(*l*)												
O2	6(*d*)		0.7904(4)	0.1161(4)	0.2449(7)	0.2079	0.8355	0.1701	0.2222	-0.53	-0.63	-0.13	1.01	0.20
O3	6(*d*)		0.5308(3)	0.3274(3)	0.9437(6)	0.9067	0.5340	0.2625	0.8832	-0.04	0.76	0.21	0.77	0.18
		12(*l*)												
O4	6(*d*)		0.5373(4)	0.1976(4)	0.1773(7)	0.1403	0.5340	0.2625	0.1168	0.04	-0.76	0.21	0.77	0.18
S1	3(*c*)		0.3486(1)	0.0	0.7607(5)	0.7237	0.3328	0.0	0.722	0.19	0.0	0.02	0.19	0.17
		6(*i*)												
S2	3(*c*)		0.6831(1)	0.0	0.3167(5)	0.2797	0.6672	0.0	0.278	0.19	0.0	0.02	0.19	0.16
N2	3(*c*)	3(*g*)	0.1119(4)	0.0	0.515(9)	0.478	0.1119	0.0	0.5	0.0	0.0	-0.2	0.2	0.22
O5	3(*c*)		0.4592(5)	0.0	0.8457(8)	0.8087	0.4504	0.0	0.7772	0.1	0.0	0.28	0.3	0.22
		6(*i*)												
O6	3(*c*)		0.5584(4)	0.0	0.2912(7)	0.2542	0.5496	0.0	0.2228	0.1	0.0	0.28	0.3	0.23
O7	3(*c*)		0.3749(5)	0.0	0.6011(7)	0.5641	0.3338	0.0	0.5628	0.48	0.0	0.01	0.48	0.20
		6(*i*)												
O8	3(*c*)		0.7073(4)	0.0	0.4756(7)	0.4386	0.6662	0.0	0.4372	0.48	0.0	0.01	0.48	0.18
O9	3(*c*)		0.1324(4)	0.0	0.1165(7)	0.0795	0.1322	0.0	0.1171	0.0	0.0	-0.34	0.34	0.20
		6(*i*)												
O10	3(*c*)		0.868(4)	0.0	0.8824(7)	0.8454	0.8678	0.0	0.8829	0.0	0.0	-0.34	0.34	0.22
Al1	2(*b*)	2(*c*)	0.3333	0.6667	0.0612(3)	0.0242	0.3333	0.6667	0.0	-0.0	0.0	0.22	0.22	0.15
C1	2(*b*)	2(*d*)	0.3333	0.6667	0.5586(11)	0.5216	0.3333	0.6667	0.5	-0.0	0.0	0.19	0.19	0.16
C2	1(*a*)	1(*b*)	0.0	0.0	0.5142(12)	0.4772	0.0	0.0	0.5	0.0	0.0	-0.2	0.2	0.16
Al2	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.037	0.0	0.0	0.0	0.0	0.0	-0.33	0.33	0.14
H1	6(*d*)	6(*k*)	0.9245	0.1113	0.5092	0.4722	0.9245	0.1113	0.5	0.0	0.0	-0.25	0.25	n/d‡
H2	6(*d*)	6(*k*)	0.5729	0.138	0.5611	0.5241	0.5729	0.138	0.5	0.0	0.0	0.22	0.22	n/d
H3	6(*d*)	6(*k*)	0.7361	0.2309	0.5436	0.5066	0.7446	0.2205	0.5	0.0	0.0	0.06	0.06	n/d
H4	6(*d*)		0.869	0.08	0.848	0.811	0.835	0.17	0.817	0.0	0.0	-0.05	0.05	n/d
		12(*l*)												
H8	6(*d*)		0.801	0.26	0.214	0.177	0.835	0.17	0.183	0.0	0.0	-0.05	0.05	n/d
H5	6(*d*)	6(*j*)	0.92	0.14	0.116	0.079	0.92	0.14	0.0	0.0	0.0	0.71	0.71	n/d
H6	6(*d*)	6(*j*)	0.753	0.21	0.9	0.863	0.7446	0.2205	0.0	0.0	0.0	1.23	1.23	n/d
H7	6(*d*)	6(*j*)	0.592	0.129	0.9	0.863	0.592	0.129	0.0	0.0	0.0	1.23	1.23	n/d
H9	6(*d*)	6(*j*))	0.881	0.42	0.214	0.267	0.881	0.42	0.0	0.0	0.0	1.92	1.92	n/d

† For all atoms tending toward supergroup *P* $\bar{6}$ 2*m* except S1, S2, O5-O9 which tend toward *P* $\bar{3}$ 1*m*, see §2.8.

‡ Not determined or reported.

Table S7

Modified atomic positions in $Li_{17}Ag_3Sn_6$ based on Lupu *et al*., (2004) [170571] with hypothetical x' y' z' coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å (see footnote 4).

a = 8.063(3), c = 8.51(4) Å; $z^* = z + 0.0147$.

	Wyckoff	Position												
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Sn1	3(*c*)	3(*g*)	0.3482(16)	0.3482(16)	0.4993(11)	0.5140	0.3482	0.3482	0.5	0.0	0.0	0.12	0.12	0.01
Sn2	3(*c*)	3(*f*)	0.0	0.3158(18)	0.0013(2)	0.0160	0.0	0.3158	0.0	0.0	0.0	0.14	0.14	0.01
Ag1	1(*a*)	1(*b*)	0.0	0.0	0.5066(3)	0.5213	0.0	0.0	0.5	0.0	0.0	0.18	0.18	0.01
Ag2	2(*b*)	2(*c*)	0.3333	0.6667	0.0059(16)	0.0206	0.3333	0.6667	0.0	0.0	0.0	0.18	0.18	0.01
Li1	3(*c*)		0.356(4)	0.356(4)	0.144(6)	0.1587	0.358	0.358	0.164	-0.02	-0.02	-0.05	0.06	n/d‡
		6(*i*)												
Li4	3(*c*)		0.358(5)	0.358(5)	0.815(5)	0.8297	0.356	0.356	0.835	0.02	0.02	-0.05	0.06	n/d
Li2	3(*c*)		0.0	0.304(5)	0.326(6)	0.3407	0.0	0.3055	0.337	0.0	-0.01	0.03	0.03	n/d
		6(*i*)												
Li3	3(*c*)		0.307(5)	0.0	0.651(6)	0.6657	0.3055	0.0	0.663	0.01	0.0	0.02	0.02	n/d
Li5	2(*b*)		0.3333	0.6667	-0.322(6)	-0.3073	0.3333	0.6667	-0.3325	0.0	0.0	0.21	0.21	n/d
		4(*h*)												
Li6	2(*b*)		0.6667	0.3333	0.343(6)	0.3577	0.6667	0.3333	0.3325	0.0	0.0	0.21	0.21	n/d
Li7	1(*a*)†	1(*a*)	0.0	0.0	-0.132(7)	-0.1173	0.0	0.0	0	0.0	0.0	1.00	1.00	n/d

† A missing Li8 located at ~0, 0, 0.132 would correspond to an earlier $Li_{18}Ag_3Sn_6$ composition noted by Lupu *et al*., (2004) and fully satisfy $P\bar{6}2m$ symmetry .

‡ Not determined or reported.

