Supplementary Publication of Tables 1S – 22S

Systematic Prediction of New Ferroelectrics in Space Group *P*3

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Abstract

The current release of the Inorganic Crystal Structure Database contains a total of 57 entries under space group *P*3 that correspond to 50 different materials. Twenty one structures reported with this space group satisfy the criteria for ferroelectricity, at a confidence level that depends on the reliability of the underlying structural determination. One ferroelectric discovered earlier is also listed. In addition, the database contains 19 entries that probably should be assigned to a centrosymmetric space group, 7 that are polar but probably not ferroelectric and 2 that are without atomic coordinates. Seven entries are either duplicates or present additional structural studies of the same material. Structures in space group *P*3 identified as potentially new ferroelectrics include $LiAsCu_{0.93}$, Na_2UF_6, BiTeI, $BaGe_4O_9$, α-UMo_2O_8, Cu_2SiS_3, $Co(IO_3)_2$, $Sr_7Al_{12}O_{25}$, KSn_2F_5, $YbIn_2S_4$, $Na_5CrF_2(PO_4)_2$, $Sn(ClO_2)_2(ClO_4)_6$, Eu_3BWO_9, $Li(H_2O)_4B(OH)_4{\cdot}2H_2O$, $Mn_3V_{1/2}(SiO_4)O(OH)_2$, $Ca_6(Si_2O_7)(OH)_6$, $Na_{6.9(2)}[Al_{5.6(1)}Si_{6.4(1)}O_{24}](S_2O_3)_{1.0(1)}{\cdot}2H_2O$, $BaCa_2In_6O_{12}$, $Ni(H_2O)_6[Sb(OH)_6]_2$, $Sr_4Cr_3O_9$ and $Cu_5O_2(VO_4)_2{\cdot}CuCl_2$.

Table 1S *Atomic positions for $LiAsCu_{0.93}$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 4.125, c = 9.025 Å

(uncertainties not provided by authors)

	Wyckoff positions $P3, P\bar{3}$	x	y	z^*	$z´$	$\Delta z^{\cong}$
Li1	1(a), 1(a)	0	0	0.008[A]	0	0.072
Li2	1(a)	0	0	0.331	0.335	-0.036
	2(c)					
Li3	1(a)	0	0	0.661	0.665	-0.036
As1	1(b)	1/3	2/3	-0.025	0	-0.226
	2(d)					
Cu2	1(c)	2/3	1/3	0.040(4)	0	0.361
As2	1(b)	1/3	2/3	0.691(4)	0.678	0.122
	2(d)					
As3	1(c)	2/3	1/3	0.336(3)	0.322	0.122
Cu1	1(b)	1/3	2/3	0.326(3)	0.348	-0.199
	2(d)					
Cu3	1(c)	2/3	1/3	0.630(2)	0.652	-0.199

[≅] $z^* = z - 0.025$; $\Delta z = (z^* - z´)c$.

[A] Uncertainties in z(Li) coordinates not given.

Table 2(*a*)S *Atomic positions for $BaGe_4O_9$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 11.61(2), *c* = 4.74(1) Å

	Wyckoff positions *P*3,*P*321	*x*	*y*	*z*	*z´*	Δz[†]
Ba,Ba[‡]	3(*d*),3(*f*)	0.3341(4)	0.3334(5)	0	0	0
Ge1,Ge4	1(*a*),1(*a*)	0	0	-0.093(3)	0	0.441
Ge2	1(*b*)	2/3	1/3	0.006(4)	-0.048	0.256
Ge3	2(*d*)					
Ge3	1(*b*)	1/3	2/3	0.102(3)	0.048	0.256
Ge4,Ge2	3(*d*),3(*f*)	0.8148(7)	0.8200(6)	0.411(3)	½	-0.422
Ge5	3(*d*)	0.6674(7)	0.5131(6)	0.505(3)	0.456	0.232
Ge1	6(*g*)					
Ge6	3(*d*)	0.5180(6)	0.6719(7)	0.593(3)	0.544	0.232
O1	3(*d*)	0.846(3)	0.929(4)	0.119(8)	0.238	-0.56
O1	6(*g*)					
O6	3(*d*)	0.926(4)	0.843(4)	-0.357(8)	-0.238	-0.56
O2	3(*d*)	0.584(5)	0.407(5)	0.216(11)	0.260	-0.21
O4	6(*l*)					
O4	3(*d*)	0.551(4)	0.556(4)	-0.304(8)	-0.260	-0.21
O3	3(*d*)	0.775(3)	0.652(3)	0.310(8)	0.409	-0.47
O2	6(*g*)					
O7	3(*d*)	0.665(7)	0.808(7)	0.493(18)	0.591	-0.47
O5	3(*d*)	0.474(6)	0.735(6)	-0.102(13)	0.075	-0.84
O3	6(*g*)					
O9	3(*d*)	0.753(5)	0.484(5)	-0.253(10)	-0.075	-0.84
O8,O5	3(*d*),3(*f*)	0.406(4)	0.588(4)	0.327(9)	½	-0.82

[†] $\Delta z = (z - z´)c$.

[‡] First atom in space group *P*3 as designated by Robbins *et al.* (1966), second atom in space group *P*321 as by Shashkov *et al.* (1985), see Table 2(*b*)S.

Table 2(*b*)S *Atomic positions for $BaGe_4O_9$ in space group P321*

a = 11.608(6), c = 4.768(2) Å

	x	*y*	*z*
Ba;[≅] Ba	0.3320(1)	0.3320(1)	0
Ge1;Ge5&6	0.6620(1)	0.5129(1)	0.4075(2)
Ge2;Ge4	0.8213(2)	0.8213(2)	½
Ge3;Ge2&3	1/3	2/3	0.8980(4)
Ge4;Ge1	0	0	0
O1;O1&6	0.8484(4)	0.9382(8)	0.766(1)
O2;O3&7	0.6753(8)	0.7887(9)	0.308(2)
O3;O5&9	0.7493(9)	0.4866(8)	0.325(2)
O4;O2&8	0.5879(8)	0.4073(9)	-0.123(2)
O5;O4	0.5188(11)	0.5188(11)	½

[≅] Equivalent positions of authors' coordinates, for ready comparison with Table 2(*a*)S. Second entry is atom designation in that table for space group *P*3, see §2.4.

Table 3S *Atomic positions for a-UMo_2O_8 at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 17.300(10), *c* = 6.145(1) Å

