Supplementary Data

Systematic Prediction of New Ferroelectrics in Space Groups $P3_1$ and $P3_2$

Table S1 – S31

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Abstract

Release 2002/2 of the Inorganic Crystal Structure Database contains 62 entries in space group $P3_1$ and 10 in space group $P3_2$ on 49 different materials including 8 families with 2 or more isostructural members. Sixteen new structure types satisfy the structural criteria for ferroelectricity, each with a confidence level that depends necessarily on the reliability of each determination. $LaBGeO_5$, a mineral with stillwellite structure, was previously reported as ferroelectric and forms an additional family with 7 other members or related structures that satisfy the criteria. Ten structures reported in space group $P3_1$ or $P3_2$ are dubious or incorrect with atomic coordinates that satisfy supergroup symmetry. One material is probably pyroelectric but unlikely to become ferroelectric and three others are either incompletely solved or refined. Among the predicted new ferroelectrics are Cu_2BaGeS_4, $Fe_3(Fe,Si)O_4(OH)_5$, Se_4S_5, $K_2HCr_2AsO_{10}$, IV-$RbNO_3$, $Rb_2Sc(NO_3)_5$, Na_3ReO_5, $Nd_{14}(GeO_4)_2(BO_3)_6O_8$, $CsHgCl_3$, $Ba_2Cu_2AlF_{11}$, KYF_4, $SrS_2O_6{\cdot}4H_2O$, $Cu_3PbTeO_6(OH)_2$, $ReH(CO)_4$, $Ni(NH_3)_5Ni(NH_3)_4Mo(CN)_8{\cdot}2H_2O$ and the 6T polytype of $Ca_{1.89}Ta_{1.80}Sm_{0.16}Ti_{0.10}O_7$, in addition to β-$LaBSiO_5$, $PbBAsO_5$ and $BaBAsO_5$ in the stillwellite family.

Table captions

Table S1(*a*). Atomic positions for Cu_2SrSnS_4 at room temperature (Teske, 1976), with hypothetical *x´y´ z´* coordinates and the Δx, Δy, Δz displacements in Å.

Table S1(*b*). Atomic positions for Cu_2SrGeS_4 at room temperature (Teske, 1979) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S1(*c*). Atomic positions for $Cu_2BaGeSe_4$ at room temperature (Tampier & Johrendt, 2001) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S2. Atomic positions in cronstedtite-3T at room temperature (Smrčok *et al.,* 1994) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S3. Atomic positions for S_5Se_4 at room temperature (Geller & Lind, 1970) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{iso} displacements in Å.

Table S4. Atomic positions for $CsNO_3$ in phase II at room temperature (Pohl & Gross, 1993) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S5(*a*). Atomic positions in $(NH_4)_2Tm(NO_3)_5$ at room temperature (Manek & Meyer, 1993*a*) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

Table S5(*b*). Atomic positions for $Rb_2Y(NO_3)_5$ at room temperature (Manek & Meyer, 1993*b*) with hypothetical *z´* coordinates and both polar and u^{33} displacements in Å.

Table S5(*c*). Atomic positions for $Rb_2Sc(NO_3)_5$ at room temperature (Meyer & Stockhause, 1994) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S6. Atomic positions for Na_3ReO_5 at room temperature (Vielhaber & Hoppe, 1992) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S7. Atomic positions in $Nd_{14}(GeO_4)_2(BO_3)_6O_8$ at 295 K (Ilyukhin & Dzhurinskii, 1994) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

Table S8(*a*). Atomic positions for $CsHgCl_3$ at room temperature (Albarski *et al.,* 2000) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

Table S8(*b*). Atomic positions for $Cs_{0.7}(NH_4)_{0.3}HgCl_3$ at room temperature (Kabadou *et al.,* 1998) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

Table S9. Atomic positions for $Ba_2Cu_2AlF_{11}$ at room temperature (Dupont *et al.*, 1998) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and polar u^{33} displacements in Å.

Table S10. Atomic positions for $SrS_2O_6{\cdot}4H_2O$ at room temperature (Fábry, 1995) with hypothetical *x´*, *y´, z´* coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

Table S11. Atomic positions for $Cu_3Pb(TeO_6)(OH)_2$, parakhinite, at room temperature (Burns *et al.,* 1995) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å.

Table S12. Atomic positions for $ReH(CO)_4$ at room temperature (Masciocchi *et al*., 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S13. Atomic positions in $Ni_2(NH_3)_9[Mo(CN)_8]\cdot 2H_2O$ at 153 K (Meske & Babel, 1999) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

Table S14(*a*). Atomic positions for the 6T polytype of $Ca_{1.89}Ta_{1.80}Sm_{0.16}Ti_{0.10}O_7$ at room temperature (Grey & Roth, 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in $Å^2$

Table S14(*b*). As in Table S14(*a*) but with an origin shift of +(⅓, ⅔, 1/6).

Table S15(*a*). Atomic positions for $(Ce,La)BSiO_5$ at room temperature (Callegari *et al.,* 1992) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S15(*b*). Atomic positions for $(Ce,La)BSiO_5$ at room temperature (Burns *et al.,* 1993) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

Table S15(*c*). Atomic positions for $LaBGeO_5$ at room temperature [Kaminskii *et al.*, (1990) and Belokoneva *et al*., (1991)] with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

Table S16(*a*). Atomic positions for $PrBGeO_5$ phase II at 923 K (Belokoneva *et al.,* 1998) with hypothetical z' coordinates and both polar and u_{eq} displacements in Å.

Table S16(*b*). Atomic positions in $PrBGeO_5$ phase III at 293 K (Belonkeva *et al*., 1998) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

Table S17(*a*). Atomic positions for $LaBSiO_5$ at 293 K (Ono *et al*., 1996) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

Table S17(*b*). Atomic positions for $LaBSiO_5$ at room temperature (Samygina *et al.,* 1993) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S17(*c*). Atomic positions for $LaBSiO_5$ at 273 K (Belokonova *et al.,* 1996) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S17(*d*). Atomic positions for $LaBSiO_5$ at 473 K (Belokonova *et al.,* 1996) determined in space group $P3_121$ with u^{33} displacements in Å.

Table S18(*a*). Atomic positions for $LaBSiO_5$ at 296 K (Chi *et al*., 1997) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

Table S18(*b*). Atomic positions for $PbBAsO_5$ at room temperature (Park & Bluhm, 1996*a*) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

Table S18(*c*). Atomic positions for $BaBAsO_5$ at room temperature (Park & Bluhm, 1996*b*) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

Table S19. Atomic positions for $KTlF_4$ at room temperature (Hebecker, 1975) with hypothetical z' x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S20(*a*). Atomic positions for Fe_7Se_8 at room temperature with hypothetical x', y', z' coordinates and Δx, Δy, Δz displacements in Å (Andresen & Leciejewicz, 1964) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S21. Atomic positions for B_2O_3 at room temperature (Gurr *et al.*, 1970) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S22. Atomic positions for mineral combeite, $Na_2Ca_2Si_3O_9$ at room temperature (Fischer & Tillmanns, 1983) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S23. Atomic positions for $Ti_6C_{3+\delta}$ at room temperature (Kukol' *et al.*, 1995) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S24. Atomic positions for $IrGe_4$ at room temperature (Panday & Schubert, 1969) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S25. Atomic positions for Nb_6C_5 at room temperature (Christensen, 1985) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

Table S26. Atomic positions in mineral sheldrickite $NaCa_3(CO_3)_2F_3{\cdot}H_2O$ at room temperature (Grice *et al*., 1997) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S27. Atomic positions for high pressure phase I of ZnTe at room temperature (Kusaba & Weidner, 1994) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S28. Atomic positions in $CaCO_3{\cdot}H_2O$ at room temperature (Effenberger, 1981) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S29. Atomic positions for $Li_7Cu_7Si_5$ at room temperature Pavlyuk *et al*., (1995) with *B* parameters in Å

Table S30. Atomic positions proposed by Pauling & Kamb (1982) for lithiophorite $Li_6Al_{14}(OH)_{42}Mn_{21}O_{42}$ at room temperature.