Table S8(*a*)

Seven independent determinations of the Cronstedtite structure, with averaged *x*,*y*,*z* coordinates. [18193 *et alii*]

$a \approx 5.5$, $c \approx 7.1$ Å

***x*-coords.**	Fe1,Si 2(*b*)	Fe2 3(*c*)	O1 3(*c*)	O2 1(*a*)	O3 2(*b*)	O4 3(*c*)	H1 1(*a*)	H2 3(*c*)
ICSD#								
18193	⅓	0.6667	0.52	0.0000	0.3333	0.3333	n/d†	n/d
89909	⅓	0.66520(7)	0.4416(6)	0.0000	0.3333	0.3321(3)	n/d	n/d
89910	⅓	0.66522(6)	0.4433(4)	0.0000	0.3333	0.3320(3)	0.000	0.343(6)
158233	⅓	0.6653(1)	0.4432(6)	0.0000	0.3333	0.3318(6)	0.000	0.348
158234	⅓	0.6653(1)	0.4432(6	0.0000	0.3333	0.3322(6)	0.000	0.348
158235	⅓	0.6654(3)	0.448(1)	0.0000	0.3333	0.3318(6)	0.000	0.348
158236	⅓	0.6651(1)	0.444(1)	0.0000	0.3333	0.333(1)	0.000	0.348
Average	0.3333	0.6655	0.4547	0.0000	0.3333	0.3324	0.0000	0.347
***y*-coords.**								
18193	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	n/d	n/d
89909	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	n/d	n/d
89910	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.0000	0.0000
158233	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.0000	0.000
158234	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.000	0.000
158235	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.000	0.000
158236	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.000	0.000
Average	0.6667	0.0000	0.0000	0.0000	0.6667	0.0000	0.0000	0.0000
***z*-coords.**								
18193	0.091	0.5	0.000	0.34	0.34	0.649	n/d	n/d
89909	0.1014(1)	0.5	0.0235(3)	0.3508(5)	0.3457(5)	0.6412(3)	n/d	n/d
89910	0.1038(1)	0.5	0.0290(3)	0.3556(5)	0.3510(5)	0.6436(4)	0.25(1)	0.757(8)
158233	0.1018(2)	0.5	0.102(1)	0.351(5)	0.3458(4)	0.6388(6)	0.233	0.745
158234	0.102(1)	0.5	0.102(1)	0.3514(7)	0.3458(4)	0.6391(3)	0.223	0.745
158235	0.1029(3)	0.5	0.1029(3)	0.353(1)	0.349(1)	0.641(13)	0.205	0.755
158236	0.1021(3)	0.5	0.1021(3)	0.348(2)	0.342(1)	0.6402(9)	0.224	0.796
Average	0.1007	0.5	0.0598	0.3506	0.3463	0.6421	0.227	0.760

† Not determined or reported.

Table S8(*b*)

Averaged atomic coordinates for Cronstedtite structure [18193 *et alii*], with hypothetical $x'\,y'\,z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

$a \approx 5.512(1)$, $c \approx 7.106(1)$ Å; $z^* = z - 0.0018$ excluding z(H) coordinates.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Fe1/Si	2(*b*)	2(*c*)	0.3333	0.6667	0.1007	0.1007	0.3333	0.6667	0	0.0	0.0	0.716	0.716	0.44
Fe2	3(*c*)	3(*g*)	0.6655	0.0	0.5	0.5	0.6655	0.0	0.5	0.0	0.0	0.000	0.000	n/d†
O1	3(*c*)	3(*f*)	0.4547	0.0	0.0598	0.0598	0.4547	0.0	0	0.0	0.0	0.425	0.425	n/d
O2	1(*a*)	1(*b*)	0.0	0.0	0.3506	0.3506	0.0	0.0	0.5	0.0	0.0	-1.062	1.062	n/d
O3	2(*b*)	2(*d*)	0.3333	0.6667	0.3463	0.3463	0.3333	0.6667	0.5	0.0	0.0	-1.092	1.092	n/d
O4	3(*c*)	3(*g*)	0.3324	0.0	0.6421	0.6421	0.3324	0.0	0.5	0.0	0.0	1.010	1.010	n/d
H1	1(*a*)	1(*a*)	0.0	0.0	0.227	0.227	0.0	0.0	0	0.0	0.0	1.613	1.613	n/d
H2	3(*c*)	3(*g*)	0.347	0.0	0.760	0.760	0.347	0.0	0.5	0.0	0.0	1.848	1.848	n/d

† Not determined or reported.

Table S9

Modified atomic positions for Yb_2O_2S based on Ballestracci & Rossat-Mignod (1969) [23583] with hypothetical $x'\,y'\,z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

$a = 3.726$, c = 6.509 Å; $z^* = z + 0.21$ based only on Yb. Identical 1(*a*), 2(*c*) and 2(*d*) positions in supergroups $P\bar{3}1m$ and $P\bar{6}2m$ result in each exhibiting an identical fit.

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Yb	2(*b*)	2(*d*)	0.3333	0.6667	0.29	0.5	0.3333	0.6667	0.5	0.0	0.0	0.00	0.00	n/d†
O	2(*b*)	2(*c*)	0.3333	0.6667	0.62	0.83	0.3333	0.6667	1.0	0.0	0.0	-1.11	1.11	n/d
S	1(*a*)	1(*a*)	0.0	0.0	0.0	0.21	0.0	0.0	0.0	0.0	0.0	1.37	1.37	n/d

† Not determined or reported.

Table S10(*a*)

Modified atomic positions for $K_3V_5O_{14}$ based on Byström & Evans' (1959) study [24068], with hypothetical $x'\,y'\,z'$ coordinates, and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 8.6796(20), c = 4.9914(8) Å; $z^* = z + 0.035$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K1	3(*c*)	3(*f*)	0.605	0.0	0.0	0.035	0.605	0.0	0.0	0.0	0.0	0.17	0.17	0.11
V1	2(*b*)	2(*d*)	0.3333	0.6667	0.471	0.506	0.3333	0.6667	0.5	0.0	0.0	0.03	0.03	0.11
V2	3(*c*)	3(*g*)	0.231	0.0	0.472	0.507	0.231	0.0	0.5	0.0	0.0	0.03	0.03	0.11
O1	2(*b*)	2(*c*)	0.3333	0.6667	0.796	0.831	0.3333	0.6667	1.0	0.0	0.0	-0.84	0.84	0.11
O2	3(*c*)		0.24	0.0	0.782	0.817	0.201	0.0	0.7075	0.34	0.0	0.55	0.65	0.11
		6(*i*)												
O3	3(*c*)		0.838	0.0	0.367	0.402	0.799	0.0	0.2925	0.34	0.0	0.55	0.65	0.11
O4	6(*d*)	6(*k*)	0.469	0.177	0.366	0.401	0.469	0.177	0.5	0.0	0.0	-0.49	0.49	0.11

Table S10(*b*)

Modified atomic positions for $K_3V_5O_{14}$ based on Evans & Brusewitz's (1994) study [75219], with hypothetical $x'\,y'\,z'$ coordinates, and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 8.6901(5), c = 5.0063(8) Å; $z^* = z$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K1	3(*c*)[†]	3(*f*)	0.6080(4)	0.0	0.0001(7)	0.608	0.0	0.0	0.0	0.0	0.0	0.0	0.03
V1	2(*b*)		0.3333	0.6667	0.5194(6)	0.3333	0.6667	0.5194	0.0	0.0	0.0	0.0	0.01
		4(*h*)											
V3	2(*b*)		0.3333	0.6667	0.4806(6)	0.3333	0.6667	0.4806	0.0	0.0	0.0	0.0	0.01
V2	3(*c*)		0.2292(2)	0.0	0.516	0.2292	0.0	0.516	0.0	0.0	0.0	0.0	0.01
		6(i)											
V4	3(*c*)		0.2292(2)	0.0	0.484	0.2292	0.0	0.484	0.0	0.0	0.0	0.0	0.01
O1	2(*b*)		0.3333	0.6667	0.194(2)	0.3333	0.6667	0.194	0.0	0.0	0.0	0.0	0.03
		4(*h*)											
O5	2(*b*)		0.3333	0.6667	0.806	0.3333	0.6667	0.806	0.0	0.0	0.0	0.0	0.03
O2	3(*c*)		0.25(2)	0.0	0.19(2)	0.25	0.0	0.19	0.0	0.0	0.0	0.0	0.04
		6(*i*)											
O6	3(*c*)		0.25(2)	0.0	0.81(2)	0.25	0.0	0.81	0.0	0.0	0.0	0.0	0.04
O3	3(*c*)		0.831(1)	0.0	0.566(3)	0.831	0.0	0.566	0.0	0.0	0.0	0.0	0.03
		6(*i*)											
O7	3(*c*)		0.831(1)	0.0	0.434(3)	0.831	0.0	0.434	0.0	0.0	0.0	0.0	0.03
O4	6(*d*)		0.461(1)	0.169(1)	0.637(1)	0.461	0.169	0.637	0.0	0.0	0.0	0.0	0.02
		12(*l*)											
O8	6(*d*)		0.461(1)	0.169(1)	0.363(1)	0.461	0.169	0.363	0.0	0.0	0.0	0.0	0.02

[†] This K 3(*c*) location only was listed; a related K2 ion in 3(*c*) is necessary for charge balance, *cf.* Table S10(*a*).