	Wyckoff position $P3, P\bar{3}$	*x*	*y*	*z*[*]	*z´*	Δz[†]
U1	1(*a*), 1(*b*)	0	0	0.536(2)	½	0.22
U2	1(*b*) 2(*d*)	1/3	2/3	-0.016	0	-0.10
U3	1(*c*)	2/3	1/3	-0.016	0	-0.10
U4	3(*d*) 6(*g*)	0	1/3	0.263(2)	0.251	0.08
U5	3(*d*)	1/3	1/3	-0.239(2)	-0.251	0.07
Mo1	3(*d*) 6(*g*)	0.2308(8)	0.1592(8)	0.229(2)	0.249	0.12
Mo4	3(*d*)	0.0625(8)	0.2283(8)	-0.268(2)	-0.248	0.12
Mo2	3(*d*) 6(*g*)	0.2673(8)	0.4323(8)	0.244(2)	0.262	-0.11
Mo5	3(*d*)	0.4365(8)	0.1755(8)	-0.279(2)	-0.261	-0.11
Mo3	3(*d*) 6(*g*)	0.6020(8)	0.0993(8)	0.265(2)	0.242	0.14
Mo6	3(*d*)	0.1098(8)	0.5015(8)	-0.219(2)	-0.242	0.14
O1	3(*d*) 6(*g*)	0.123(8)	0.078(8)	0.364(2)	0.315	0.30
O13	3(*d*)	0.044(9)	0.115(9)	-0.266[‡]	-0.315	0.30
O2	3(*d*) 6(*g*)	0.234(9)	0.226(9)	-0.016[‡]	0	-0.10
O15	3(*d*)	0.008(8)	0.237(8)	-0.016[‡]	0	-0.10
O3	3(*d*) 6(*g*)	0.251(8)	0.242(8)	0.424(2)	0.500	-0.47
O16	3(*d*)	0.027(9)	0.235(9)	0.434(2)	0.500	-0.47
O4	3(*d*) 6(*g*)	0.287(13)	0.104(12)	0.234[‡]	0.250	-0.10
O14	3(*d*)	0.177(8)	0.280(8)	-0.266[‡]	-0.250	-0.10
O5	3(*d*) 6(*g*)	0.280(8)	0.549(8)	0.194(2)	0.230	-0.22
O17	3(*d*)	0.559(8)	0.272(8)	-0.266[‡]	-0.230	-0.22
O6	3(*d*) 6(*g*)	0.250[‡]	0.370(9)	-0.016[‡]	0	-0.10
O20	3(*d*)	0.392(8)	0.104(9)	-0.016[‡]	0	-0.10
O7	3(*d*) 6(*g*)	0.285(9)	0.395(9)	0.484[‡]	0.500	-0.10
O19	3(*d*)	0.400(8)	0.116(8)	0.484[‡]	0.500	-0.10

O8	3(*d*)	0.149(8)	0.342(8)	0.284(2)	0.275	0.06
	6(*g*)					
O18	3(*d*)	0.380(9)	0.230(9)	-0.266‡	-0.275	0.06
O9	3(*d*)	0.617(8)	0.205(8)	0.234‡	0.250	-0.10
	6(*g*)					
O21	3(*d*)	0.218(8)	0.576(8)	-0.266‡	-0.250	-0.10
O10	3(*d*)	0.644(8)	0.103(8)	-0.016‡	0	-0.10
	6(*g*)					
O23	3(*d*)	0.070(9)	0.432(9)	-0.016‡	0	-0.10
O11	3(*d*)	0.497(8)	0.027(8)	0.234‡	0.250	-0.10
	6(*g*)					
O22	3(*d*)	0.022(8)	0.535(8)	-0.206(2)	-0.250	-0.10
O12	3(*d*)	0.659(8)	0.099(8)	0.484‡	0.500	-0.10
	6(*g*)					
O24	3(*d*)	0.110(9)	0.460(9)	0.484‡	0.500	-0.10

† $\Delta z = (z^{*} - z')c$, with $z^{*} = z - 0.016$; authors' atomic numbering retained.

‡ Values fixed at 0, ¼, ½ or ¾ and not varied in refinement.

Table 4S *Atomic positions for Cu_2SiS_3 at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 10.981(3), c = 6.046(1) Å

	Wyckoff position *Cmc*2_1, *Cmcm*	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
Cu	8(*b*), 8(*g*)	0.162(1)	0.839(1)	0.309(1)	¼	0.36
Si	4(*a*), 4(*c*)	0	0.332(1)	0.300	¼	0.30
S1	8(*b*), 8(*g*)	0.158(1)	0.814(1)	0.691(1)	¾	-0.36
S2	4(*a*), 4(*c*)	0	0.345(2)	0.679(1)	¾	-0.31

$^{\cong}$ $\Delta z = (z^* - z\hat{})c$, with $z^* = z + 0.300$

Table 5S *Atomic positions for $Sr_7Al_{12}O_{25}$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 17.910, *c* = 7.160 Å [uncertainties not given]

	Wyckoff position *P*3,*P*321	*x*	*y*	*z*[*]	*z´*	Δz[†]
Sr1	3(*d*),3(*e*)	0.5539(5)	0.4789(5)	-0.0058	0	-0.042
Sr2	3(*d*) W1[‡]	0.1484(4)	0.2558(5)	0.1484(3)	0.1582	-0.070
Sr5	3(*d*)	0.2578(4)	0.1093(4)	0.3320(4)	0.3418	-0.070
Sr3	3(*d*) W1	0.4140(5)	0.2246(4)	0.8125(4)	0.8261	-0.097
Sr4	3(*d*)	0.1904(4)	0.4111(5)	0.6602(3)	0.6739	-0.098
Sr6	3(*d*),3*f*	0.0781(5)	0.5605(5)	0.4795(3)	½	-0.147
Sr7[|]	1(*a*),1(*b*)	0	0	0.4451(4)	½	-0.393
Sr8	1(*a*),1(*a*)	0	0	0.0462(5)	0	0.331
Sr9	1(*b*) 2(*d*)	1/3	2/3	0.7762(5)	0.8352	-0.423
Sr11	1(*c*)	2/3	1/3	0.1057(5)	0.1648	-0.423
Sr10	1(*b*) 2(*d*)	1/3	2/3	0.3853(3)	0.3346	0.363
Sr12	1(*c*)	2/3	1/3	0.7161(4)	0.6654	0.363
Al1	3(*d*),3(*f*)	0.2636(5)	0.2792(5)	0.5234(5)	½	0.168
Al2	3(*d*) 6(*g*)	0.0527(5)	0.6484(5)	0.8574(5)	0.8340	0.168
Al6	3(*d*)	0.3857(5)	0.3134(5)	0.1895(5)	0.1660	0.168
Al3	3(*d*) W1	0.0781(5)	0.1953(5)	0.7080(5)	0.7149	-0.049
Al4	3(*d*)	0.1953(5)	0.1171(5)	0.7783(5)	0.7852	-0.049
Al5	3(*d*) W1	0.4687(5)	0.2138(5)	0.3731(5)	0.3812	-0.058
Al10	3(*d*)	0.2558(5)	0.4707(5)	0.1104(5)	0.1187	-0.059
Al9	3(*d*) 6(g)	0.4062(5)	0.0527(5)	0.6221(5)	0.6670	-0.321
Al11	3(*d*)	0.0751(5)	0.3896(5)	0.2881(5)	0.3330	-0.321
Al7	3(*d*),3(*e*)	0.2792(5)	0.0156(5)	0.9570(5)	0	-0.308
Al8	3(*d*),3(*f*)	0.5449(5)	0.4082(5)	0.4453(5)	½	-0.392
Al12	3(*d*),3(*e*)	0.4501(5)	0.5888(5)	0.0361(5)	0	0.258
O1	3(*d*) W1	0.2509(8)	0.1015(8)	0.9580(8)	-0.0357	-0.045
O14	3(*d*)	0.1503(8)	0.2509(8)	0.5293(8)	0.5357	-0.045
O2	3(*d*) W2	0.0625(8)	0.4687(8)	0.1846(8)	0.1885	-0.028
O4	3(*d*)	0.5986(8)	0.0615(8)	0.3076(8)	0.3115	-0.028