Table S31. Atomic positions in $K_5CoW_{12}O_{40}{\cdot}20H_2O$ at room temperature (Muncaster *et al.*, 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

Table S1(*a*)
Atomic positions for Cu_2SrSnS_4 at room temperature (Teske, 1976), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 6.290$, $c = 15.578$ Å.† $z^* = z - 0.0814$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz
Cu1	3(*a*)	0.2578(5)	0.2469(5)	0.2560(2)	0.2907	0.3113	0.2554	-0.207	-0.405	0.009
	6(*c*)‡									
Cu2	3(*a*)	-0.3235(5)	0.0849(5)	0.0786(2)	-0.2907	0.0206	0.0779	-0.207	0.404	0.011
Sn	3(*a*),3(*a*)	⅓	0.3736(1)	-0.0000(2)	0.3535	0.3535	0	-0.127	0.126	0.000
Sr	3(*a*),3(*b*)	-0.1065(5)	⅔	0.1686	0	~0.6667	1/6	-0.670	~0	0.030
S2	3(*a*)	-0.1219(1)	0.1735(8)	0.2129(3)	-0.2461	0.0426	0.2137	0.781	0.823	-0.012
	6(*c*)									
S1	3(*a*)	0.3702(7)	0.1578(7)	0.1189(3)	0.2461	0.2887	0.1196	0.781	-0.823	-0.011
S3	3(*a*)	0.9827(7)	0.4284(7)	-0.0021(3)	0.8808	0.5561	-0.0012	0.641	-0.803	-0.014
	6(*c*)									
S4	3(*a*)	0.6838(7)	0.7789(7)	0.0003(3)	0.5561	0.8808	0.0012	0.803	-0.641	-0.014

† Lattice parameter uncertainties and thermal/static displacements u^{ij} not given.

‡ See footnote 1 for equivalent positions in space- and supergroup.

Table S1(*b*)
Atomic positions for Cu_2SrGeS_4 at room temperature (Teske, 1979) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

$a = 6.143$, $c = 15.282$ Å.† $z^* = -(z + 0.0837)$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_2$,$P3_221$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Cu1	3(a)	0.2539(5)	0.2554(5)	0.7439(2)	0.2936	0.3132	0.7441	-0.232	0.562	-0.003	0.13
Cu2	6(c) 3(a)	-⅓	0.0774(4)	0.9223(2)	-0.2936	0.0196	0.9225	-0.232	-0.562	-0.003	0.13
Ge	3(a),3(a)	0.3333	0.3824(2)	0.0001(2)	0.3579	0.3579	0	-0.147	0.147	0.002	0.08
Sr	3(a),3(b)	-0.1133(2)	⅔	0.8337	0	0.6667	⅚	-0.639	0	0.006	0.10
S1	3(a)	0.3765(8)	0.1790(8)	0.8858(3)	0.2627	0.2979	0.8858	0.699	-0.730	0	0.08
S2	6(c) 3(a)	-0.1489(7)	0.1541(7)	0.7809(3)	-0.2627	0.0352	0.7809	0.699	0.730	0	0.05
S3	3(a)	0.0006(7)	0.4325(7)	0.9962(3)	-0.1168	0.5503	0.9961	0.721	-0.724	0.001	0.11
S4	6(c) 3(a)	0.6680(7)	0.7658(7)	0.0039(3)	0.5503	0.8832	0.0039	0.723	-0.721	0.001	0.10

† Uncertainties not given.

Table S1(*c*)
Atomic positions for $Cu_2BaGeSe_4$ at room temperature (Tampier & Johrendt, 2001) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

a = 6.490(1), c = 16.355(3) Å with $z^* = -(z + 0.0837)$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Cu1†	3(*a*)	0.2534(4)	0.2477(4)	0.7566(1)	0.2908	0.3116	0.7566	-0.243	-0.417	0.000	0.13
Cu2	6(*c*) 3(*a*)	0.6719(4)	0.0853(4)	0.5766(1)	-0.2908	0.0208	0.5766	-0.242	0.417	0.000	0.13
Ge	3(*a*),3(*b*)	0.3333(3)	0.3824(3)	0.4997(1)	0.3579	0.3579	½	-0.159	0.159	-0.005	0.08
Ba	3(*a*),3(*a*)	-0.1164(2)	0.6668(1)	0.6667	0	0.6668	⅔	0.755	-0.002	0.006	0.10
Se1	3(*a*)	0.3002(3)	0.1445(3)	0.3853(1)	0.2390	0.2556	0.3858	0.397	-0.721	-0.008	0.08
Se2	6(*c*) 3(*a*)	0.3666(3)	0.1777(3)	0.6137(1)	0.2556	0.2390	0.6142	0.720	-0.398	-0.008	0.05
Se3	3(*a*)	0.9998(3)	0.4341(3)	0.5038(1)	0.8839	0.5506	0.5044	0.752	-0.756	-0.010	0.11
S4	6(*c*) 3(*a*)	0.6671(3)	0.7680(3)	0.4950(1)	0.5506	0.8839	0.4956	0.756	-0.752	-0.010	0.10

† Atom numbering in equivalent positions corresponding to Cu_2SrGeS_4 in Table S1(*b*).

Table S2

Atomic positions in cronstedtite-3T at room temperature (Smrčok *et al.,* 1994) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

$a = 5.497(2)$, $c = 21.355(7)$ Å with $z^* = z + 0.02011$, $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1,P3_212$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Fe1†	3(*a*),3(*b*)	0.8909(2)	0.1132(5)	0.18511	0.8889	0.1111	1/6	0.01	0.01	0.39	0.16
Fe2	3(*a*),3(*b*)	0.2258(2)	0.7784(4)	0.18346(6)	0.2237	0.7763	1/6	0.01	0.01	0.36	0.16
Fe3	3(*a*),3(*b*)	0.5607(2)	0.4481(4)	0.18352(6)	0.5563	0.4437	1/6	0.02	0.02	0.36	0.16
Si1/Fe	3(*a*),3(*a*)	0.8915(5)	0.4447(6)	0.05169(7)	0.8908	0.4454	0	0.01	-0.01	1.10	0.13
Si2/Fe	3(*a*),3(*a*)	1.5564(2)	0.7781(2)	0.05169(7)	1.5563	0.7782	0	0.00	-0.00	1.10	0.12
O1	3(*a*)	0.784(1)	0.112(1)	0.0262(3)	0.836	0.277	0.0639	-0.29	-0.90	-0.80	0.16
OH2	6(*c*) 3(*a*)	0.558(1)	0.112(1)	0.2317(2)	0.723	0.164	0.2694	-0.91	-0.29	-0.80	0.12
O2	3(*a*),3(*a*)	1.224(1)	0.672(1)	0.0270(3)	1.264	0.632	0	-0.22	0.22	0.58	0.16
O3	3(*a*)	0.664(1)	0.550(1)	0.0263(3)	0.611	0.664	0.0639	0.29	-0.62	-0.80	0.16
OH3	6(*c*) 3(*a*)	0.223(1)	0.442(1)	0.2317(3)	0.336	0.389	0.2694	-0.62	0.29	-0.80	0.17
OH1	3(*a*)	0.221(1)	0.113(1)	0.1352(2)	0.220	0.111	0.1185	0.01	0.01	0.36	0.17
OH4	6(*c*) 3(*a*)	0.892(1)	0.781(1)	0.2315(2)	0.889	0.780	0.2148	0.02	0.01	0.36	0.13
O4	3(*a*)	-0.109(1)	0.441(1)	0.1340(2)	0.055	0.440	0.1672	-0.90	0.01	-0.71	0.17
O5	6(*c*) 3(*a*)	0.562(1)	-0.218(1)	0.1329(2)	0.560	-0.055	0.1661	0.01	-0.90	-0.71	0.17

† Occupancies: Fe1, 1.048(9); Fe2, 1.040(9); Fe3, 1.033(9);

Si1/Fe, 0.75(1) Si + 0.25 Fe; Si2/Fe, 0.76(1) + 0.24 Fe.