Table S11

Modified atomic positions for $Na_2ZnCl_4(H_2O)_3$ based on Brehler's (1960) study [24269], with hypothetical $x'\,y'\,z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å, with respect to $P\bar{6}2m$ supergroup symmetry. (see footnote 4).

a = 6.876(5), c = 5.955(5) Å; $z^* = z$ - 0.060.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Na	2(*b*)	2(*c*)	0.3333	0.6667	0.16	0.10	0.3333	0.6667	0.0	-0.0	0.0	0.60	0.60	0.21
Zn	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.06	0.0	0.0	0.0	0.0	0.0	-0.36	0.36	0.21
Cl1	1(*a*)	1(*b*)	0.0	0.0	0.38	0.32	0.0	0.0	0.5	0.0	0.0	-1.07	1.07	0.21
Cl2	3(*c*)	3(*g*)	0.315	0.0	0.89	0.83	0.315	0.0	0.5	0.0	0.0	1.97	1.97	0.21
O	3(*c*)	3(*g*)	0.5	0.0	0.37	0.31	0.5	0.0	0.5	0.0	0.0	-1.13	1.13	0.21

Table S12

Modified atomic positions for Lizardite 9*T*, $Mg_2Fe_{0.1}Al_{1.27}Si_{1.4}O_{4.6}(OH)_{4.4}$, based on Jahanbagloo & Zolti's (1968) results [24427], with hypothetical $x'\,y'\,z'$ coordinates and subcell Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 5.295(4), $c \approx$ 7.11(7) Å; $z^* = z$ - 0.0330. Full cell c = 63.99(60) Å, see §3.5.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Mg1,Fe1,Al1	3(*c*)	3(*f*)	0.6667	0.0	0.0513(9)	0.0183	0.6667	0.0	0.0	0.0	0.0	0.13	0.13	0.14
Al2,Si1	2(*b*)	2(*c*)	0.3333	0.6667	0.009(6)	-0.0240	0.3333	0.6667	0.0	0.0	0.0	-0.17	0.17	0.13
O1	3(*c*)	3(*f*)	0.46(2)	0.0	0.0	-0.0330	0.46	0.0	0.0	0.0	0.0	-0.23	0.23	0.17
O2	2(*b*)	2(*c*)	0.3333	0.6667	0.0353(8)	0.0023	0.3333	0.6667	0.0	0.0	0.0	0.02	0.02	0.18
O3	1(*a*)	1(*a*)	0.0	0.0	0.0353(8)	0.0023	0.0	0.0	0.0	0.0	0.0	0.02	0.02	0.18
O4	3(*c*)	3(*f*)	0.3333	0.0	0.067(1)	0.0340	0.3333	0.0	0.0	0.0	0.0	0.24	0.24	0.19

Table S13

Modified atomic positions for AuCd based on Alasafi & Schubert (1977), [58408], with hypothetical x' y' z' coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 8.1047(6), c = 5.7974(5) Å; z^* = z - 0.1114.

	Wyckoff	Position												
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Au1	1(*a*)	1(*a*)	0.0	0.0	0.197	0.0856	0.0	0.0	0.0	0.0	0.0	0.50	0.50	0.16
Au2	2(*b*)	2(*c*)	0.3333	0.6667	0.042	-0.0694	0.3333	0.6667	0.0	0.0	0.0	-0.40	0.40	0.16
Au3	3(*c*)		0.643	0.0	0.752	0.6406	0.665	0.0	0.646	-0.18	0.0	-0.03	0.18	0.16
		6(*k*)												
Au4	3(*c*)		0.312	0.0	0.46	0.3486	0.334	0.0	0.354	-0.18	0.0	-0.03	0.18	0.16
Cd1	1(*a*)	1(*b*)	0.0	0.0	0.687	0.5756	0.0	0.0	0.5	0.0	0.0	0.44	0.44	0.16
Cd2	2(*b*)	2(*d*)	0.3333	0.6667	0.546	0.4346	0.3333	0.6667	0.5	0.0	0.0	-0.38	0.38	0.15
Cd3	3(*c*)		0.649	0.0	0.252	0.1406	0.664	0.0	0.1485	-0.12	0.0	-0.13	0.18	0.16
		6(*k*)												
Cd4	3(*c*)		0.312	0.0	0.955	0.8436	0.327	0.0	0.8515	-0.12	0.0	-0.13	0.18	0.18

Table S14

Modified atomic positions for synthetic holtedahlite $Mg_{12}(HPO_4)(PO_4)_5(OH)_6$, based on Rømming & Raade (1989), [64769], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 11.186(3), c = 4.977(1) Å; $z^* = z - 0.0880$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Mg1	6(*d*)	6(*j*)	0.6705(1)	0.1461(2)	0.0	-0.0880	0.6705	0.1461	0	0	0	-0.438	0.438	0.09
Mg2	6(*d*)	6(*k*)	0.8246(1)	0.1457(1)	0.5065(3)	0.4185	0.8246	0.1457	0.5000	0	0	-0.406	0.406	0.11
P1	1(*a*)	1(*b*)	0.0	0.0	0.7287(5)	0.6407	0.0	0.0	0.5000	0	0	0.700	0.700	0.08
P2	2(*b*)	2(*d*)	0.6667	0.3333	0.4781(4)	0.3901	0.6667	0.3333	0.5000	0	0	-0.547	0.547	0.08
P3	3(*c*)	3(*f*)	0.6609(1)	0.6609(1)	0.0323(4)	-0.0557	0.6609	0.6609	0	0	0	-0.277	0.277	0.07
O1	3(*c*)	3(*g*)	0.1285(4)	0.1285(4)	0.634(9)	0.546	0.1285	0.1285	0.5000	0	0	0.229	0.229	0.11
O3	3(*c*)	3(*f*)	0.7326(3)	0.7326(3)	0.2973(7)	0.2093	0.7326	0.7326	0	-0.776	-1.884	1.042	1.286	0.10
O4	6(*d*)		0.8706(3)	0.244(3)	0.8674(5)	0.7794	0.7956	0.2425	0.7495	0.840	0.017	0.149	0.935	0.09
		12(*l*)												
O2	6(*d*)		0.7207(3)	0.2409(3)	0.3685(6)	0.2805	0.7956	0.2425	0.2505	-0.838	-0.018	0.149	0.934	0.10
O8	3(*c*)		0.2805(4)	0.2805(4)	0.1975(8)	0.1095	0.3266	0.3266	0.2539	-0.516	-0.516	-0.719	1.012	0.11
		6(*l*)												
O7	3(*c*)		0.3727(3)	0.3727(3)	0.6898(7)	0.6018	0.3266	0.3266	0.7461	0.516	0.516	-0.718	1.012	0.09
O5	3(*c*)	3(*f*)	0.528(3)	0.528(3)	0.0981(8)	0.0101	0.528	0.528	0	0.313	0.313	0.050	0.617	0.10
O6	2(*b*)	2(*d*)	0.6667	0.3333	0.7893(8)	0.7013	0.6667	0.3333	0.5000	0	0	1.002	1.002	0.13
O9	1(*a*)	1(*a*)	0.0	0.0	0.044(2)	-0.044	0	0	0	0	0	-0.219	0.219	0.19
H1	3(*c*)	3(*g*)	0.438	0.438	0.632	0.544	0.438	0.438	0.5000	0	0	0.219	0.219	0.14
H2	3(*c*)	3(*f*)	0.229	0.229	0.183	0.095	0.229	0.229	0	0	0	0.473	0.473	0.14