O3	3(*d*)	0.6552(8)	0.0468(8)	0.9561(8)	0.9618	-0.039
	W2					
O11	3(*d*)	0.0478(8)	0.3925(8)	0.5332(8)	0.5382	-0.038
O5	3(*d*)	0.3974(8)	0.1328(8)	0.5127(8)	0.5180	-0.038
	W3					
O10	3(*d*)	0.2626(8)	0.3916(8)	0.9766(8)	0.9820	-0.039
O6	3(*d*)	0.2783(8)	0.2031(8)	0.6465(8)	0.6797	-0.238
	6(g)					
O8	3(*d*)	0.2890(8)	0.2705(8)	0.2871(8)	0.3203	-0.238
O7	3(*d*)	0.0722(8)	0.2724(8)	0.8467(8)	0.8598	-0.093
	W4					
O16	3(*d*)	0.3173(8)	0.3759(8)	0.6270(8)	0.6402	-0.093
O9	3(*d*)	0.5214(8)	0.0830(8)	0.6231(8)	0.6655	-0.303
	W5					
O12	3(*d*)	0.1826(8)	0.4160(8)	0.2920(8)	0.3345	-0.303
O13	3(*d*)	0.4355(8)	0.5156(8)	0.8633(8)	0.8345	0.206
	W6					
O24	3(*d*)	0.1875(8)	0.6406(8)	0.1943(8)	0.1655	0.206
O15	3(*d*)	0.4150(8)	0.2314(8)	0.1963(8)	0.1924	0.028
	W7					
O22	3(*d*)	0.6386(8)	0.4453(8)	0.3115(8)	0.3076	0.028
O17	3(*d*)	0.3798(8)	0.0566(8)	0.8672(8)	0.8330	0.245
	W8					
O19	3(*d*)	0.0136(8)	0.2861(8)	0.2012(8)	0.1670	0.245
O18	3(*d*)	0.5166(8)	0.3056(8)	0.5303(8)	0.5313	-0.007
	W2					
O23	3(*d*)	0.2177(8)	0.5234(8)	0.9678(8)	0.9687	-0.007
O20	3(*d*)	0.1230(8)	0.1455(8)	0.8643(8)	0.8580	0.045
	W9					
O21	3(*d*)	0.1376(8)	0.0253(8)	0.6484(8)	0.6420	0.045
O25[††]	1(*a*),1(*b*)	0	0	0.5563(8)	½	0.403
O26	1(*a*),1(*a*)	0	0	0.9360(8)	0	-0.458
O27	1(*b*)	1/3	2/3	0.8857(8)	0.8302	0.397
	2(*d*)					
O29	1(*c*)	2/3	1/3	0.2253(8)	0.1698	0.397
O28	1(*b*)	1/3	2/3	0.2763(8)	0.3401	0.457
	2(*d*)					
O30	1(*c*)	2/3	1/3	0.5961(8)	0.6599	0.457

[†] $\Delta z = (z^* - z')c$, with $z^* = z - 0.0058$.

[‡] Nonspace group relations: W1, *y*,*x*,½-*z*; W2, *y*, $\bar{x}$,½-*z*; W3, *y*, *y*-*x*,½-*z*; W4, *y*-*x*,*x*, ½-*z*; W5, *y*, $\bar{x}$, $\bar{z}$; W6, $\bar{y}$, *y*-*x*, $\bar{z}$; W7, *y*,*x*-*y*,½-*z*; W8 *y*,*x*-*y*, $\bar{z}$.

[††] Sr7-Sr12 and O25-O30 sites are each reported 50% occupied.

Table 6S *Atomic positions for KSn_2F_5 at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 7.291(1), c = 9.861(2) Å

	Wyckoff position $P3,P\bar{3}$	x	y	z^*	$z´$	Δz †
Sn1	3(d) 6(g)	0.3269(1)	-0.0078(1)	0.3254	0.3254	0
Sn2	3(d)	-0.3380(1)	-0.0014(1)	-0.3254(1)	-0.3254	0
K1	1(a),1(a)	0	0	-0.0218(12)	0	-0.215
K2	1(b) 2(d)	1/3	2/3	-0.0029(18)	-0.0154	0.123
K3	1(c)	2/3	1/3	0.0279(11)	0.0154	0.124
F1[A]	1(b) 2(d),2(c) ††	1/3	2/3	-0.2945(23)	-0.2893	-0.051
F3	1(a)	0	0	0.2841(18)	0.2893	-0.051
F2	1(b) 2(d)	1/3	2/3	0.2808(14)	0.2904	-0.095
F8[A]	1(c)	2/3	1/3	-0.300(6)	-0.2904	-0.095
F4	3(d) 6(g)	0.6606(8)	0.1061(8)	0.2823(10)	0.2836	-0.013
F5[A]	3(d)	0.2267(17)	0.9939(14)	-0.2848(14)	-0.2836	-0.012
F6	3(d) 6(g)	0.6479(13)	0.0166(12)	-0.1251(20)	-0.1237	-0.014
F7	3(d)	0.6722(7)	0.6963(9)	0.1222(13)	0.1237	-0.015

† $\Delta z = (z^* - z´)c$, with $z^* = z - 0.3417$.

[A] The F1, F5 and F8 sites are reported respectively as 63, 94 and 27% occupied.

†† Only one of each 2(c) and 2(d) position is occupied.

Table 7S *Atomic positions for $YbIn_2S_4$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 20.859(8), c = 3.8743(9) Å

	Wyckoff position *P*3,*P*321	*x*	*y*	z^*	*z´*	$\Delta z^\dagger$
Yb1	1(*a*),1(*a*)	0	0	0	0	0
Yb2	1(*c*)	2/3	1/3	0	0	0
Yb3	1(*b*) 2(*d*)	1/3	2/3	0	0	0
Yb4	3(*d*),3(*f*)	0.0083(2)	0.345(3)	0.51(1)	½	0.04
Yb5	3(*d*),3(*f*)	0.348(2)	0.333(4)	0.498(1)	½	-0.008
Yb6	3(*d*),3(*e*)	0.002(3)	0.356(4)	0.995(1)	0	-0.019
In1	3(*d*)	0.220(3)	0.113(4)	-0.473(9)	-0.58	0.43
In4	3(*d*) 6(*a*)‡	0.1212(5)	0.2126(4)	0.19(2)	0.08	0.43
In2	3(*d*)	0.4623(7)	0.2329(8)	0.12(3)	0.053	0.26
In5	3(*d*) 6(*a*)‡	0.2351(4)	0.4424(2)	-0.485(2)	-0.553	0.263
In3	3(*d*)	0.5573(4)	0.4324(3)	-0.494(2)	-0.505	0.043
In6	3(*d*) 6(*a*)‡	0.1141(6)	0.561(1)	0.016(2)	0.005	0.043
S1	3(*d*),3(*f*)	0.248(3)	0.224(3)	0.017(8)	0	0.066
S2	3(*d*) 6(*g*)	0.551(4)	0.307(3)	-0.53(1)	-0.502	-0.11
S9	3(*d*)	0.357(1)	0.571(4)	0.474(8)	0.502	-0.11
S3	3(*d*),3(*f*)	0.094(3)	0.105(3)	0.48(1)	½	-0.08
S4	3(*d*) 6(*g*)	0.460(3)	0.361(2)	0.004(8)	0.022	-0.068
S11	3(*d*)	0.317(1)	0.422(2)	0.039(7)	0.022	0.068
S5	3(*d*) 6(*g*)	0.142(2)	0.304(1)	-0.498(7)	-0.479	-0.074
S10	3(*d*)	0.356(4)	0.154(5)	0.46(1)	0.479	-0.074
S6	3(*d*), 3(*f*)	0.026(2)	0.49(2)	0.491(9)	½	-0.035
S7	3(*d*), 3(*e*)	0.181(2)	0.022(4)	0.03(1)	0	0.12
S8	3(*d*),6(*g*)††	0.156(2)	0.467(2)	0.137(7)	0	0.53
S12	3(*d*), 3(*e*)	0.630(3)	0.496(3)	0.002(8)	0	0.008

† $\Delta z = (z^* - z^\wedge)c$.