Table S3

Atomic positions for S_5Se_4 at room temperature (Geller & Lind, 1970) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 7.85(1), c = 4.62(1) Å with $z^* = z + 0.3788$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_112$	Site occupancy S/Se	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
S/Se1	3(*a*),3(*a*)	0.40/0.60	0.001(1)	0.121(1)	0.378	-0.061	0.061	⅓	0.48	0.48	0.21	0.26
S/Se2	3(*a*) 6(*c*)†	0.167/0.083	0.667(1)	0.453(1)	0.270(8)	0.667	0.453	0.251	0.00	0.00	0.09	0.27
S/Se4	3(*a*)	0.167/0.083	0.547(1)	0.333(1)	0.436(8)	0.547	0.333	0.417	0.00	0.00	0.09	0.27
S/Se3	3(*a*) 6(*c*)	0.167/0.083	0.597(1)	0.403(1)	0.353(8)	0.563	0.351	0.417	0.27	0.41	-0.06	0.27
S/Se5	3(*a*)	0.167/0.083	0.528(1)	0.264(1)	0.520(8)	0.563	0.212	0.583	-0.27	0.41	-0.06	0.27
S/Se6	3(*a*),3(*b*)	0.60/0.40	0.460(1)	0.780(1)	0.208(8)	0.413	0.827	$^1/_6$	0.37	-0.37	0.19	0.27

† See footnote 1 for equivalent positions in space- and supergroup.

Table S4
Atomic positions for $CsNO_3$ in phase II at room temperature (Pohl & Gross, 1993) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 10.902(2), c = 7.740(2) Å, with $z^* = z - 0.1523$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Cs1	3(*a*),3(*b*)	0.4481(1)	0.5557(1)	0.5004(3)	0.5019	0.5019	½	-0.59	0.59	0.01	0.17
Cs2	3(*a*)	0.1205(1)	0.2220(1)	-0.1523	0.1683	0.3093	-0.1500	-0.52	-0.95	-0.02	0.17
	6(*c*)										
Cs3	3(*a*)	-0.2161(1)	0.2282(1)	0.4810(1)	-0.1683	0.1410	0.4833	-0.52	0.95	-0.02	0.17
N1	3(*a*),3(*a*)	0.4629(7)	0.5933(7)	0.009(2)	0.5281	0.5281	0	-0.71	0.71	0.07	0.18
N2	3(*a*)	0.1085(7)	0.2034(7)	0.379(1)	0.1688	0.3034	0.378	-0.66	-1.09	0.01	0.16
	6(*c*)										
N3	3(*a*)	-0.2290(9)	0.2345(7)	-0.043(2)	-0.1688	0.1345	-0.044	-0.66	1.09	0.01	0.20
O1	3(*a*)	0.4417(7)	0.6650(8)	0.115(1)	0.3324	0.6669	0.123	1.19	-0.02	-0.06	0.23
	6(*c*)										
O9	3(*a*)	0.6689(6)	0.2231(6)	-0.131(1)	0.6669	0.3324	-0.123	0.02	-1.19	-0.06	0.21
O2	3(*a*)	0.4004(10)	0.4650(7)	0.015(2)	0.5305	0.5080	0.061	-1.42	-0.47	-0.36	0.31
	6(*c*)										
O3	3(*a*)	0.5510(7)	0.6605(8)	-0.107(1)	0.5080	0.5305	-0.061	0.47	1.42	-0.36	0.23
O4	3(*a*),3(*b*)	0.0045(6)	0.1134(6)	-0.540(1)	0.0590	0.0590	½	-0.59	0.59	-0.31	0.20
O5	3(*a*),3(*b*)	0.2265(5)	0.2314(7)	-0.579(1)	0.2290	0.2289	½	-0.03	0.02	-0.61	0.25
O6	3(*a*)	0.0828(10)	0.2565(8)	0.250(1)	0.0951	0.3368	0.344	-0.13	-0.88	-0.73	0.28
	6(*c*)										
O8	3(*a*)	-0.1073(7)	0.3216(7)	-0.104(1)	-0.0951	0.2417	-0.010	-0.13	0.87	-0.73	0.25
O7	3(*a*),3(*a*)	-0.2474(13)	0.1638(9)	0.079(1)	-0.2056	0.2056	0	-0.46	-0.46	0.61	0.31

Table S5(*a*)
Atomic positions in $(NH_4)_2Tm(NO_3)_5$ at room temperature (Manek & Meyer, 1993*a*) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 11.2376(8), c = 9.301(1) Å, with $z^* = z + 0.1979$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_12$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Tm	3(*a*),3(*a*)	0.6634(1)	0.9965(1)	0.3398	0.6634	0	⅓	0	-0.04	0.06	0.18
N(H_4)1	3(*a*)	0.6032(9)	0.669(1)	0.676(1)	0.6364	0.730	0.749	-0.37	-0.68	-0.68	0.24
	6(*c*)										
N(H_4)2	3(*a*)	0.7905(7)	0.6695(8)	0.177(1)	0.7298	0.6364	0.251	0.68	0.37	-0.69	0.26
N1	3(*a*)	0.594(1)	0.029(1)	0.631(1)	0.679	0.049	0.622	-0.96	-0.23	0.08	0.23
	6(*c*)										
N3	3(*a*)	0.070(1)	0.764(1)	0.387(1)	0.049	0.679	0.378	0.24	-0.96	0.02	0.14
O1	3(*a*)	0.9983(7)	0.5115(6)	0.859(1)	0.022	0.5994	0.887	-0.25	-0.99	-0.26	0.23
	6(*c*)										
O7	3(*a*)	0.958(1)	0.6652(9)	0.4192(1)	-0.022	0.5773	0.446	-0.25	0.99	-0.25	0.11
O2	3(*a*)	0.962(1)	0.666(1)	0.921(1)	0.905	0.696	0.883	0.64	-0.34	0.35	0.33
	6(*c*)										
O8	3(*a*)	0.1518(7)	0.8212(6)	0.489(1)	0.095	0.851	0.450	0.64	-0.34	0.36	0.22
O3	3(*a*)	0.9580(9)	0.5238(9)	0.084(1)	0.8828	0.6159	0.077	0.85	-1.04	0.07	0.18
	6(*c*)										
O9	3(*a*)	0.1916(9)	0.2921(9)	0.5966(9)	0.2668	0.3841	0.590	-0.85	-1.04	0.06	0.21
N2	3(*a*),3(*a*)	0.915(1)	0.999(1)	0.4039(9)	0.915	0	⅓	0	0.01	0.66	0.19
O4	3(*a*)	0.1127(8)	0.912(1)	0.749(1)	0.1079	0.910	0.691	0.05	0.02	0.54	0.24
	6(*c*)										
O5	3(*a*)	0.8970(9)	0.8003(8)	0.699(1)	0.8921	0.798	0.642	0.06	0.02	0.53	0.25
O6	3(*a*),3(*a*)	0.9927(8)	0.0198(7)	0.755(1)	0	0.0198	⅔	-0.08	0	0.82	0.27
N4	3(*a*)	0.7524(9)	0.4193(9)	0.609(1)	0.7504	0.4184	0.634	0.02	0.01	-0.23	0.24
	6(*c*)										
N5	3(*a*)	0.330(1)	0.5825(9)	0.009(1)	0.332	0.5816	0.033	-0.02	0.01	-0.22	0.22
O10	3(*a*)	0.7602(9)	0.5321(8)	0.655(1)	0.7560	0.4208	0.657	0.05	1.25	-0.02	0.26
	6(*c*)										
O15	3(*a*)	0.331(2)	0.6906(9)	0.007(1)	0.335	0.5792	0.009	-0.05	1.25	-0.02	0.24
O11	3(*a*)	0.866(1)	0.422(1)	0.599(1)	0.859	0.432	0.665	0.08	0.11	-0.61	0.29
	6(*c*)										
O13	3(*a*)	0.1483(9)	0.5820(9)	0.603(1)	0.1412	0.573	0.668	0.08	0.10	-0.61	0.24
O12	3(*a*)	0.6855(7)	0.3263(9)	0.925(1)	0.5829	0.2877	0.922	1.15	0.43	0.03	0.25
	6(*c*)										
O14	3(*a*)	0.2491(9)	0.4802(9)	0.082(1)	0.2877	0.5829	0.078	-0.43	-1.15	0.04	0.24