Table S15

Modified atomic positions for Satterlyite - $Fe_{0.77}Mg_{0.23})_{12}(PO_3OH)(PO_4)_5((OH)O)_6$, based on Kolitsch *et al.* (2002) [94842], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 11.355(1), c = 5.0394(5 Å; z^* = z - 0.0926.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Fe1, Mg1	6(*d*)	6(*j*)	0.6708(3)	0.1492(3)	0.989(4)	0.8964	0.6708	0.1492	1.0	0.0	0.0	-0.52	0.52	0.1
Fe2, Mg2	6(*d*)	6(*k*)	0.8249(3)	0.1462(3)	0.4956(5)	0.4030	0.8249	0.1462	0.5	0.0	0.0	-0.49	0.49	0.09
P1	1(*a*)	1(*b*)	0.0	0.0	0.7218(19)	0.6292	0.0	0.0	0.5	0.0	0.0	0.65	0.65	0.09
P2	2(*b*)	2(*d*)	0.6667	0.3333	0.4727(14)	0.3801	0.6667	0.3333	0.5	0.0	0.0	-0.60	0.60	0.08
P3	3(*c*)	3(*f*)	0.6516(5)	0.6516(5)	0.0222(11)	-0.0704	0.6516	0.6516	0.0	0.0	0.0	-0.36	0.36	0.08
O1	3(*c*)	3(*g*)	0.1276(16)	0.1276(16)	0.6303(5)	0.5377	0.1276	0.1276	0.5	0.0	0.0	0.19	0.19	0.14
O3	3(*c*)	3(*f*)	0.7317(16)	0.7317(16)	0.2797(3)	0.1871	0.7317	0.7317	0.0	0.0	0.0	-0.30	1.42	0.11
O2	6(*d*)	12(*l*)	0.7237(13)	0.2454(13)	0.3645(3)	0.2719	0.7982	0.2476	0.2536	-0.85	-0.02	0.09	0.87	0.11
O4	6(*d*)		0.8728(12)	0.2498(12)	0.8573(2)	0.7647	0.7982	0.2476	0.7464	0.85	0.02	0.09	0.87	0.11
O5	3(*c*)	3(*f*)	0.5267(15)	0.5267(15)	0.0949(4)	0.0023	0.5765	0.5765	0.0	-0.57	-0.57	0.01	0.99	0.12
O7	3(*c*)	3(*g*)	0.3738(16)	0.373816)	0.675(3)	0.5824	0.4235	0.4235	0.5	-0.43	-0.43	0.42	0.86	0.11
O6	2(*b*)	2(*c*)	0.6667	0.3333	0.9838(4)	0.8912	0.6667	0.3333	1.0	0.0	0.0	-0.55	0.55	0.13
O8	3(*c*)	3(*f*)	0.2766(15)	0.2766(15)	0.1838(3)	0.0912	0.2766	0.2766	0.0	0.0	0.0	0.93	0.93	0.11
O9	1(*a*)	1(*a*)	0.0	0.0	0.0305(8)	-0.0621	0.0	0.0	0.0	0.0	0.0	-0.31	0.31	0.2
H1	3(*c*)	3(*g*)	0.437(4)	0.437(4)	0.584(10)	0.491	0.437	0.4371	0.5	0.0	0.0	-0.05	0.05	n/d†
H2	3(*c*)	3(*f*)	0.195(4)	0.195(4)	0.096(9)	0.003	0.195	0.195	0.0	0.0	0.0	0.02	0.02	n/d

† Not determined or reported.

Table S16

Modified atomic positions for $[(CH_3)_4N]_2(Mo_3Se_{13})$**,** based on Liao, Li & Kanatzidis' (1995) study, [66870], with hypothetical $x'\ y'\ z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

.
a = 11.578(1), c = 6.11(2) Å; z^* = z - 0.0183.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Mo1	3(*c*)	3(*g*)	0.0	0.1388(3)	0.5262	0.5079	0.0	0.1388	0.5	0.0	0.00	0.05	0.05	0.14
Se1	1(*a*)	1(*a*)	0.0	0.0	0.827(1)	0.8087	0.0	0.0	1.0	0.0	0.0	-1.17	1.17	0.17
Se2	3(*c*)	6(*i*)	-0.2596(4)	0.0	0.562(1)	0.5438	-0.2158	0.0	0.6677	-0.51	0.0	-0.76	0.92	0.17
Se3	3(*c*)		-0.1719(4)	0.0	0.2265(9)	0.2083	-0.2158	0.0	0.3323	0.51	0.0	-0.76	0.92	0.16
Se4	3(*c*)	6(*i*)	0.0	0.3585(4)	0.423(1)	0.4048	0.0	0.3321	0.3165	0.0	0.31	0.54	0.62	0.20
Se5	3(*c*)		0.0	0.3057(4)	0.79(1)	0.7718	0.0	0.3321	0.6835	0.0	-0.31	0.54	0.62	0.19
N1	2(*b*)	2(*c*)	0.3333	0.6667	0.014(8)	-0.0043	0.3333	0.6667	0.0	-0.0	0.0	0.03	0.03	0.19
C1	2(*b*)	2(*d*)	0.3333	0.6667	0.74(1)	0.7217	0.3333	0.6667	0.5	-0.0	0.0	1.35	1.35	0.04
C2	6(*d*)	6(*j*)	0.208(5)	0.657(5)	0.055(7)	0.0367	0.208	0.792	0.0	0.0	-1.56	0.22	1.58	0.25

Table S17

Modified atomic positions for $TiD_{0.093}O_{0.3}$, based on the results of Kajitani *et al*. (1991), [71816], with hypothetical $x'\ y'\ z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 5.158(4), c = 4.812(3) Å; z^* = z - 0.0433.

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ti1	3(*c*)	6(*k*)	0.3403(13)	0.0	0.2299(4)	0.1866	0.3368	0.0	0.2510	0.02	0.0	-0.31	0.31	0.14
Ti2	3(*c*)		0.6667(15)	0.0	-0.2721(4)	-0.3154	0.6632	0.0	-0.2510	0.02	0.0	-0.31	0.31	0.03
O1	2(*b*)	4(*h*)	0.3333	0.6667	0.4443(34)	0.4010	0.3333	0.6667	0.2221	0.0	0.0	0.86	0.86	0.08
O3	2(*b*)		0.3333	0.6667	0.0	-0.0433	0.3333	0.6667	-0.2221	0.0	0.0	0.86	0.86	0.01
O2	1(*a*)	1(*b*)	0.0	0.0	0.4443(65)	0.4010	0.0	0.0	0.5	0.0	0.0	-0.48	0.48	0.08
O4	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.0433	0.0	0.0	0.0	0.0	0.0	-0.21	0.21	0.01
D1	2(*b*)	2(*c*)	0.3333	0.6667	0.0	-0.0433	0.3333	0.6667	0.0	0.0	0.0	-0.21	0.21	0.2
D2	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.0433	0.0	0.0	0.0	0.0	0.0	-0.21	0.21	0.2