‡ Note the *z* coordinate relation in 6(*g*) is replaced here by *z* and ~(½- *z*).

†† All sites in position 6(*g*) with $z \lessapprox -0.137$ are unoccupied.

Table 8S *Atomic positions for $Na_5CrF_2(PO_4)_2$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 10.576(3), c = 6.669(2) Å

	Wyckoff position *P*3,*P*312	*x*	*y*	*z*	*z´*	$\Delta z^{\dagger}$
Cr	3(*d*),3(*j*)	0.1675(3)	0.3343(3)	0	0	0
P1	3(*d*) 6(*l*)[A]	0.4823(2)	0.5163(2)	0.2502(3)	0.2502	0
P2	3(*d*)	0.2948(2)	0.1458(2)	-0.2502(3)	-0.2502	0
Na1	3(*d*) 6(*l*)[A]	0.4932(8)	0.4770(9)	0.760(1)	0.7606	-0.01
Na2	3(*d*)	0.3520(8)	0.1651(8)	0.239(1)	0.2394	-0.01
Na3	3(*d*),3(*j*)	0.169(1)	0.334(1)	0.499(2)	½	0.00
Na4	1(*a*),1(*b*)	0	0	0.439(2)	½	-0.41
Na5	1(*b*),1(*d*)	1/3	2/3	0.581(1)	½	0.54
Na6	1(*c*),1(*f*)	2/3	1/3	0.508(3)	½	0.05
Na7	1(*c*),1(*e*)	2/3	1/3	-0.007(2)	0	-0.05
Na8	1(*a*), 1(*a*)	0	0	-0.004(2)	0	-0.03
Na9	1(*b*),1(*c*)	1/3	2/3	0.028(2)	0	0.19
O1	3(*d*),3(*j*)	0.4124(7)	0.5043(7)	0.4598(9)	½	-0.268
O2	3(*d*) 6(*l*)	0.5561(6)	0.4241(6)	0.255(1)	0.2447	0.070
O8	3(*d*)	0.4632(7)	0.2334(6)	-0.2342(9)	-0.2447	0.070
O3	3(*d*)	0.5856(6)	0.6844(6)	0.2118(8)	0.2089	0.019
O5	3(*d*)	0.2502(6)	0.2601(6)	-0.206(1)	-0.2089	0.019
O4	3(*d*)	0.3694(5)	0.4634(6)	0.0807(8)	0.0757	0.033
O6	3(*d*)	0.2296(7)	0.0354(6)	-0.0707(9)	-0.0757	0.033
O7	3(*d*),3(*j*)	0.2342(6)	0.0707(6)	-0.4401(8)	½	0.399
F1	3(*d*)	0.183(1)	0.4717(8)	-0.199(1)	-0.2000	0.010
F2	3(*d*)	0.144(1)	0.191(1)	0.201(1)	0.2000	0.010

† $\Delta z = (z - z')c$.

A The atomic coordinates of the P1,Na1 and also P2,Na2 pairs have a Wyckoff 6(*l*) position relationship.

Table 9S *Atomic positions for $Sn(ClO_2)_2(ClO_4)_6$ at 213 K with hypothetical z´ coordinates and polar displacements in Å*

a = 15.913(5), c = 7.452(1) Å

	Wyckoff position *P*3,*P*312	*x*	*y*	*z*	*z´*	Δz †
Sn1	1(*a*),1(*a*)	0	0	0.025	0	0.19
Sn2	1(*b*),1(*d*)	1/3	2/3	0.5232(9)	½	0.17
Sn3	1(*c*),1(*e*)	2/3	1/3	-0.049(1)	0	-0.37
Cl1	3(*d*) 6(*l*)	0.175(1)	0.177(1)	0.245(2)	0.209	0.27
Cl2	3(*d*)	0.189(1)	0.019(1)	-0.172(2)	-0.209	-0.27
Cl3	3(*d*) 6(*l*)	0.307(1)	0.476(1)	0.296(3)	0.283	0.10
Cl4	3(*d*)	0.148(1)	0.496(1)	-0.269(2)	-0.283	0.10
Cl5	3(*d*) 6(*l*)	0.693(1)	0.169(2)	0.192(4)	0.172	0.15
Cl6	3(*d*)	0.501(1)	0.144(1)	-0.152(4)	-0.172	0.15
Cl7	3(*d*) 6(*l*)	0.327(1)	0.336(1)	-0.227(4)	0.284	0.42
Cl8	3(*d*)	0.710(2)	0.701(3)	0.340(6)	-0.284	0.42
O1	3(*d*) 6(*l*)	0.120(2)	0.072(3)	0.202(5)	0.216	-0.10
O8	3(*d*)	0.227(5)	0.134(5)	-0.230(8)	-0.216	-0.10
O2	3(*d*) 6(*l*)	0.221(4)	0.240(3)	0.107(6)	0.058	0.36
O6	3(*d*)	0.212(3)	-0.003(3)	-0.010(6)	-0.058	0.36
O3	3(*d*) 6(*l*)	0.247(4)	0.182(4)	0.365(6)	0.365	0.04
O7	3(*d*)	0.189(3)	-0.009(3)	-0.366(1)	-0.365	0.04
O9	3(*d*) 6(*l*)	0.354(3)	0.573(3)	0.350(6)	0.340	0.07
O13	3(*d*)	0.247(3)	0.554(3)	-0.331(5)	-0.340	0.07
O10	3(*d*) 6(*l*)	0.335(4)	0.428(4)	0.415(7)	0.417	-0.02
O14	3(*d*)	0.086(3)	0.445(3)	-0.420(6)	-0.417	-0.02
O11	3(*d*) 6(*l*)	0.207(3)	0.441(4)	0.305(8)	0.221	0.63
O15	3(*d*)	0.136(4)	0.442(4)	-0.137(4)	-0.221	0.63
O12	3(*d*) 6(*l*)	0.335(3)	0.472(3)	0.109(6)	0.171	-0.45
O16	3(*d*)	0.118(4)	0.565(4)	-0.232(7)	-0.171	-0.45

O17	3(*d*) 6(*l*)	0.631(3)	0.213(3)	0.125(5)	0.162	-0.28
O21	3(*d*)	0.557(3)	0.245(3)	-0.200(5)	-0.162	-0.28
O18	3(*d*) 6(*l*)	0.709(4)	0.124(4)	0.043(8)	0.084	-0.31
O22	3(*d*)	0.454(3)	0.086(3)	-0.125(6)	-0.084	-0.31
O19	3(*d*) 6(*l*)	0.636(3)	0.1393)	0.357(6)	0.330	0.20
O23	3(*d*)	0.563(4)	0.106(4)	-0.304(7)	-0.330	0.20
O20	3(*d*) 6(*l*)	0.777(5)	0.234(5)	0.231(8)	0.312	-0.61
O24	3(*d*)	0.434(3)	0.124(3)	-0.394(6)	-0.312	-0.61
O25	3(*d*),3(*j*)[A]	0.627(3)	0.645(3)	0.217(5)	0	1.62

[†] $\Delta z = (z^{*} - z')c$, with $z^{*} = z - 0.119$.

[A] The 3 missing O atoms would satisfy Wyckoff position 6(*l*) in space group *P*312 if O26 were placed in position 3(*d*) of space group *P*3 and paired with O25.