Table S5(*b*)
Atomic positions for $Rb_2Y(NO_3)_5$ at room temperature (Manek & Meyer, 1993*b*) with hypothetical x', y', z' coordinates and both polar and u^{33} displacements in Å

a = 11.2376(8), c = 9.301(1) Å with $z^* = z$ - 0.0350 and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Rb1‡	3(*a*),3(*b*)	0.6673(3)	0.0622(2)	0.7582(3)	0.6673	0	5/6	0	0.70	-0.70	0.25
Rb2	3(*a*)	0.2049(2)	0.3332(9)	0.9251(3)	0.1062	0.3370	0.9173	1.11	-0.04	0.77	0.22
	6(*c*)										
Y	3(*a*)	0.3408(2)	0.0075(2)	0.0905(0)	0.3370	0.1062	0.0827	0.04	-1.11	0.77	0.18
N1	3(*a*)	0.247(1)	0.583(1)	0.358(2)	0.332	0.584	0.296	-0.95	-0.01	0.58	0.21
	6(*c*)										
N5	3(*a*)	0.584(2)	0.253(2)	0.099(2)	0.668	0.252	0.037	-0.95	0.01	0.58	0.26
N2	3(*a*),3(*b*)	0.084(2)	0.003(1)	0.160(1)	0	0.003	1/6	0.94	0	-0.06	0.21
N3	3(*a*),3(*b*)	0.308(2)	0.076(1)	0.805(2)	0.308	0	5/6	0	0.85	-0.26	0.23
N4	3(*a*),3(*a*)	0.026(2)	0.433(1)	0.713(2)	0	0.433	⅔	0.29	0	0.43	0.22
O1	3(*a*)	0.417(1)	0.550(1)	0.686(1)	0.498	0.535	0.760	-0.91	0.17	-0.69	0.24
	6(*c*)										
O12	3(*a*)	0.044(1)	0.480(1)	0.834(1)	-0.037	0.465	0.907	0.91	0.17	-0.68	0.29
O2	3(*a*)	0.234(1)	0.765(1)	0.064(1)	0.298	0.730	-0.019	-0.72	0.39	0.77	0.22
	6(*c*)										
O15	3(*a*)	0.694(2)	0.361(2)	0.103(2)	0.730	0.298	0.019	-0.40	0.71	0.78	0.37
O3	3(*a*)	0.332(1)	0.645(1)	0.008(1)	0.261	0.609	-0.007	0.80	0.40	0.14	0.25
	6(*c*)										
O14	3(*a*)	0.580(8)	0.427(1)	0.689(1)	0.652	0.391	0.674	-0.81	0.40	0.14	0.26
O4	3(*a*)	0.200(1)	0.114(1)	0.167(9)	0.180	0.224	0.129	0.22	-1.23	0.35	0.24
	6(*c*)										
O7	3(*a*)	0.333(1)	0.160(1)	-0.091(1)	0.224	0.180	-0.129	1.23	-0.22	0.35	0.22
O5	3(*a*)	0.094(1)	0.899(1)	0.121(1)	0.142	0.898	0.052	-0.54	0.01	0.64	0.23
	6(*c*)										
O9	3(*a*)	0.293(1)	0.104(1)	0.685(1)	0.245	0.103	0.615	0.54	0.01	0.65	0.24
O6	3(*a*),3(*b*)	0.002(2)	0.980(1)	0.517(2)	0	0	½	0.02	-0.22	0.16	0.29
O8	3(*a*)	0.305(2)	-0.032(1)	0.840(1)	0.153	-0.193	0.779	1.71	1.81	0.57	0.25
	6(*c*)										
O11	3(*a*)	-0.001(1)	-0.507(1)	0.616(1)	-0.153	-0.346	0.555	1.71	-1.81	0.57	0.24
O10	3(*a*)	0.029(2)	0.323(1)	0.685(1)	0.135	0.353	0.759	-1.19	-0.38	-0.69	0.26
	6(*c*)										
O13	3(*a*)	-0.240(1)	0.247(2)	0.500(2)	-0.135	0.217	0.574	-1.18	0.38	-0.69	0.25

‡ Rb1, Rb2 and Y coordinates presented in equivalent locations for comparison with Table 6S(*a*).

Table S5(*c*)
Atomic positions for $Rb_2Sc(NO_3)_5$ at room temperature (Meyer & Stockhause, 1994) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 11.034(1), c = 9.474(1) Å, $z^* = z$ - 0.0098 with $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_112$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Sc	3(*a*) 6(*c*)	0.6669(3)	0.0154(2)	0.4905	0.6668	0.0328	0.4991	0.01	-0.19	-0.08	0.23
Rb2	3(*a*)	0.9499(2)	0.3334(2)	0.1590	0.9672	0.3332	0.1676	-0.19	0.01	-0.08	0.29
Rb1	3(*a*),3(*a*)	1.6666(1)	0.8026(9)	-0.0098	1.6461	0.8231	0	0.23	-0.23	-0.09	0.24
N1	3(*a*) 6(*c*)	0.4145(9)	0.4338(9)	0.884	0.5008	0.3434	0.864	-0.95	0.99	0.19	0.24
N3	3(*a*)	0.747(1)	0.413(1)	0.823	0.6566	0.4992	0.803	0.99	-0.95	0.19	0.20
N2	3(*a*) 6(*c*)	-0.0821(8)	0.6861(8)	0.0979	0.1058	0.6379	0.1067	-2.07	0.53	-0.08	0.16
N5	3(*a*)	0.3442(9)	0.5896(9)	0.2179	0.5321	0.6379	0.2266	-2.07	-0.53	-0.08	0.23
N4	3(*a*),3(*b*)	0.0891(9)	0.0779(9)	0.0949	0.056	0.1112	1/6	0.36	-0.37	-0.68	0.20
O1	3(*a*) 6(*c*)	0.4899(7)	0.4952(7)	-0.0099	0.5039	0.5258	-0.0542	-0.15	-0.34	0.42	0.26
O3	3(*a*)	0.4436(8)	0.4821(8)	0.7653	0.4742	0.4961	0.7209	-0.34	-0.15	0.42	0.20
O2	3(*a*) 6(*c*)	0.3049(8)	0.3206(7)	-0.0876	0.1603	0.3330	-0.0779	1.60	-0.14	-0.08	0.26
O4	3(*a*)	0.3174 (7)	0.3454(7)	0.4015	0.1728	0.3330	0.4112	1.60	0.14	-0.08	0.28
O5	3(*a*) 6(*c*)	-0.1567(7)	0.6715(7)	-0.0078	-0.1707	0.6961	0.0558	0.15	-0.27	-0.60	0.21
O6	3(*a*)	0.8153(8)	0.1087(8)	-0.1195	0.8293	0.1333	-0.0558	-0.15	-0.27	-0.60	0.18
O7	3(*a*) 6(*c*)	0.7685(7)	0.5193(9)	-0.2523	0.6667	0.3848	-0.2425	1.12	1.48	-0.09	0.23
O8	3(*a*)	0.5648(7)	0.4164(8)	0.2326	0.6667	0.2819	0.2424	-1.12	1.48	-0.09	0.26
O9	3(*a*),3(*a*)	0.6399(8)	1.3071(9)	0.5988	0.6490	1.2980	⅔	-0.10	0.10	-0.64	0.31
O10	3(*a*) 6(*c*)	0.1224(8)	0.2023(7)	0.1367	0.0740	0.1227	0.1962	0.53	0.88	-0.56	0.29
O12	3(*a*)	0.0256(9)	0.0309(8)	-0.2556	0.0740	-0.0487	-0.1962	-0.53	0.88	-0.56	0.27
O11	3(*a*),3(*a*)	0.8679(8)	1.8139(9)	0.745	0.8939	1.7879	⅔	-0.29	0.29	0.74	0.28
O15	3(*a*),3(*a*)	1.3644(8)	0.693(1)	-0.098	1.3716	0.6858	0	-0.08	0.08	-0.93	0.32
O13	3(*a*),3(*a*)	0.2550(8)	0.4657(7)	0.1755	0.2402	0.4804	1/6	0.16	-0.16	0.08	0.28
O14	3(*a*),3(*a*)	1.1486(9)	0.5381(8)	-0.099	1.1245	0.5622	0	0.27	-0.27	-0.94	0.26