Table S18

Modified atomic positions for $Cs_4Au_6S_5$, based on Klepp & Weithaler (1996) [82557], with hypothetical $x'\ y'\ z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 10.243(3), c = 5.29(2) Å; z^* = z - 0.0762.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cs1	1(*a*)	1(*b*)	0.0	0.0	0.835(1)	0.911	0.0	0.0	1.0	0.0	0.0	-0.47	0.47	0.19
Cs2	3(*c*)	3(*g*)	0.0	0.6009(3)	0.552(6)	0.628	0.0	0.6009	0.5	0.0	0.0	0.68	0.68	0.16
Au1	6(*d*)	6(*j*)	0.7142(1)	0.5444(1)	0.077	0.153	0.7142	0.5444	0.0	0.0	0.0	0.81	0.81	0.14
S1	2(*b*)	2(*d*)	0.3333	0.6667	0.85(3)	0.926	0.3333	0.6667	1.0	-0.0	0.0	-0.39	0.39	0.16
S2	3(*c*)	3(*f*)	0.752(1)	0.752(1)	0.305(2)	0.381	0.752	0.752	0.5	0.0	0.0	-0.63	0.63	0.18

Table S19

Modified atomic positions for $Ba_{10}Cl_{3.7}F_{31.3}Fe_3Mn_3$, based on Darriet *et al.* (1996), [82861], with hypothetical $x'\ y'\ z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 11.075(2), c = 8.173(2) Å; z^* = z - 0.0042.

	Wyckoff Position														
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
Ba1	2(*b*)	2(*c*)	0.6667	0.3333	0.0	-0.0042	0.6667	0.3333	0.0	0.0	0.0	-0.18	0.18	0.13	1
Ba2	2(*b*)	2(*d*)	0.6667	0.3333	0.5024(2)	0.4982	0.6667	0.3333	0.5	0.0	0.0	-0.17	0.17	0.18	1
Ba3	3(*c*)		0.7322(1)	0.0	0.7835(2)	0.7793	0.7499	0.0	0.7819	-0.20	0.0	-0.02	0.20	0.13	1
		6(*k*)													
Ba4	3(*c*)		0.2325(1)	0.0	0.2198(3)	0.2156	0.2501	0.0	0.2181	-0.19	0.0	-0.02	0.19	0.15	0.85
Ba5[†]	3(*c*)	*nr*.Ba4	0.2448(6)	0.0	0.2844(12)	0.2802	0.2501	0.0	0.2181	-0.06	0.0	0.49	0.54	0.15	0.15
Fe1	3(*c*)		0.6071(1)	0.0	0.2611(3)	0.2569	0.6002	0.0	0.2184	0.08	0.0	0.31	0.32	0.12	1
		6(*k*)													
Mn1	3(*c*)		0.4068(2)	0.0	0.8244(4)	0.8202	0.3998	0.0	0.7816	0.08	0.0	0.32	0.33	0.13	0.85
Mn2	3(*c*)	*nr*.Mn1	0.386(14)	0.0	0.7414(7)	0.7375	0.3998	0.0	0.7816	-0.15	0.0	-0.33	0.33	0.14	0.15
F1	6(*d*)		0.8487(5)	0.4488(5)	0.7414(7)	0.7372	0.9002	0.4556	0.6929	-0.57	-0.08	0.40	0.73	0.14	0.5
		12(*l*)	ok												
F7	6(*d*)		0.4379(14)	0.9653(18)	0.3556(20)	0.3514	0.4446	0.9002	0.3071	-0.07	0.72	0.36	0.78	0.21	0.5
F2	6(*d*)		0.8547(6)	0.2428(6)	0.9514(7)	0.9472	0.8025	0.2665	0.8461	0.58	-0.26	0.83	0.97	0.14	1
		12(*l*)													
F4	6(*d*)		0.7976(6)	0.5123(6)	0.2592(10)	0.2550	0.8025	0.5360	0.1539	-0.05	-0.26	0.86	0.91	0.19	1
F3	3(*c*)	(3*f*)	0.5376(12)	0.0	0.0409(13)	0.0367	0.5	0.0	0.	0.42	0.0	0.33	0.53	0.23	1
F5	3(*c*)	3(*g*)	0.6806(17)	0.0	0.4711(15)	0.4669	0.5	0.0	0.5	1.21	0.0	-0.24	1.23	0.28	1
F6	3(*c*)		0.7613(8)	0.0	0.1557(13)	0.1515	0.7556	0.0	0.2734	0.06	0.0	2.52	2.52	0.16	1
		6(*k*)													
Cl1/F8	3(*c*)		0.2501(6)	0.0	0.609(7)	0.6048	0.2444	0.0	0.7266	0.06	0.0	2.52	2.52	0.2	**0.85/0.15**
Cl2	1(*a*)	1(*a*)	0.0	0.0	0.9319(8)	0.9277	0.0	0.0	1.0	0.0	0.0	-0.59	0.59	0.15	1
Cl3	1(*a*)	*nr*.F9	0.0	0.0	0.4549(66)	0.4507	0.0	0.0	0.5	0.0	0.0	-0.40	0.4	0.2	0.85
F9	1(*a*)	1(*a*)	0.0	0.0	[0.3214(33)]	[0.3172]	0.0	0.0	0.xxx	0.0	0.0	2.02	2.02	0.2	0.15

[†] Ba4 and Ba5 appear only ~0.55 Å; Mn1, Mn2 ~0.724 Å; F7, F7 ~0.67 Å and F9, Cl3 ~1.09 Å apart.

Table S20

Modified atomic positions for NiTi**,** based on Gong *et al.* (2006) [156442], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4)**.**

a = 7.384, c = 5.461 Å; $z^* = z + 0.0453$

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ti1	1(*a*)	1(*a*)	0.0	0.0	0.0	0.0453	0.0	0.0	0.0	0.0	0.0	0.247	0.25	n/d†
Ti2	2(*b*)	2(*d*)	0.3333	0.6667	-0.09	-0.0448	0.3333	0.6667	0.0	0.0	0.0	-0.245	0.25	n/d
Ti3	3(*c*)	6(*i*)	0.322	0.0	0.299	0.3443	0.332	0.0	0.3480	-0.074	0.0	-0.020	0.08	n/d
Ti4	3(*c*)		0.658	0.0	0.603	0.6483	0.668	0.0	0.6520	-0.074	0.0	-0.020	0.08	n/d
Ni1	1(*a*)	1(*b*)	0.0	0.0	0.536	0.5813	0.0	0.0	0.5	0.0	0.0	0.444	0.44	n/d
Ni2	2(*b*)	2(*d*)	0.3333	0.6667	0.377	0.4223	0.3333	0.6667	0.5	0.0	0.0	-0.424	0.42	n/d
Ni3	3(*c*)	6(*i*)	0.316	0.0	0.818	0.8633	0.339	0.0	0.8615	-0.170	0.0	0.010	0.17	n/d
Ni4	3(*c*)		0.638	0.0	0.095	0.1403	0.661	0.0	0.1385	-0.170	0.0	0.010	0.17	n/d

† Not determined or reported.

Table S21

Modified atomic positions for $V[C(NH_2)_3](SO_4)_2(H_2O)_6$ based on Tragenna-Piggott *et al*. (2004) [170206], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å, except u_{iso} for H atoms undetermined. (see footnote 4)**.**

a = 11.8116(4), c = 9.0311(3) Å; $z^* = z + 0.0010$.