Table 10S *Atomic positions for $Li(H_2O)_4B(OH)_4{\cdot}2H_2O$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 6.5534(5), c = 6.1740(7) Å

	Wyckoff position *P*3,*P*321	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
O1	1(*a*)	0	0	0.2465	0.272	-0.157
	2(*c*)					
O2	1(*a*)	0	0	0.7025(5)	0.728	-0.157
O3	1(*c*)	2/3	1/3	0.4715(4)	0.434	0.231
	2(*d*)					
O5	1(*b*)	1/3	2/3	0.6033(5)	0.565	0.231
O4	3(*d*)	0.8915(2)	0.5275(2)	0.7914(4)	0.803	-0.074
	6(*g*)					
O6	3(*d*)	0.0261(2)	0.4302(2)	0.1848(4)	0.196	-0.074
B	1(*c*)	2/3	1/3	0.7100(5)	0.712	-0.012
	2(*d*) [A]					
Li	1(*b*)	1/3	2/3	0.2860(8)	0.288	-0.012
H1	1(*a*),1(*b*)	0	0	0.573(9)	½	0.45
H2	3(*d*)	0.11(2)	0.09(2)	0.75(1)	0.771	-0.13
	6(*g*)					
H3	3(*d*)	0.013(7)	0.122(7)	0.208(7)	0.229	-0.13
H4	3(*d*)	0.57(1)	0.20(1)	0.437(1)	0.386	0.31
	6(*g*)					
H6	3(*d*)	0.394(7)	0.589(7)	0.664(6)	0.613	0.31
H5	3(*d*)	0.746(6)	0.107(5)	0.776(4)	0.747	0.18
	6(*g*)					
H7	3(*d*)	0.929(5)	0.419(5)	0.283(5)	0.253	0.18
H8	3(*d*),3(*e*)	0.458(5)	0.017(5)	0.078(5)	0	0.48

$^{\cong}$ $\Delta z = (z^* - z´)c$, with $z^* = z - 0.0035$.

[A] For disorder by B and Li over the 2(*d*) site at $T \, f \, T_c$.

Table 11S *Atomic positions for $Ca_6(Si_2O_7)(OH)_6$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 10.035(5), c = 7.499(3) Å

	Wyckoff position $P3,P\bar{6}$	x	y	z	$z´$	$\Delta z^{\cong}$
Ca1	3(*d*),3(*j*)	0.6689(2)	0.0455(2)	-0.0037(3)	0	-0.028
Ca2	3(*d*),3(*k*)	0.6665(3)	0.0426(3)	0.5071(3)	½	0.053
Ca3	3(*d*) 6(*l*)	0.0492(3)	0.3886(3)	0.2497(3)	0.2491	0.004
Ca4	3(*d*) 6(*l*)	0.0397(3)	0.3738(3)	-0.2485(3)	-0.2491	0.004
Si1	1(*c*) 2(*h*)	2/3	1/3	-0.2810(9)	-0.2776	-0.025
Si2	1(*c*) 2(*h*)	2/3	1/3	0.2742(9)	0.2776	-0.025
Si3	1(*b*),1(*c*)	1/3	2/3	0.0330(6)	0	0.247
Si4	1(*b*),1(*d*)	1/3	2/3	0.4693(6)	½	-0.230
O1	1(*c*) 2(*h*)	2/3	1/3	-0.492(2)	-0.377	-0.86
O2	1(*b*) 2(*h*)	1/3	2/3	0.262(2)	0.377	0.86
O3	3(*d*) 6(*l*)	0.5960(9)	0.147(1)	0.237(1)	0.232	0.04
O4	3(*d*) 6(*l*)	0.5910(8)	0.1475(8)	-0.227(1)	-0.232	0.04
O5	3(*d*) 6(*l*)	0.1592(8)	0.5556(8)	-0.015(1)	0	-0.11
O6	3(*d*) 6(*l*)	0.1564(8)	0.5594(8)	0.527(1)	½	0.21
O7	3(*d*) 6(*l*)	0.2229(8)	0.3028(8)	0.264(1)	0.257	0.05
O8	3(*d*) 6(*l*)	0.2087(9)	0.2681(8)	-0.250(1)	-0.257	0.05
O9	3(*d*),3(*j*)	0.9278(9)	0.2062(8)	0.011(1)	0	0.08
O10	3(*d*),3(*k*)	0.9278	0.2072	0.502(1)	½	0.01
H1[A]	3(*d*) 6(*l*)	0.152	0.158	-0.259	-0.249	-0.07
H4	3(*d*) 6(*l*)	0.148	0.161	0.239	0.249	0.07
H2	3(*d*),3(*j*)	0.158	0.004	0.011	0	0.09
H3	3(*d*),3(*k*)	0.167	0.014	0.514	½	0.09

$^{\cong}$ $\Delta z = (z^* - z´)c$, with $z^* = z + 0.0084$.

[A] H atom positions from difference syntheses, uncertainties not reported.

Table 12S *Atomic positions for $Na_{6.9}[Al_{5.6}Si_{6.4}O_{24}](S_2O_3)\cdot 2H_2O$ at 193 K with hypothetical z´ coordinates and polar displacements in Å*

a = 12.624(2), c = 5.170(1) Å

	Wyckoff position $P3,P\bar{3}$	x	y	z^*	$z´$	Δz ≅
Al1	3(*d*) 6(*g*)	0.9258(3)	0.5869(3)	0.2281	0.2522	-0.125
Al2	3(*d*)	0.0769(3)	0.4134(3)	0.724(1)	0.7478	-0.125
Si1	3(*d*) 6(*g*)	0.6711(2)	0.5892(3)	0.231(2)	0.2545	-0.119
Si2	3(*d*)	0.3288(2)	0.4128(3)	0.7225(9)	0.7455	-0.119
O1	3(*d*) 6(*g*)	0.7970(7)	0.5946(5)	0.312(2)	0.247	0.34
O2	3(*d*)	0.2021(7)	0.4017(6)	0.819(2)	0.753	0.34
O3	3(*d*) 6(*g*)	0.8834(6)	0.4349(7)	0.278(2)	0.276	0.01
O4	3(*d*)	0.1211(6)	0.5664(6)	0.725(2)	0.724	0.01
O5	3(*d*) 6(*g*)	0.9696(7)	0.6391(7)	0.917(2)	0.749	0.87
O6	3(*d*)	0.0271(7)	0.3452(7)	0.420(2)	0.251	0.87
O7	3(*d*) 6(*g*)	0.6748(6)	0.6340(7)	0.937(2)	0.751	0.97
O8	3(*d*)	0.3119(6)	0.3556(7)	0.436(2)	0.249	0.97
Na1	1(*b*) 2(*d*)	1/3	2/3	0.859(2)	0.754	0.54
Na2	1(*b*)	2/3	1/3	0.352(2)	0.246	0.55
Na3	3(*d*) 6(*g*)	0.8662(4)	0.7214(4)	0.697(1)	0.755	-0.30
Na4	3(*d*)	0.1284(4)	0.2601(4)	0.187(1)	0.245	-0.30
O9	3(*d*) 6(*g*)	0.6910(37)	0.3039(36)	0.786(5)	0.739	0.24
O10	3(*d*)	0.3158(45)	0.6909(42)	0.308(5)	0.261	0.24
S1	1(*a*) 2(c)	0	0	0.896[A]	0.828	0.35
S4/O	1(*a*)	0	0	0.240(6)	0.172	0.35
S2/O	1(*a*),1(*b*)	0	0	0.568(3)	½	0.35
S3/O	3(*d*) 6(*g*)	0.9352(9)	0.0628(11)	0.240(6)	0.234	0.03
S5/O	3(*d*)	0.8725(13)	0.9324(16)	0.772(5)	0.766	0.03

≅ $\Delta z = (z^* - z´)c$, with $z^* = z + 0.0041$.