Table S6

Atomic positions for Na_3ReO_5 at room temperature (Vielhaber & Hoppe, 1992) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 5.544(1), c = 13.580(7) Å, with $z^* = z - 0.0042$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Re	3(*a*),3(*a*)	0.7092(2)	0.0417(2)	0.333	0.7092	0	⅓	0	0.23	0	0.11
Na1	3(*a*),3(*b*)	0.623(4)	0.941(3)	0.834(2)	0.623	0	0.833	0	-0.33	0.01	0.17
Na3	3(*a*) 6(*c*)	0.405(3)	0.372(3)	0.748 (2)	0.349	0.325	0.751	0.31	0.26	-0.04	0.18
Na2	3(*a*)	0.277(3)	0.293(3)	0.246(1)	0.325	0.349	0.249	-0.27	-0.31	-0.04	0.14
O1	3(*a*) 6(*c*)	0.492(4)	0.513(4)	0.896(2)	0.452	0.590	0.915	0.22	-0.43	-0.26	0.17
O5	3(*a*)	-0.177(4)	0.334(4)	0.732(1)	-0.137	0.410	0.751	-0.22	-0.42	-0.26	0.09
O2	3(*a*),3(*a*)	0.171(4)	0.830(4)	0.774(2)	0	0.830	⅔	0.95	0	1.45	0.13
O3	3(*a*) 6(*c*)	0.848(4)	0.851(4)	0.270(2)	0.810	0.744	0.301	0.21	0.59	-0.42	0.19
O4	3(*a*)	0.028(4)	0.364(3)	0.335(2)	0.066	0.256	0.366	-0.21	-0.59	-0.42	0.15

Table S7

Atomic positions in $Nd_{14}(GeO_4)_2(BO_3)_6O_8$ at 295 K (Ilyukhin & Dzhurinskii, 1994) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 9.945(3), c = 25.992(7) Å with $z^* = z - 0.0122$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Nd1	3(*a*)	0.1487(2)	0.7674(5)	0.1022	0.1184	0.7152	0.1120	0.30	0.52	-0.25	0.06
	6(*c*)										
Nd7	3(*a*)	-0.0881(2)	0.5446(2)	0.2115(1)	-0.1184	0.5968	0.2213	0.30	-0.52	-0.25	0.08
Nd2	3(*a*)	0.0643(2)	0.3274(2)	0.2852(1)	0.0360	0.3519	0.2670	-0.28	-0.24	0.32	0.08
	6(*c*)										
Nd11	3(*a*)	-0.0077(2)	0.3404(2)	0.0786(1)	-0.0360	0.3159	0.0664	-0.28	0.24	0.32	0.07
Nd3	3(*a*)	-0.1181(2)	0.9293(2)	0.0955(1)	-0.1428	-0.0999	0.1079	0.25	0.29	-0.32	0.10
	6(*c*)										
Nd5	3(*a*)	0.1674(2)	0.0136(2)	0.2130(1)	0.1428	0.0429	0.2254	0.25	-0.29	-0.32	0.06
Nd4	3(*a*)	0.5928(2)	0.1164(2)	0.2884(1)	0.5834	0.1543	0.2773	0.09	-0.38	0.29	0.08
					0.5804	0.1526	0.2674	0.12	-0.36	0.55	
	6(*c*)										
Nd14	3(*a*)†	0.4259(3)	-0.3912(2)	0.0672(4)	0.4166	-0.4291	0.0561	0.09	0.38	0.29	0.06
Nd14′		0.4319(6)	-0.3915(6)	0.0870(6)	0.4196	-0.4277	0.0659	0.12	0.36	0.55	0.04
Nd6	3(*a*)	0.3627(2)	0.7354(2)	0.2164(1)	0.3248	0.7695	0.2319	0.38	-0.34	-0.40	0.08
	6(*c*)										
Nd9	3(*a*)	-0.2868(2)	0.4788(2)	0.0860(1)	-0.3248	0.4447	0.1015	0.38	0.34	-0.40	0.07
Nd8	3(*a*)	0.7882(2)	0.8628(2)	0.2862(1)	0.7544	0.8988	0.2766	0.34	-0.35	0.25	0.07
	6(*c*)										
Nd12	3(*a*)	0.2793(2)	0.1803(2)	0.0664(1)	0.2456	0.1444	0.0568	0.34	0.35	0.25	0.06
Nd10	3(*a*)	0.4828(2)	0.4147(2)	0.2507(2)	0.4694	0.4498	0.2525	0.13	-0.35	-0.05	0.07
	6(*c*)										
Nd13	3(*a*)	0.5440(2)	0.0155(2)	0.0791(2)	0.5306	-0.0196	0.0809	0.13	0.35	-0.05	0.09
Ge1	3(*a*)	0.1366(3)	-0.2253(3)	0.3050(2)	0.1192	-0.2112	0.3048	-0.30	0.21	0.01	0.07
	6(*c*)										
Ge2	3(*a*)‡	-0.1970(3)	0.1018(3)	0.6955(2)	-0.2112	0.1192	0.6952	-0.30	0.21	0.01	0.06
O1	3(*a*)	0.140(2)	-0.223(2)	0.374(1)	0.081	-0.174	0.3737	0.59	0.49	0.01	0.07
	6(*c*)										
O23	3(*a*)	-0.022(2)	-0.206(2)	-0.0401(9)	-0.081	-0.255	-0.0404	-0.59	0.49	0.01	0.12
O2	3(*a*)	0.001(3)	-0.182(3)	0.278(1)	0.041	-0.198	0.279	-0.40	0.16	0.04	0.11
	6(*c*)										
O21	3(*a*)	-0.081(2)	-0.255(2)	0.0519(9)	-0.041	-0.239	0.054	-0.40	0.16	-0.04	0.06