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
V1	1(*a*)	1(*b*)	0.0	0.0	0.5404(10)	0.5414	0.0	0.0	0.5	0	0	0.36	0.36	0.02
V2	2(*b*)	2(*d*)	0.3333	0.6667	0.4762(7)	0.4771	0.3333	0.6667	0.5	0	0	-0.21	0.21	0.02
S1	3(*c*)		0.0	0.3495(5)	0.7844(3)	0.7859	0.0	0.3330	0.7849	0	0.19	0.01	0.19	0.02
		6(*k*)												
S2	3(*c*)		0.0	0.6835(5)	0.2156(3)	0.2160	0.0	0.6670	0.2151	0	0.19	0.01	0.19	0.02
O1	3(*c*)		0.0	0.1398(2)	0.418(3)	0.419	0.0	0.1395	0.3763	0	0	0.38	0.38	0.03
		6(*k*)												
O2	3(*c*)		0.0	-0.1392(19)	0.6652(3)	0.6665	0.0	-0.1395	0.6237	0	0	0.39	0.39	0.03
O3	6(*d*)		0.4688(16)	0.6596(14)	0.3525(19)	0.3532	0.4725	0.6651	0.3765	-0.04	0.06	-0.21	0.22	0.03
		12(*l*)												
O4	6(*d*)		0.4761(17)	0.802(16)	0.5996(18)	0.6007	0.4725	0.8075	0.6235	0.04	-0.06	-0.21	0.22	0.03
O5	6(*d*)		0.3429(15)	0.1174(16)	0.7457(2)	0.7471	0.3338	0.1175	0.7309	0.11	0	0.15	0.19	0.03
		12(*l*)												
O8	6(*d*)		-0.1177(16)	0.6753(15)	0.2848(2)	0.2853	-0.1175	0.6662	0.2691	0	0.11	0.15	0.19	0.03
O6	3(*c*)		0.0	0.4556(18)	0.697(3)	0.698	0.0	0.4481	0.7282	0	0.09	-0.27	0.28	0.03
		6(*k*)												
O9	3(*c*)		0.0	0.5595(17)	0.2406(2)	0.2411	0.0	0.5519	0.2718	0	0.09	-0.28	0.29	0.03
O7	3(*c*)		0.0	0.3751(2)	0.9409(3)	0.9427	0.0	0.3339	0.9416	0	0.49	0.01	0.49	0.05
		6(*k*)												
O10	3(*c*)		0.0	0.7073(19)	0.0576(2)	0.0578	0.0	0.6661	0.0584	0	0.49	-0.01	0.49	0.04
N1	6(*d*)	6(*i*)	-0.112(2)	0.888(2)	0.0232(3)	0.0232	-0.112	0.888	0.0	0	0	0.21	0.21	0.03
N2	6(*d*)	6(*i*)	0.4407(2)	0.7817(2)	0.9774(3)	0.9793	0.4407	0.8814	0.0	0.39	0.39	0.19	0.70	0.04
C1	1(*a*)	1(*a*)	0.0	0.0	0.0231(5)	0.0231	0.0	0.0	0.0	0	0	0.21	0.21	0.02
C2	2(*b*)	2(*c*)	0.3333	0.6667	0.9789(3)	0.9808	0.3333	0.6667	1.0	0	0	0.17	0.17	0.03
H1	6(*d*)		-0.0672(12)	0.132(3)	0.373(3)	0.374	-0.0675	0.1405	0.341	0	0.10	0.30	0.32	n/d
		12(*l*)												
H2	6(*d*)		-0.0679(12)	-0.208(2)	0.691(4)	0.692	-0.0675	-0.2080	0.659	0	0	-0.29	0.29	n/d
H6	6(*d*)		0.472(3)	0.867(2)	0.628(4)	0.629	0.468	0.8717	0.656	0.05	0.06	-0.24	0.26	n/d
		12(*l*)												
H3	6(*d*)		0.464(2)	0.5913(17)	0.316(3)	0.317	0.468	0.5963	0.344	-0.05	-0.06	-0.24	0.26	n/d
H5	6(*d*)		0.534(2)	0.795(3)	0.644(3)	0.645	0.5351	0.802	0.6	-0.01	-0.08	0.14	0.16	n/d
		12(*l*)												
H4	6(*d*)		0.5363(19)	0.7271(16)	0.323(3)	0.324	0.5351	0.7331	0.4	0.01	-0.07	-0.14	0.15	n/d
H7	6(*d*)		0.1828(18)	0.892(14)	0.015(3)	0.015	0.2678	0.838	0.015	-1.00	0.64	0.01	1.43	n/d
		12(*l*)												
H9	6(*d*)		0.5148(18)	0.783(2)	0.985(5)	0.987	0.4298	0.838	0.985	1.00	-0.65	0.01	1.44	n/d
H8	6(*d*)	6(*i*)	0.433(2)	0.851(18)	0.978(5)	0.980	0.428	0.856	1.0	0.06	-0.06	-0.18	0.19	n/d

Table S22

Modified atomic positions for the mineral Långbanite $Mn_{13}SbSi_{12}O_{24}$, based on Moore *et al.* (1991) [69610], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4)**.**

a = 11.563(2), c = 11.100(2) Å; $z^* = z - 0.0098$.