[A] Uncertainty not reported.

Table 13S *Atomic positions for $Ba_{0.85}Ca_{2.15}In_6O_{12}$ with hypothetical z´ coordinates and polar displacements in Å*

a = 9.8880(1), c = 3.2170(1) Å

	Wyckoff position $P3,P\bar{3}$	x	y	z^*	$z´$	Δz [≅]
Ba1	1(*a*)	0	0	0.723(4)	0.742	-0.06
	2(*c*)					
Ba2	1(*a*)	0	0	0.240(7)	0.258	-0.06
Ba/Ca	1(*a*),1(*a*)	0	0	-0.046(5)	0	-0.15
Ca1	1(*b*)	1/3	2/3	0.285(5)	0.261	0.08
	2(*d*)					
Ca2	1(*c*)	2/3	1/3	0.763(7)	0.739	0.08
In1	3(*d*)	0.3492(4)	-0.0005(4)	0.268	0.252	0.05
	6(*g*)					
In2	3(*d*)	0.6545(4)	0.0068(4)	0.765(2)	0.748	0.05
O1	3(*d*)	0.1910(5)	0.3040(4)	0.268(5)	0.246	0.07
	6(*g*)					
O2	3(*d*)	0.8052(6)	0.6976(6)	0.777(4)	0.754	0.07
O3	3(*d*)	0.5293(6)	0.3970(6)	0.266(5)	0.247	0.06
	6(*g*)					
O4	3(*d*)	0.4669(6)	0.6003(7)	0.772(5)	0.753	0.06

[≅] $\Delta z = (z^* - z´)c$, with $z^* = z + 0.0183$.

Table 14S *Atomic positions for $Ni(H_2O)_6[Sb(OH)_6]_2$ with hypothetical z´ coordinates and polar displacements in Å*

a = 16.060(3), c = 9.792(1) Å

	Wyckoff position $P3,P\bar{3}$	x	y	z^*	$z´$	$\Delta z^{\cong}$
Sb1	1(*a*),1(*a*)	0	0	0.0337	0	0.330
Sb2	1(*c*) 2(*d*)	2/3	1/3	-0.0546(2)	-0.0431	-0.113
Sb3	1(*b*)	1/3	2/3	0.0316(6)	0.0431	-0.113
Ni1	3(*d*) 6(*g*)	0.3379(2)	0.0080(2)	0.0026(5)	0.0097	-0.069
Ni2	3(*d*)	0.6639(3)	-0.0065(2)	-0.0168(4)	-0.0097	-0.069
O1	3(*d*) 6(*g*)	0.032(1)	0.117(1)	-0.086(2)	-0.116	0.29
O2	3(*d*)	0.114(1)	0.08(1)	0.146(1)	-0.116	0.29
O3	3(*d*) 6(*g*)	0.579(1)	0.221(1)	-0.166(2)	-0.159	-0.07
O5	3(*d*)	0.302(1)	0.554(1)	0.152(1)	0.159	-0.07
O4	3(*d*) 6(*g*)	0.697(1)	0.254(1)	0.061(1)	0.068	-0.069
O6	3(*d*)	0.364(1)	0.783(1)	-0.075(1)	-0.068	-0.069
O7	3(*d*) 6(*g*)	0.315(1)	0.097(1)	-0.125(2)	-0.113	-0.118
O17	3(*d*)	0.633(1)	-0.126(1)	0.101(1)	0.113	-0.113
O8	3(*d*) 6(*g*)	0.426(1)	0.116(1)	0.127(1)	0.132	-0.059
O18	3(*d*)	0.553(1)	-0.091(1)	-0.138(2)	-0.132	-0.059
O9	3(*d*) 6(*g*)	0.454(1)	0.036(1)	-0.113(2)	-0.109	-0.044
O13	3(*d*)	0.582(1)	0.027(2)	0.104(2)	0.109	-0.044
O10	3(*d*) 6(*g*)	0.363(1)	-0.085(1)	0.122(2)	0.124	-0.020
O14	3(*d*)	0.693(1)	0.111(1)	-0.126(1)	-0.124	-0.020
O11	3(*d*) 6(*g*)	0.253(1)	-0.107(1)	-0.122(1)	-0.113	-0.088
O15	3(*d*)	0.781(1)	0.081(1)	0.104(2)	0.113	-0.088
O12	3(*d*) 6(*g*)	0.215(1)	-0.028(1)	0.125(2)	0.135	-0.093
O16	3(*d*)	0.754(1)	-0.032(2)	-0.144(2)	-0.135	-0.093
Sb4	1(*a*),1(*b*)	0	0	0.5311(3)	½	0.305

Sb5	1(*c*)	2/3	1/3	0.4522(2)	0.4599	-0.075
Sb6	2(*d*) 1(*b*)	1/3	2/3	0.5324(3)	0.5401	-0.075
Sb7	3(*d*)	0.3283(1)	-0.0066(1)	0.5041(4)	0.5104	-0.062
Sb8	6(*g*) 3(*d*)	0.6678(2)	0.0055(1)	0.4833(2)	0.4896	-0.062
O19	3(*d*)	0.064(1)	0.112(1)	0.400(2)	0.422	-0.220
O20	6(*g*) 3(*d*)	0.115(1)	0.042(1)	0.645(2)	0.668	-0.220
O21	3(*d*)	0.550(1)	0.269(1)	0.569(1)	0.609	-0.392
O23	6(*g*) 3(*d*)	0.263(1)	0.550(1)	-0.351(1)	-0.391	0.392
O22	3(*d*)	0.623(1)	0.220(1)	-0.664(1)	-0.626	-0.367
O24	6(*g*) 3(*d*)	0.395(1)	0.778(1)	0.411(2)	0.374	0.367
O25	3(*d*)	0.260(1)	0.039(1)	0.378(2)	0.388	-0.103
O35	6(*g*) 3(*d*)	0.607(1)	-0.108(1)	0.601(1)	0.612	-0.103
O26	3(*d*)	0.378(1)	0.113(1)	0.612(1)	0.620	-0.08
O36	6(*g*) 3(*d*)	0.551(1)	-0.040(1)	0.371(2)	0.380	-0.08
O27	3(*d*)	0.447(1)	0.060(1)	0.381(1)	0.390	-0.088
O31	6(*g*) 3(*d*)	0.618(1)	0.074(1)	0.601(1)	0.610	-0.088
O28	3(*d*)	0.400(1)	-0.050(1)	0.619(1)	0.630	-0.103
O32	6(*g*) 3(*d*)	0.732(1)	0.116(1)	0.360(1)	0.370	-0.103
O29	3(*d*)	0.281(1)	-0.123(1)	0.380(1)	0.392	-0.118
O33	6(*g*) 3(*d*)	0.779(1)	0.055(1)	0.596(1)	0.608	-0.118
O30	3(*d*)	0.211(1)	-0.074(1)	0.615(1)	0.626	-0.103
O34	6(*g*) 3(*d*)	0.707(1)	-0.067(1)	0.364(2)	0.374	-0.103

≅ $\Delta z = (z^* - z')c$, with $z^* = z + 0.0337$.