O3	3(*a*)	0.323(3)	-0.095(3)	0.283(1)	0.342	-0.040	0.247	-0.19	-0.55	0.94	0.14
					0.314	-0.047	0.247	0.09	-0.48	0.94	0.14
	6(*c*)										
O24	}	-0.361(4)	0.673(4)	0.122(1)	-0.342	0.618	0.086	-0.19	0.55	0.94	0.37
O24′	} 3(*a*)††	-0.304(5)	0.687(5)	0.123(1)	-0.314	0.639	0.087	0.10	0.48	0.94	0.37
O4	3(*a*)	0.078(2)	0.583(2)	0.2873(9)	0.142	0.638	0.3141	-0.64	-0.55	0.70	0.09
	6(*c*)										
O22	3(*a*)	-0.207(3)	-0.449(2)	-0.0078(7)	-0.142	-0.504	0.0190	-0.64	0.55	0.70	0.05
O5	3(*a*)	-0.205(3)	0.112(3)	0.1258(1)	-0.235	0.084	0.1321	0.30	0.28	-0.16	0.14
	6(*c*)										
O17	3(*a*)	0.265(3)	0.291(3)	0.195(1)	0.235	0.319	0.2012	0.30	0.28	-0.16.	0.16
O6	3(*a*)	0.619(3)	-0.043(3)	0.220(1)	0.694	0.016	0.219	0.75	-0.59	0.03	0.12
	6(*c*)										
O16	3(*a*)	-0.769(2)	0.382(2)	0.116(1)	-0.694	0.322	0.115	-0.75	0.59	0.03	0.11
O7	3(*a*)	0.840(21)	0.278(2)	0.2230(8)	0.836	0.286	0.181	0.04	0.08	1.09	0.08
	6(*c*)										
O15	3(*a*)	-0.832(4)	0.458(3)	0.194(1)	-0.836	0.450	0.152	0.04	0.08	1.09	0.19
O8	3(*a*)	0.949(3)	0.057(3)	0.216(1)	0.917	-0.022	0.213	0.32	0.79	0.08	0.14
	6(*c*)										
O34	3(*a*)	-0.885(2)	0.981(2)	0.1233(8)	-0.917	0.061	0.120	0.32	0.79	0.08	0.03
O9	3(*a*)	0.526(2)	0.785(2)	0.314(1)	0.513	0.748	0.262	0.13	0.49	1.34	0.12
	6(*c*)										
O12	3(*a*)	0.501(3)	0.198(3)	0.1220(9)	0.513	0.235	0.071	-0.12	-0.48	1.34	0.10
O10	3(*a*)	0.345(3)	0.532(2)	0.288(1)	0.308	0.551	0.290	-0.41	0.17	-0.05	0.10
	6(*c*)										
O18	3(*a*)	-0.270(3)	0.262(3)	0.0417(9)	-0.308	0.243	0.0432	0.19	0.56	-0.04	0.09
O11	3(*a*)	0.407(3)	0.592(3)	0.377(1)	0.359	0.611	0.379	0.48	-0.19	-0.06	0.15
	6(*c*)										
O20	3(*a*)	-0.310(2)	0.272(2)	-0.0489(7)	-0.359	0.253	-0.046	0.49	0.19	-0.06	0.03
O13	3(*a*)	0.640(3)	0.400(3)	0.177(1)	0.621	0.407	0.193	0.19	-0.07	-0.42	0.13
	6(*c*)										
O32	3(*a*)	-0.601(3)	0.792(3)	0.124(1)	-0.621	0.786	0.140	0.19	0.06	-0.42	0.09
O14	3(*a*)	0.453(2)	0.170(2)	0.2151(9)	0.440	0.134	0.168	0.13	0.36	1.22	0.09
					0.473	0.125	0.184	-0.20	0.45	0.80	
	6(*c*)										
O25	}	-0.427(4)	0.658(5)	0.213(2)	-0.440	0.694	0.166	-0.13	-0.36	1.22	0.09
O25′	} 3(*a*)††	-0.492(5)	0.606(7)	0.180(3)	-0.473	0.652	0.149	-0.19	-0.46	0.81	0.20
O19	3(*a*)	-0.062(2)	0.343(2)	-0.0141(7)	-0.051	0.328	-0.028	-0.11	0.13	0.36	0.00
	6(*c*)										
O29	3(*a*)	0.312(3)	0.960(3)	0.042(1)	0.328	-0.051	0.028	-0.11	0.13	0.36	0.09

O26	3(*a*)††	-0.166(4)	0.728(4)	0.176(2)	-0.054	0.593	0.194	-1.11	1.34	-0.48	0.09
O26′		-0.248(7)	0.679(7)	0.216(2)	-0.095	0.548	0.214	-1.52	1.30	0.04	0.17
O33	6(*c*) 3(*a*)	-0.058(2)	0.511(2)	0.1196(8)	0.054	0.647	0.139	-1.11	-1.35	-0.48	0.000
					0.095	0.643	0.119	-1.52	-1.31	0.04	
O27	3(*a*)	0.151(2)	-0.232(2)	0.689(1)‡	0.127	-0.205	0.689	0.24	-0.26	0.00	0.06
O28	6(*c*) 3(*a*)	-0.177(2)	0.103(2)	0.311(1)	-0.205	0.127	0.311	0.24	-0.24	0.00	0.08
O30	3(*a*)	0.002(3)‡	-0.073(3)‡	0.052(1)	0.074	-0.022	0.005	-0.72	-0.51	1.22	0.23
O31	6(*c*) 3(*a*)	0.030(3)	0.147(3)	0.042(1)	-0.022	0.074	-0.005	0.52	-0.73	1.22	0.11
B1	3(*a*)	0.428(3)	0.632(3)	0.827(1)‡	0.337	0.580	-0.172	0.90	0.52	-0.01	0.10
B2	6(*c*) 3(*a*)	0.527(3)	0.247(3)	0.172(3)	0.580	0.337	0.172	-0.53	-0.90	-0.01	0.09
B3	3(*a*)	0.221(4)	0.377(4)	0.668(1)‡	0.227	0.336	0.667	-0.06	0.41	0.03	0.11
B5	6(*c*) 3(*a*)	-0.103(3)	0.704(3)	0.001(1)	-0.109	0.664	0.000	0.06	0.40	0.03	0.08
B4	3(*a*)	-0.218(3)	0.291(3)	0.4925(9)‡	-0.291	0.308	0.4924	0.73	-0.17	0.01	0.06
B6	6(*c*) 3(*a*)	-0.328(3)	0.675(5)	0.174(1)	0.599	0.692	0.174	0.73	-1.17	0.01	0.13

† Nd14 occupancy, 63(3)%; Nd14′, 37(3)%. Atomic numbering at partially occupied sites differs from that in the original report.

‡ Reported z(Ge2) replaced by ½ + z; z(O27) by ½ + z; x(O30) by ½ + x, y(O30) by ½ + y z(B1) by ½ + z, z(B3) by ½ + z and z(B4) by ½ + z.

†† O24-O26, O24′ - O26′ each reported with 50% occupancy, see also first footnote above.

Table S8(*a*)
Atomic positions for $CsHgCl_3$ at room temperature (Albarski *et al.,* 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 13.287(1), c = 9.4081(4) Å, with $z^* = z + 0.52031$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_2,P3_212$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Cs1‡	3(*a*),3(*a*)	0.22689(15)	0.10862(18)	0.0177(3)	0.22367	0.11184	0	0.04	-0.04	0.17	0.24
Cs3	3(*a*),3(*a*)	0.5539(2)	1.10489(14)	0.3218(3)	0.5529	1.10586	⅓	0.01	-0.01	-0.11	0.25
Cs2	3(*a*),3(*a*)	0.23131(16)	0.44379(14)	0.3495(2)	-0.77811	0.77811	⅔	-0.13	-0.13	0.15	0.22
Hg3	3(*a*),3(*b*)	0.88846(6)	1.77468(8)	0.83242(13)	0.88771	1.77543	5/6	0.01	-0.01	-0.01	0.18
Hg1	3(*a*),3(*b*)	0.22078(9)	-0.22014(6)	0.16386(6)	0.22046	-0.22046	1/6	0.01	0.01	-0.03	0.17
Hg2	3(*a*),3(*b*)	0.88926(7)	0.44713(7)	0.50311 (4)	0.89093	0.44546	½	-0.02	0.02	0.03	0.18
Cl6	3(*a*),3(*a*)	1.9093(6)	0.9830(5)	0.0158(7)	1.9282	0.9641	0	-0.25	0.25	0.15	0.22
Cl9	3(*a*) 6(*c*)	0.0552(6)	0.7744(6)	-0.0037(8)	0.0774	0.7820	-0.0050	-0.30	-0.10	0.01	0.25
Cl2	3(*a*)	-0.7896 (5)	-0.0995(6)	0.3395(7)	-0.7820	-0.0774	0.3383	-0.10	-0.29	0.01	0.24
Cl1	3(*a*),3(*a*)	1.2309(5)	0.6262(6)	0.0336(7)	1.2381	0.6190	0	-0.10	0.10	0.32	0.20
Cl5	3(*a*) 6(*c*)	0.9189 (5)	0.2657(6)	0.3193(6)	0.8921	0.2764	0.3336	0.36	-0.13	-0.13	0.23
Cl7	3(*a*)	0.8653(7)	0.6050(6)	0.6522(7)	0.8921	0.6157	0.6664	-0.36	-0.14	-0.13	0.26
Cl3	3(*a*),3(*a*)	-0.2731 (6)	0.2847(4)	0.6045(7)	-0.2789	0.2789	⅔	0.08	0.08	-0.59	0.23
Cl4	3(*a*) 6(*c*)	0.0273(6)	0.5784(4)	0.3410(6)	0.0382	0.5852	0.3314	-0.14	-0.09	0.09	0.23
Cl8	3(*a*)	0.0490(8)	0.4461(6)	0.6783(8)	0.0382	0.4529	0.6686	0.14	-0.09	0.09	0.24

‡ Atoms in the order and setting of Table S8(*b*) but numbered as in Albarski *et al.* (2000).