	Wyckoff	Position												
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Mn1	3(*c*)	3(*f*)	0.8312(3)	0.0	0.995(5)	0.9852	0.8312	0.0	0.0	0.0	0.0	-0.16	0.16	0.03
Mn5	3(*c*)	3(*g*)	0.3396(1)	0.0	0.4922(3)	0.4824	0.3396	0.0	0.5	0.0	0.0	-0.20	0.20	0.01
Mn2	6(*d*)	6(*j*)	0.5002(2)	0.3284(1)	0.9878(2)	0.9780	0.5002	0.3284	0.0	0.0	0.0	-0.24	0.24	0.01
Mn4	6(*d*)		0.3297(1)	0.155(1)	0.2593(1)	0.2495	0.4169	0.1612	0.2691	-1.01	-0.07	-0.22	1.07	0.0
		12(*l*)												
Mn9	6(*d*)		0.5041(2)	0.1674(2)	0.7212(2)	0.7114	0.4169	0.1612	0.7309	1.01	0.07	-0.22	1.07	0.02
Mn3	3(*c*)		0.5272(1)	0.0	0.2561(2)	0.2463	0.6801	0.0	0.2619	-1.77	0.0	-0.17	1.78	0.0
		6(*i*)												
Mn8	3(*c*)		0.167(3)	0.0	0.7324(2)	0.7226	0.3199	0.0	0.7381	-1.77	0.0	-0.17	1.78	0.02
Mn6	3(*c*)	3(*g*)	0.8363(2)	0.0	0.4995(3)	0.4897	0.8363	0.0	0.5	0.0	0.0	-0.11	0.11	0.01
Mn7	6(*d*)	6(*k*)	0.4948(1)	0.3252(1)	0.4862(2)	0.4764	0.4948	0.3252	0.5	0.0	0.0	-0.26	0.26	0.01
Sb	3(*c*)	3(*f*)	0.3436(5)	0.0	0.991	0.9812	0.3436	0.0	1.0	0.0	0.0	-0.21	0.21	0.01
Si1	1(*a*)	1(*a*)	0.0	0.0	0.2286(5)	0.2188	0.0	0.0	0.0	0.0	0.0	2.43	2.43	0.01
Si2	2(*b*)	2(*c*)	0.6667	0.3333	0.2319(5)	0.2221	0.6667	0.3333	0.0	0.0	-0.0	2.47	2.47	0.01
Si3	3(*c*)	3(*g*)	0.668(3)	0.0	0.7529(4)	0.7431	0.668	0.0	0.5	0.0	0.0	2.70	2.70	0.01
O1	1(*a*)		0.0	0.0	-0.9224(16)	-0.9322	0.0	0.0	-0.8487	0.0	0.0	-0.92	0.92	0.01
		2(*e*)												
O20	1(*a*)		0.0	0.0	0.7749(29)	0.7651	0.0	0.0	0.8487	0.0	0.0	-0.93	0.93	0.16
O2	2(*b*)		0.6667	0.3333	-0.9188(10)	-0.9286	0.6667	0.3333	-0.8370	0.0	0.0	-1.02	1.02	0.01
		4(*h*)												
O19	2(*b*)		0.6667	0.3333	0.7551(14)	0.7453	0.6667	0.3333	0.8370	0.0	0.0	-1.02	1.02	0.04
O3	3(*c*)	3(*f*)	0.4947(7)	0.0	0.0821(9)	0.0723	0.4947	0.0	-0.0719	0.0	0.0	0.80	0.80	0.01
O10	3(*c*)		0.6996(7)	0.0	0.2259(8)	0.2161	0.6024	0.0	0.2614	1.12	0.0	-0.50	1.22	0.01
		6(*i*)												
O16	3(*c*)		0.7946(29)	0.0	0.7031(23)	0.6933	0.7946	0.0	0.7386	0.0	0.0	-0.50	0.50	0.07
O4	6(*d*)	6(*j*)	0.3458(6)	0.1449(7)	0.085(6)	0.0752	0.3355	0.1645	0.0	0.12	1.90	0.83	2.13	0.01
O5	3(*c*)		0.1923(10)	0.0	0.9015(9)	0.8917	0.1620	0.0	0.8112	0.35	0.0	0.89	0.96	0.02
		6(*i*)												
O8	3(*c*)		0.1317(6)	0.0	0.2792(7)	0.2694	0.1620	0.0	0.1889	0.35	0.0	0.89	0.96	0.01
O6	3(*c*)	3(*f*)	0.6696(8)	0.0	0.8975(11)	0.8877	0.6696	0.0	1.0000	0.00	0.0	-1.25	1.25	0.01
O9	3(*c*))		0.3587(6)	0.0	0.2887(6)	0.2789	0.3447	0.0	0.2983	0.16	0.0	0.73	0.75	0.0
		6(*i*)												
O15	3(*c*)		0.3308(19)	0.0	0.6921(13)	0.6823	0.3447	0.0	0.7017	0.16	0.0	-0.73	0.75	0.04
O7	6(*d*)	6(*j*))	0.4879(7)	0.1489(8)	0.896(6)	0.8862	0.4879	0.1489	1.0000	0.0	0.0	-1.26	1.26	0.01
O11	3(*c*)	3(*g*)	0.5441(7)	0.0	0.4348(9)	0.4250	0.5441	0.0	0.5	0.0	0.0	-0.83	0.83	0.01
O12	6(*d*)		0.5342(5)	0.3291(6)	0.2821(5)	0.2723	0.4881	0.3209	0.2941	0.32	0.09	-0.24	0.44	0.01
		12(*l*)												
O18	6(*d*)		0.4419(27)	0.313(3)	0.694(17)	0.6842	0.4881	0.3209	0.7059	0.32	-0.09	-0.24	0.37	0.14
O13	6(*d*)	6(*k*)	0.3252(6)	0.1841(6)	0.4355(6)	0.4257	0.3252	0.1841	0.5	0.0	0.0	-0.82	0.82	0.01
O14	3(*c*)	3(*g*)	0.1388(10)	0.0	0.5605(9)	0.5507	0.1388	0.0	0.5	0.0	0.0	0.56	0.56	0.02
O17	6(*d*)	6(*k*)	0.5293(7)	0.1929(7)	0.5424(7)	0.5326	0.5293	0.1929	0.5	0.0	0.0	0.36	0.36	0.01

Table S23

Modified atomic positions for $Ba_{21}Al_{40}$ based on Amerioun *et al.* (2004) [170238], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4)**.**

a = 10.5681(14), c = 17.205(6) Å; $z^* = z - 0.0102$ $z^* = z - 0.0957$

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ba1	3(*c*)		0.3295(6)	0.0	0.0006(13)	-0.0951	0.3323	0.0	0.0537	-0.03	0.0	-2.56	2.56	0.02
		6(*k*)												
Ba4	3(*c*)		0.665(7)	0.0	-0.1068(6)	-0.2025	0.6678	0.0	-0.0537	-0.03	0.0	-2.56	2.56	0.01
Ba3	3(*c*)†		0.3321(7)	0.0	0.3913(6)	0.2956	0.3308	0.0	0.3561	0.01	0.0	-1.04	1.04	0.01
		6(*k*)												
Ba7	3(*c*)		0.6706(7)	0.0	0.6792(4)	0.5835	0.6692	0.0	0.6440	0.01	0.0	-1.04	1.04	0.01
Ba2	3(*c*)	3(*g*)	0.3228(8)	0.0	0.607(5)	0.5113	0.5	0.0	0.5	-1.87	0.0	0.19	1.88	0.01
Ba5	2(*b*)		0.6667	0.3333	0.1048(6)	0.0091	0.6667	0.3333	-0.1076	0.0	0.0	2.01	2.01	0.01
		4(*h*)												
Ba8	2(*b*)		0.6667	0.3333	0.3200(1)	0.2243	0.6667	0.3333	0.1076	0.0	0.0	2.01	2.01	0.01
Ba6	1(*a*)		0.0	0.0	0.1066(8)	0.0109	0.0	0.0	-0.1082	0.0	0.0	2.05	2.05	0.01
		2(*e*)												
Ba9	1(*a*)		0.0	0.0	0.3231(7)	0.2274	0.0	0.0	0.1082	0.0	0.0	2.05	2.05	0.01
Al1	1(*a*)		0.0	0.0	0.6920(5)	0.5963	0.0	0.0	0.5790	0.0	0.0	0.30	0.30	0.02
		2(*e*)												
Al11	1(*a*)		0.0	0.0	-0.4659(4)	-0.5616	0.0	0.0	-0.5790	0.0	0.0	0.30	0.30	0.02
Al2	2(*b*)	2(*d*)	0.6667	0.3333	0.6532(3)	0.5575	0.6667	0.3333	0.5000	0.0	0.0	0.99	0.99	0.01
Al3	3(*c*)		0.3309(3)	0.3309(3)	0.3307(4)	0.2350	0.4101	0.4101	0.2712	-0.84	-0.84	-0.62	1.58	0.01
		6(*k*)												
Al10	3(*c*)†		0.4892(4)	0.4892	-0.2117(2)	-0.3074	0.4101	0.4101	-0.2712	-0.84	-0.84	-0.62	1.58	0.01
Al4	1(*a*)	1(*a*)	0.0	0.0	0.9007(5)	0.8050	0.0	0.0	1.0	0.0	0.0	-3.35	3.35	0.01
Al5	2(*b*)	2(*c*)	0.6667	0.3333	0.9036(3)	0.8079	0.6667	0.3333	1.0	0.0	0.0	-3.31	3.31	0.01
Al6	3(*c*)	3(*f*)	0.3342(3)	0.3342(3)	0.0976(3)	0.0019	0.5	0.5	0.0	1.75	1.75	0.03	3.03	0.01
Al7	3(*c*)		0.1942(4)	0.0	0.7940(3)	0.6983	0.2175	0.0	0.6574	-0.25	0.0	0.70	0.74	0.01
		6(*k*)												
Al13	3(*c*)†		0.7591(4)	0.0	0.4793(2)	0.3836	0.7854	0.0	0.3426	-0.28	0.0	0.71	0.76	0.02
Al8	6(*d*)		0.8363(4)	0.3363(3)	0.7853(2)	0.6896	0.8266	0.3364	0.6384	0.10	0.0	0.88	0.89	0.01
		12(*l*)												
Al12	6(*d*)		0.8168(3)	0.4803(3)	0.5086(2)	0.4129	0.8266	0.4853	0.3616	-0.10	-0.05	0.88	0.89	0.02
Al9	6(*d*)	6(*k*)	0.1551(4)	0.3328(3)	0.2112(2)	0.1155	0.1626	0.3253	0.0	-0.08	0.08	1.99	1.99	0.01

† Coordinates of the form 0, x, z in space group $P31m$ are equivalent to x, 0, z or x, x, -z.