Table 15S *Atomic positions for $Cu_5O_2(VO_4)_2 \cdot CuCl_2$ with hypothetical z´ coordinates and polar displacements in Å*

a = 6.375(1), c = 8.399(1) Å

	Wyckoff position *P*3,*P*312	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
Cu1	1(*a*) 2(*g*)	0	0	0.2242	0.2081	0.135
V2	1(*a*)	0	0	-0.192(2)	-0.2081	0.135
Cu2	3(*d*),3(*k*)	0.338(2)	0.161(2)	0.504(2)	½	0.04
Cu3	1(*c*) 2(*i*)	2/3	1/3	-0.2266(9)	-0.2093	-0.145
V1	1(*c*)	2/3	1/3	0.192(2)	0.2093	-0.145
Cu4[A]	1(*b*) 2(*h*)	1/3	2/3	0.2419	0.2432	-0.011
Cu5[A]	1(*b*)	1/3	2/3	-0.2444[≅≅]	-0.2432	-0.011
O1	1(*a*),1(*a*)	0	0	0.009(9)	0	0.08
O4	1(*c*),1*e*	2/3	1/3	-0.001(8)	0	-0.01
O2	1(*c*),1*f*	2/3	1/3	-0.437(6)	½	0.53
O3	1(*a*),1(*b*)	0	0	0.468(8)	0	0.27
O5	3(*d*) 6(*l*)	0.379(8)	0.186(9)	0.255(4)	0.25	0.04
O6[¶]	3(*d*)	0.8	0.6	-0.245	-0.25	0.04
Cl1	1(*b*),1(*d*)	1/3	2/3	0.4956	½	-0.04
Cl2	1(*b*),1(*c*)	1/3	2/3	-0.0079	0	-0.07

[≅] $\Delta z = (z^* - z')c$, with $z^* = z + 0.2242$.

[A] The occupancy of the Cu4 site is reported as 69 %, that of the Cu5 site as 32 %. The Cu1, V2 and Cu3,V1 atoms form nonidentical pairs in space group *P*312. The table assumes misidentification of, or exchanged identities between, Cu and V, see §2.21.

[≅≅] Uncertainties not given for *z*(Cu4), *z*(Cu5), *z*(Cl1) or *z*(Cl2).

[¶] O6 is missing from the authors' list of coordinates; the values given for it in the table are assumed, see §2.21.

Table 16S *Atomic positions at room temperature for the mineral olgite,*

$Na(Sr_{0.52}Ba_{0.48})(Sr_{0.58}Na_{0.42})(Na_{0.81}Sr_{0.19})[PO_{3.40}][P_{0.76}O_{3.88}]$,

with hypothetical z´ coordinates and polar displacements in Å

a = 5.565(2), c = 7.050(3) Å

	Wyckoff position *P*3,*P*321	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
*M*1[A]	1(*a*),1(*a*)	0	0	0.0083	0	0.059
*M*2	1(*c*) 2(*d*)	2/3	1/3	0.3351(7)	0.3389	-0.026
*M*3	1(*b*)	1/3	2/3	0.657(1)	0.6611	-0.026
Na	1(*a*),1(*b*)	0	0	0.499(4)	½	-0.007
P1	1(*b*) 2(*d*)	1/3	2/3	0.222(2)	0.218	0.028
P2	1(*c*)	2/3	1/3	0.786(1)	0.782	0.028
O1	3(*d*) 6(*g*)	0.823(6)	0.191(6)	0.699(3)	0.700	-0.007
O2	3(*d*)	0.198(4)	0.816(4)	0.299(2)	0.300	-0.007
O3	1(*b*) 2(*d*)	1/3	2/3	0.004(3)	0	0.028
O4	1(*c*)	2/3	1/3	0.001(5)	0	0.007

$^{\cong}$ $\Delta z = (z^* - z´)c$, with $z^* = z + 0.0083$.

[A] *M*1 reported with 62% Sr, 48% Ba; *M*2 with 58% Sr, 42% Na; *M*3 with 81% Na, 19% Sr; P1 with 76%; O1 with 80% and O3 with 88% occupancy.

Table 17S *Atomic positions for $LaNb_7O_{19}$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 6.2531(2), *c* = 20.0685(10) Å

	Wyckoff position $P3,P\bar{6}$	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
La1	1(*a*)	0	0	-0.1533	-0.1558	0.049
	2(*g*)					
Nb5	1(*a*)	0	0	0.1582(1)	0.1558	0.049
La2	1(*c*)	2/3	1/3	0.1533(1)	0.1558	-0.049
	2(*i*)					
Nb6	1(*c*)	2/3	1/3	-0.1583(1)	-0.1558	-0.049
Nb1	3(*d*),3(*j*)	0.3334(2)	0.3111(1)	0.0000(1)	0	0
Nb3	3(*d*),3(*k*)	0.3334(2)	0.0306(2)	0.5000(1)	½	0
Nb2	3(*d*)	0.3335(2)	0.0286(2)	0.3117(1)	0.3117	0.001
	6(*l*)					
Nb4	3(*d*)	0.3333(2)	0.0287(2)	-0.3118(1)	-0.3117	0.001
O1	3(*d*),3(*j*)	0.088(1)	0.422(1)	-0.0002(4)	0	0.004
O3	3(*d*),3(*k*)	0.084(1)	0.668(1)	0.5001(5)	½	0.002
O2	3(*d*)	0.084(1)	0.667(1)	0.3061(4)	0.3060	0.003
	6(*l*)					
O4	3(*d*)	0.085(1)	0.666(1)	-0.3058(4)	-0.3060	0.003
O5	3(*d*)	0.392(1)	0.289(1)	-0.0948(3)	-0.0945	0.005
	6(*l*)					
O6	3(*d*)	0.275(1)	0.231(1)	0.0943(3)	0.0945	0.005
O7	3(*d*)	0.279(1)	0.038(1)	0.2083(3)	0.2085	-0.005
	6(*l*)					
O10	3(*d*)	0.389(1)	0.093(1)	-0.2088(4)	-0.2085	0.005
O8	3(*d*)	0.300(1)	0.035(1)	-0.4028(4)	-0.4026	-0.003
	6(*l*)					
O9	3(*d*)	0.367(1)	0.068(1)	0.4025(4)	0.4026	-0.003
O11	1(*a*)	0	0	-0.0217(6)	-0.0221	0.008
O15	1(*c*)	2/3	1/3	0.0225(6)	0.0221	0.008
O12	1(*a*)	0	0	0.3165(6)	0.3167	-0.003
O18	1(*c*)	2/3	1/3	-0.3168(7)	-0.3168	-0.003
O13	1(*a*)	0	0	0.4901(7)	0.4899	0.004
O17	1(*c*)	2/3	1/3	-0.4897(6)	-0.4899	0.004
O14	1(*a*)	0	0	-0.2852(6)	-0.2847	-0.010
O16	1(*c*)	2/3	1/3	0.2842(6)	0.2847	-0.010

$^{\cong}$ $\Delta z = (z^* - z´)c$, with $z^* = z - 0.1533$.