Table S8(*b*)
Atomic positions for $Cs_{0.7}(NH_4)_{0.3}HgCl_3$ at room temperature (Kabadou *et al.,* 1998) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 13.295(11), c = 9.419(8) Å, with z^* = z + 0.0012 and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_2$,$P3_212$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Cs1†	3(*a*),3(*a*)	0.2226(4)	0.0997(5)	-0.0185(8)	0.2149	0.1074	0	0.10	-0.10	-0.17	0.21
Cs3	3(*a*),3(*a*)	0.2163(5)	0.4372(3)	0.3476(9)	0.2178	0.4357	⅓	-0.02	0.02	0.14	0.20
Cs2	3(*a*),3(*a*)	0.5575(3)	1.1066(3)	0.3383(9)	0.5547	1.1094	⅓	0.04	-0.04	0.05	0.20
Hg3	3(*a*),3(*b*)	0.8875(2)	1.7741(2)	-0.1642(2)	0.8872	1.7744	⅚	0.01	-0.01	0.02	0.19
Hg1	3(*a*),3(*b*)	0.2245(2)	-0.2195(2)	0.1631(2)	0.2220	-0.2220	⅙	0.03	0.03	-0.03	0.19
Hg2	3(*a*),3(*b*)	0.8919(2)	0.4450(2)	0.5004(3)	0.8913	0.4456	½	0.01	-0.01	0.00	0.18
Cl1	3(*a*),3(*a*)	1.8984(1)	0.9366	-0.0533(2)	1.8900	0.9450	0	0.11	-0.11	0.04	0.23
Cl2	3(*a*) 6(*c*)	0.0591	0.7746	-0.0153	0.0751	0.7794	-0.0031	-0.21	-0.06	-0.11	0.25
Cl5	3(*a*)	-0.7841	-0.0910	0.3242	-0.7794	-0.0751	0.3364	-0.06	-0.21	-0.11	0.24
Cl3	3(*a*) 6(*c*)	0.8932	0.2801	0.3291	0.8866	0.2616	0.3365	0.09	0.25	-0.07	0.25
Cl6	3(*a*)	0.8800	0.6435	0.6562	0.8866	0.6250	0.6635	-0.09	0.25	-0.07	0.25
Cl4	3(*a*),3(*a*)	-0.2616	0.3133	0.6439	-0.2874	0.2874	0.6667	0.34	0.34	-0.21	0.24
Cl8	3(*a*),3(*a*)	1.2237	0.6163	0.0569	1.2267	0.6133	0	-0.04	0.04	0.54	0.23
C17	3(*a*) 6(*c*)	0.0155	0.5979	0.3435	0.0385	0.5850	0.3355	-0.31	0.17	0.07	0.23
Cl9	3(*a*)	0.0615	0.4665	0.6725	0.0385	0.4535	0.6645	0.31	0.17	0.07	0.26
H1	3(*a*),3(*a*)	0.2225	0.0996	0.8860	0.2147	0.1074	0	0.10	-0.10	-1.07	0.22
H2	3(*a*),3(*a*)	0.2827	0.0944	0.0146	0.2514	0.1257	0	0.42	-0.42	0.14	0.22
H3	3(*a*),3(*a*)	0.1568	0.0398	0.0146	0.1311	0.0655	0	0.34	-0.34	0.14	0.22
H4	3(*a*),3(*a*)	0.2281	0.1657	0.0141	0.2625	0.1313	0	-0.45	0.46	0.13	0.22
H5	3(*a*) 6(*c*)	0.5574	0.1066	0.2425	0.5846	0.1011	0.2795	-0.36	0.07	-0.35	0.22
H8	3(*a*)	0.4893	0.0955	0.3503	0.5165	0.1011	0.3872	-0.36	-0.07	-0.35	0.22
H6	3(*a*) 6(*c*)	0.614	0.1747	0.3705	0.5789	1.1124	0.3333	0.47	0.83	0.35	0.22
H7	3(*a*)	0.5686	0.05	0.3706	0.5335	1.1124	0.3334	0.47	-0.83	0.35	0.22
H9	3(*a*) 6(*c*)	0.2162	0.437	0.2519	0.2026	0.4054	0.2692	0.18	0.42	-0.16	0.22
H10	3(*a*)	0.2164	0.3738	0.3803	0.2028	0.4054	0.3976	0.18	-0.42	-0.16	0.22
H11	3(*a*) 6(*c*)	0.1536	0.4371	0.3810	0.1712	0.4686	0.3337	-0.23	-0.42	0.45	0.22
H12	3(*a*)	0.2798	0.5	0.3804	0.2974	0.4686	0.3331	-0.23	0.42	0.45	0.22

† Cs sites occupied 70% by Cs, 30% by NH_4.

Table S9

Atomic positions for $Ba_2Cu_2AlF_{11}$ at room temperature (Dupont *et al.*, 1998) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and polar u^{33} displacements in Å

a = 7.301(1), c = 14.145(2) Å with $z = z + 0.2151$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$

	Wyckoff position $P3_2$,$P3_212$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Ba1	3(*a*),3(*b*)	-0.3482(2)	0.4640(5)	0.2151	-0.4061	0.4061	1/6	0.42	0.42	0.69	0.09
Ba2	3(*a*),3(*a*)	0.3244(2)	0.8274(2)	0.3479(1)	0.3839	0.7679	⅓	-0.43	0.43	0.21	0.12
Cu1	3(*a*)	0.3514(3)	0.3563(3)	0.4380(2)	0.3286	0.2822	0.4177	0.18	0.54	0.29	0.09
	6(*c*)										
Cu2	3(*a*)	0.9763(4)	0.2081(3)	0.2693(1)	0.9536	0.2822	0.2490	0.17	-0.54	0.29	0.09
Al	3(*a*),3(*a*)	0.8421(8)	1.8334(8)	0.4201(3)	0.8918	1.7837	⅓	-0.36	0.36	1.23	0.08
F1	3(*a*)	0.526(2)	0.248(2)	0.3973(8)	0.508	0.169	0.4129	0.13	0.58	-0.22	0.12
	6(*c*)										
F2	3(*a*)	0.680(2)	0.090(2)	0.2382(8)	0.662	0.169	0.2538	0.13	-0.58	-0.22	0.11
F3	3(*a*)	0.262(2)	0.339(2)	0.3100(9)	0.322	0.409	0.3706	-0.43	-0.51	-0.86	0.14
	6(*c*)										
F6	3(*a*)	0.028(2)	0.480(2)	0.2356(12)	0.088	0.409	0.2961	-0.44	0.52	-0.86	0.19
F4	3(*a*),3(*b*)	0.113(2)	-0.007(2)	0.4592(7)	0.071	0.035	½	0.31	-0.31	-0.58	0.09
F5	3(*a*),3(*b*)	1.205(2)	0.491(2)	0.4772(10)	1.131	0.565	½	0.54	-0.54	-0.32	0.16
F7	3(*a*),3(*a*)	0.934(2)	1.929(2)	0.3002(8)	0.954	1.909	⅓	-0.15	0.15	-0.47	0.11
F8	3(*a*)	0.909(2)	0.629(2)	0.3940(10)	0.988	0.651	0.3466	-0.58	-0.16	0.67	0.16
	6(*c*)										
F9	3(*a*)	0.585(2)	0.672(2)	0.3676(8)	0.664	0.651	0.3201	-0.58	0.15	0.67	0.12
F10	3(*a*)	0.738(2)	0.711(2)	0.5297(9)	0.766	0.714	0.5481	-0.20	-0.02	-0.26	0.12
	6(*c*)										
F11	3(*a*)	0.794(3)	0.050(2)	-0.5664(9)	0.766	0.053	-0.5481	0.20	-0.02	-0.26	0.13

Table S10

Atomic positions for $SrS_2O_6{\cdot}4H_2O$ at room temperature (Fábry, 1995) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 12.692(5), c = 19.186(9) Å with $z^* = z + 0.33011$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$