Table S24

Modified atomic positions for $Pb(C(CN)_3)_2$based on Deflon *et al.* (2006) [171702], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4)**.**

a = 14.144(5), c = 4.0902(6) Å; $z^* = z$ - 0.0290.

	Wyckoff	Position												
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Pb1	1(*a*)	1(*b*)	0.0	0.0	0.4638(2)	0.4348	.0	0.0	0.5	0.0	0.0	-0.27	0.27	0.02
Pb2	2(*b*)	2(*d*)	0.6667	0.3333	0.6241(8)	0.595	0.6667	0.3333	0.5	0.0	-0.0	0.39	0.39	0.02
C1	3(*c*)		0.0	-0.3761(7)	0.223(2)	0.194	0.0	-0.3327	0.231	0.0	1.22	-0.38	1.28	0.03
		6(*k*)												
C4	3(*c*)		0.0	0.2893(7)	-0.238(3)	0.320	0.0	0.3327	-0.231	0.0	0.06	0.23	0.24	0.03
C2	3(*c*)		0.0	-0.2812(7)	0.349(2)	-0.114	0.0	-0.2420	-0.132	0.0	-0.55	-0.89	1.05	0.02
		6(*k*)												
C5	3(*c*)		0.0	0.2028(6)	-0.085(2)	-0.267	0.0	0.2420	0.132	0.0	-0.55	-0.89	1.05	0.03
N1	3(*c*)		0.0	-0.2071(6)	0.449(2)	0.420	0.0	-0.1672	0.2113	0.0	-0.56	0.97	1.12	0.03
		6(*k*)												
N3	3(*c*)		0.0	0.1272(6)	0.0265(19)	-0.0025	0.0	0.1672	-0.2113	0.0	-0.57	0.97	1.13	0.03
C3	6(*d*)		0.4731(5)	0.3741(5)	0.1560(14)	0.127	0.4506	0.3283	0.2401	0.32	0.65	-0.34	0.92	0.02
		12(*l*)												
C6	6(*d*)		-0.0998(5)	0.2824(5)	-0.3242(15)	-0.3532	-0.1223	0.3283	-0.2401	0.32	-0.65	-0.34	0.66	0.03
N2	6(*d*)		0.5517(5)	0.3710(5)	0.1048(15)	0.0758	0.5280	0.3256	0.2526	0.34	0.64	-0.60	1.05	0.03
		12(*l*)												
N4	6(*d*)		-0.1786(5)	0.2801(6)	-0.4004(16)	-0.4294	-0.2024	0.3256	-0.2526	0.34	0.64	0.60	1.05	0.04

Table S25

Modified atomic positions for $Pb(ReO_4)_2$, based on Picard *et al.s*' (1984) data [201430], with hypothetical $x'\ y'\ z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 11.276(5), c = 5.593(3) Å; $z^* = z + 0.0909$.

	Wyckoff Position													
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Re1	3(*c*)	3(*f*)	0.3805(3)	0.0	-0.0171(16)	0.0738	0.3805	0.0	0.0	0.0	0.0	0.339	0.34	0.11
Re2	3(*c*)	3(*g*)	0.7128(2)	0.0	0.4828(16)	0.5737	0.7128	0.0	0.5	0.0	0.0	0.339	0.34	0.11
Pb1	1(*a*)	1(*a*)	0.0	0.0	0.0	0.0909	0.0	0.0	0.0	0.0	0.0	0.418	0.42	0.16
Pb2	2(*b*)	2(*d*)	0.3333	0.6667	0.4708(16)	0.5617	0.3333	0.6667	0.5	0.0	0.0	0.283	0.28	0.13
O1	3(*c*)		0.227(6)	0.0	0.119(14)	0.210	0.311	0.0	0.256	-0.947	0.0	-0.211	0.97	0.18
		6(*k*)												
O6	3(*c*)		0.395(8)	0.0	0.607(19)	0.698	0.311	0.0	0.744	0.947	0.0	-0.211	0.97	0.24
O2	6(*d*)		0.522(4)	0.140(4)	0.089(9)	0.180	0.6185	0.1475	0.239	-1.088	-0.085	-0.271	1.16	0.16
		12(*l*)												
O4	6(*d*)		0.715(5)	0.155(5)	0.611(10)	0.702	0.6185	0.1475	0.761	1.088	0.085	-0.271	1.16	0.19
O3	3(*c*)		0.727(7)	0	0.122(17)	0.213	0.789	0.0	0.258	-0.699	0.0	-0.202	0.73	0.22
		6(*k*)												
O5	3(*c*)		0.850(5)	0.0	0.607(13)	0.698	0.789	0.0	0.742	0.688	0.0	-0.202	0.72	0.16

Table S26(*a*)

Modified atomic positions for $Ag_5Pb_2O_6$ based on Byström & Evers' (1950) study [24038], with hypothetical $x'\ y'\ z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 5.939(3), c = 6.428(3) Å; z^* = z - 0.0147.

	Wyckoff Position													
	$P31m$	$P\bar{3}1m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ag1	1(*a*)		0.0	0.0	0.264	0.2493	0.0	0.0	0.264	0.0	0.0	-0.09	0.09	n/d†
		2(*e*)												
Ag2	1(*a*)		0.0	0.0	-0.264	0.7213	0.0	0.0	-0.264	0.0	0.0	-0.09	0.09	n/d
Ag3	3(*c*)	3(*g*)	0.5	0.0	0.522	0.5073	0.5	0.0	0.5	0.0	0.0	0.05	0.05	n/d
Pb	2(*b*)	2(*c*)	0.3333	0.6667	0.022	0.0073	0.3333	0.6667	0.0	0.0	0.0	0.05	0.05	n/d
O1	3(*c*)		0.603	0.0	0.215	0.2003	0.603	0.0	0.193	0.0	0.0	0.05	0.05	n/d
		6(*k*)												
O2	3(*c*)		0.397	0.0	-0.171	0.8143	0.397	0.0	-0.193	0.0	0.0	0.05	0.05	n/d

† Not determined or reported

Table S26(*b*)

Modified atomic positions for $Ag_5Pb_2O_6$ based on Yoshii *et al*.s' (2006) study [172975], with hypothetical $x'\ y'\ z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 5.9405(5), c = 6.4349(4) Å.

	Wyckoff Position				
	$P\bar{3}1m$	x	y	z	u_{iso}
Ag1	2(*e*)	0.0	0.0	0.2412(2)	0.14
Ag2	3(*f*)	0.5	0.0	0.0	0.13
Pb	2(*d*)	0.6667	0.3333	0.5	0.09
O	6(*k*)	0.6208	0.0	0.6892(2)	0.10

Table S27

Modified atomic positions for $Cd_{0.61}Pt_{3.05}Zn_{4.27}$, based on Khan & Schubert's (1970) data [654683], with hypothetical x' y' z' coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. (see footnote 4).

a = 7.050, c = 2.792 Å; $z^* = z$.

	Wyckoff	Position												
	$P31m$	$P\bar{6}2m$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cd1,Zn1	2(*b*)	2(*d*)	0.3333	0.6667	0.5	0.5	0.3333	0.6667	0.5	0.0	0.0	0.0	0.0	n/d[†]
Cd2,Zn2	3(*c*)	3(*g*)	0.735	0.0	0.5	0.5	0.735	0.0	0.5	0.0	0.0	0.0	0.0	n/d
Pt	3(*c*)	3(*f*)	0.358	0.0	0.0	0.0	0.358	0.0	0.0	0.0	0.0	0.0	0.0	n/d

[†] Not determined or reported.