Table 18S *Atomic positions for $MnSb_2O_6$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 8.8056(1), c = 4.7232(1) Å

	Wyckoff position *P*3,*P*321	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
Sb1	3(*d*)	0.69557(3)	0.69557(3)	0.0000(1)	0	0
Sb2	1(*c*)	2/3	1/3	-0.0068	-0.0068	0
Sb4	1(*b*) 2(*d*)	1/3	2/3	0.0068(1)	0.0068	0
Sb3	1(*a*)	0	0	0.5000(1)	½	0
Mn	3(*d*)	0.0001(1)	0.6317(1)	0.4999(2)	½	0.001
O1	3(*d*)	0.7752(3)	0.5545(3)	0.2196(7)	0.2178	0.010
O6	3(*d*) 6(*g*)	0.5545(4)	0.7747(4)	0.7840(8)	-0.2178	0.010
O2	3(*d*)	0.4721(4)	0.5894(4)	0.2293(7)	0.2282	0.005
O5	3(*d*) 6(*g*)	0.8815(4)	0.4091(4)	0.7729(7)	-0.2282	0.005
O3	3(*d*)	0.7876(4)	0.8963(4)	0.2647(8)	0.2632	0.007
O4	3(*d*) 6(*g*)	0.8920(4)	0.1044(4)	0.7383(8)	-0.2632	0.007

$^{\cong}$ $\Delta z = (z^* - z´)c$, with $z^* = z - 0.0068$.

Table 19S *Atomic positions for $Be_2BO_3(OH)(H_2)$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 4.434(1), c = 5.334(2) Å

	Wyckoff position *P*3,*P*321	*x*	*y*	*z*	*z´*	$\Delta z^{\cong}$
B	1(*a*),1(*b*)	0	0	½	½	0
Be1	1(*c*)	2/3	1/3	-0.3915(4)	-0.3972	0.031
Be2	1(*b*) 2(*d*)	1/3	2/3	0.4030(4)	0.3972	0.031
O	3(*d*)	0.3089(1)	-0.0001(2)	½	½	0
OH1	1(*c*)	2/3	1/3	-0.0911(3)	-0.0918	0.035
OH2	1(*b*) 2(*d*)	1/3	2/3	0.0924(3)	0.0918	0.035
H1[A]	3(*d*)	-0.438	0.427	-0.017	-0.018	0.008
H2	3(*d*) 6(*g*)	0.459	-0.444	0.020	0.018	0.008

$^{\cong}$ $\Delta z = (z - z´)c$.

[A] H atoms positions taken from Fourier difference syntheses.

Table 20S *Atomic positions $Zn_7Cu(OH)_{13}SiO(OH)_3SO_4$ with hypothetical z´ coordinates and polar displacements in Å*

a = 8.319(2), c = 7.377(1) Å

	Wyckoff position $P3,P\bar{3}$	x	y	z^*	$z´$	$\Delta z^{\cong}$
Zn1[A]	3(*d*) 6(*g*)	0.1326(1)	0.4136(1)	-0.0014(1)	-0.0005	-0.009
Zn2	3(*d*)	-0.1372(1)	-0.4266(1)	-0.0004(1)	0.0005	-0.009
Zn3	1(*a*) 2(*c*)	0	0	0.2458(3)	0.2451	0.007
Zn4	1(*a*)	0	0	-0.2440(3)	-0.2449	0.007
S	1(*b*) 2(*d*)	1/3	2/3	-0.4109(7)	-0.4012	-0.095
Si	1(*c*)	2/3	1/3	0.3915(9)	0.4012	-0.095
O1	1(*b*) 2(*d*)	1/3	2/3	-0.211(2)	-0.1865	-0.240
O2	1(*c*)	2/3	1/3	0.162(2)	0.1865	-0.240
O3	3(*d*) 6(*g*)	0.1710(8)	-0.3244(8)	-0.4781(9)	-0.4776	-0.005
OH1	3(*d*)	-0.1464(9)	0.334(1)	0.477(1)	0.4776	-0.006
OH2[¶]	1(*a*),1(*b*)	0	0	0.501(3)	½	0
OH3	3(*d*) 6(*g*)	-0.0565(8)	0.1867(8)	0.167(1)	0.1645	0.025
OH4	3(*d*)	0.0523(8)	-0.1954(8)	-0.162(1)	-0.1645	0.025
OH5	3(*d*) 6(*g*)	0.3752(7)	0.4826(8)	0.125(1)	0.1265	-0.015
OH6	3(*d*)	-0.3712(8)	-0.4716(8)	-0.128(1)	-0.1265	-0.015
H1	3(*d*) 6(*g*)	0.347(9)	0.500(9)	0.244(5)	0.2405	0.034
H2	3(*d*)	-0.370(9)	-0.413(9)	-0.237(6)	-0.2405	0.034
H3	3(*d*) 6(*g*)	-0.123(8)	0.248(8)	0.211(8)	0.2415	-0.299
H4	3(*d*)	0.05(1)	-0.252(9)	-0.272(6)	-0.2415	-0.299

[≅] $\Delta z = (z^* - z´)c$, with $z^* = z - 0.0011$.

[A] The Cu present is taken as indistinguishable from Zn, with possible ordering on Zn sites not resolved.

[¶] As given, in 3(*d*) at 0.051, 0.060, 0.500, the site results in 24 O atoms; placing OH2 in 1(*a*) corresponds to the 21 O atom formula.

Table 21S *Atomic positions for $LaTe_{0.75}Ti_{1.25}O_6$ with hypothetical z´ coordinates and polar displacements in Å*

a = 5.141(10), c = 5.218(10) Å

	Wyckoff position *P*3,*P*312	*x*	*y*	z^*	*z´*	$\Delta z^{\cong}$
La	1(*a*),1(*a*)	0	0	-0.0023	0	0.012
Te/Ti1[A]	1(*c*),1(*f*)	2/3	1/3	0.4989(2)	½	-0.006
Ti2	1(*b*),1(*d*)	1/3	2/3	0.5003(4)	½	0.002
O1	3(*d*)	0.6276	0.0027	0.2947(9)	0.2935	0.006
O2	3(*d*) 6(*l*)	0.3807	0.0025	-0.292(2)	-0.2935	0.006

$^{\cong}$ $\Delta z = (z^* - z´)c$, with z^* - 0.0023.

[A] Te occupancy is reported as 75%, Ti1 as 25%.

Table 22S *Atomic positions for $Al_4Ta_3O_{13}(OH)$ at room temperature with hypothetical z´ coordinates and polar displacements in Å*

a = 7.385-7.387(1), c = 4.515-4.516(1) Å

	Wyckoff positions $P3$, $P\bar{3}$ ‡	x	y	z	$z´$	Δz †
Ta	3(d)| 6(g)	0.1118(1)	0.3910(1)	0	-0.248	1.12
Al1	3(d)	0.423(2)	0.303(2)	0.496(2)	0.248	1.12
Al2	1(a), 1(b)	0	0	0.499(4)	½	-0.01
O1	3(d)	0.246(5)	0.062(4)	-0.270(7)	0.272	0.01
O3	3(d) 6(g)	0.192(4)	0.238(5)	0.274(7)	-0.272	0.01
O2	3(d)	0.392(5)	0.472(5)	-0.223(8)	-0.244	0.09
O4	3(d) 6(g)	0.482(5)	0.111(5)	0.265(7)	0.244	0.09
O5	1(c)	1/3	2/3	0.194(9)	0.252	-0.26
O6	1(b) 2d	2/3	1/3	-0.309(10)	-0.252	-0.26

† $\Delta z = (z^* - z´)c$

‡ Coordinates in Wyckoff position 6(g) of space group $P\bar{3}$ are

$x, y, z;\ \bar{y},\ x\text{-}y, z;\ y\text{-}x,\ \bar{x}, z;\ \bar{x},\ \bar{y},\ \bar{z};\ y,\ y\text{-}x,\ \bar{z};\ x\text{-}y, x,\ \bar{z}$.

⌈ Note approximate x,y; $y, y\text{-}x$ relationship for Al1 and Ta. With these atoms at their given locations, zero polarization results if z(Al1) = ½, whereupon Δz(Ta) = 0 and Δz(Al1) = -0.02 Å .