	Wyckoff position $P3_2$,$P3_212$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Sr1	3(*a*),3(*a*)	0.00239(9)	0.00204(7)	0.33011	0.00148	0.00295	⅓	0.01	-0.01	-0.06	0.11
Sr2	3(*a*)	0.49952(9)	0.49957(9)	0.33236(5)	0.49837	0.49959	0.33332	0.01	0.00	-0.02	0.12
	6(*c*)										
Sr3	3(*a*)	-0.49961(9)	0.50287(9)	0.99905(5)	-0.49959	0.50163	0.00001	-0.00	0.01	-0.02	0.11
Sr4	3(*a*),3(*a*)	0.49792(7)	-0.50101(7)	0.66824(6)	0.49947	-0.49947	⅔	-0.02	-0.02	0.03	0.11
O*W*1	3(*a*)	0.5923(5)	0.7280(5)	0.7065(3)	0.5978	0.7269	0.7070	-0.07	0.01	-0.01	0.16
	6(*c*)										
O*W*5	3(*a*)	0.2743(5)	0.3967(5)	0.6259(3)	0.2732	0.4022	0.6264	0.01	-0.07	-0.01	0.16
O*W*2	3(*a*)	0.5901(5)	0.3671(5)	0.2920(3)	0.4996	0.2501	0.2914	1.15	1.48	0.01	0.14
	6(*c*)										
O*W*9	3(*a*)	0.8669(5)	0.5908(5)	0.0424(3)	0.7499	0.5004	0.0419	1.48	1.15	0.01	0.16
O*W*3	3(*a*)	0.0913(5)	0.8673(5)	0.2891(3)	0.0970	0.8707	0.2893	-0.07	-0.04	-0.01	0.15
	6(*c*)										
O*W*6	3(*a*)	0.1026(5)	0.2229(5)	0.7106(3)	0.0970	0.2263	0.7107	0.07	-0.04	-0.01	0.18
O*W*4	3(*a*)	0.7224(5)	0.6332(5)	0.3734(3)	0.7247	0.6278	0.3754	-0.03	0.07	-0.04	0.15
	6(*c*)										
O*W*8	3(*a*)	0.3776(6)	0.2730(5)	0.9559(3)	0.3722	0.2753	0.9579	0.07	-0.03	-0.04	0.18
O*W*7	3(*a*)	0.3767(5)	0.6035(5)	0.0403(3)	0.3747	0.5976	0.0415	0.03	0.07	-0.02	0.15
	6(*c*)										
O*W*10	3(*a*)	0.2249(5)	0.5917(5)	0.6241(3)	0.2229	0.5976	0.6252	0.03	-0.07	-0.02	0.15
O*W*14	3(*a*)	-0.1238(5)	0.1016(5)	0.0389(3)	-0.1275	0.0971	0.0405	0.05	0.06	-0.03	0.17
	6(*c*)										
O*W*11	3(*a*)	0.2282(5)	0.0926(5)	0.6247(3)	0.2246	0.0971	0.6262	0.05	-0.06	-0.03	0.15
O*W*12	3(*a*)	0.0918(5)	0.7245(5)	0.7080(3)	0.0979	0.7227	0.7088	-0.08	0.02	-0.02	0.16
	6(*c*)										
O*W*16	3(*a*)	0.1039(5)	0.3768(5)	0.2904(3)	0.0979	0.3750	0.2912	0.08	0.02	-0.02	0.18
O*W*13	3(*a*)	0.8802(6)	0.2766(5)	0.9545(3)	0.7516	0.2515	0.9559	1.63	-0.32	-0.03	0.16
	6(*c*)										
O*W*15	3(*a*)	0.7737(5)	0.3771(6)	0.3761(3)	0.7485	0.2484	0.3774	0.32	1.63	-0.03	0.16
S1	3(*a*)	0.8439(2)	0.5334(2)	0.8353(1)	0.8456	0.5011	0.8335	-0.02	0.41	0.03	0.13
	6(*c*)										
S2	3(*a*)	0.6538(2)	0.4688(2)	0.8350(1)	0.6555	0.5011	0.8332	-0.02	-0.41	0.03	0.13
O1	3(*a*)	0.8656(5)	0.4849(5)	0.7723(3)	0.7438	0.4857	0.7700	1.55	-0.01	0.04	0.16
	6(*c*)										
O2	3(*a*)	0.8637(5)	0.4865(5)	0.8990(3)	0.7419	0.4857	0.8967	1.55	0.01	0.04	0.17

O3	3(*a*),3(*b*)	0.8995(5)	1.6658(5)	0.8349(3)	0.8551	1.7102	$^{5}/_{6}$	0.56	-0.56	0.03	0.16
O4	3(*a*)	0.6364(5)	0.5245(5)	0.8964(3)	0.7607	0.5188	0.8964	-1.58	0.07	0.00	0.17
	6(*c*)										
O5	3(*a*)	0.6338(5)	0.5131(5)	0.7702(3)	0.7581	0.5188	0.7702	-1.58	-0.07	0.00	0.17
O6	3(*a*),3(*b*)	0.5939(5)	1.3362(5)	0.8389(3)	0.6434	1.2867	$^{5}/_{6}$	-0.63	0.63	0.11	0.17
S3	3(*a*)	0.8098(2)	0.9664(2)	0.8289(1)	0.8280	0.9887	0.8326	-0.23	-0.28	-0.07	0.13
	6(*c*)										
S7	3(*a*)	0.8462(2)	0.8170(2)	0.1638(1)	0.8280	0.8393	0.1674	0.23	-0.28	-0.07	0.13
O7	3(*a*)	0.8795(5)	0.0140(5)	0.8916(3)	0.8712	-0.0025	0.8951	0.11	0.21	-0.07	0.16
	6(*c*)										
O20	3(*a*)	0.8629(5)	0.8901(5)	0.1014(3)	0.8712	0.8737	0.1049	-0.11	0.21	-0.07	0.18
O8	3(*a*)	0.8776(5)	0.0145(5)	0.7654(3)	0.8720	0.0028	0.7682	0.07	0.15	-0.05	0.18
	6(*c*)										
O19	3(*a*)	0.8663(5)	0.8809(5)	0.2290(3)	0.8720	0.8692	0.2318	-0.07	0.15	-0.05	0.16
O9	3(*a*),3(*b*)	0.7341(5)	1.8353(5)	0.8283(3)	0.8564	1.7129	$^{5}/_{6}$	-1.55	1.55	-0.10	0.16
O10	3(*a*)	0.6102(5)	0.9746(5)	0.7689(3)	0.6233	0.9883	0.7710	-0.17	-0.17	-0.04	0.18
	6(*c*)										
O23	3(*a*)	0.6363(5)	1.6213(5)	0.2270(3)	0.6233	0.6350	0.2290	0.17	-0.17	-0.04	0.16
O11	3(*a*)	0.6206(5)	0.9873(5)	0.8957(3)	0.6293	0.9977	0.8975	-0.11	-0.13	-0.03	0.17
	6(*c*)										
O22	3(*a*)	0.6379(5)	1.6211(5)	0.1007(3)	0.6293	0.6315	0.1025	0.11	-0.13	-0.03	0.17
O12	3(*a*)	0.7584(5)	0.1638(5)	0.8257(3)	0.8328	0.1261	0.8330	-0.94	0.48	-0.14	0.17
	6(*c*)										
O21	3(*a*)	0.9072(5)	0.7443(5)	0.1598(3)	0.8328	0.7067	0.1670	0.94	0.48	-0.14	0.17
O15	3(*a*),3(*b*)	0.2450(5)	0.9086(5)	0.1718(3)	0.1682	0.8318	$^{1}/_{6}$	0.97	0.97	0.10	0.17
S5	3(*a*)	0.3178(2)	0.8473(2)	0.1682(1)	0.3299	0.8285	0.1663	-0.15	0.24	0.04	0.13
	6(*c*)										
S6	3(*a*)	0.1904(2)	0.6580(2)	0.1689(1)	0.1716	0.6701	0.1670	0.24	-0.15	0.04	0.13
O13	3(*a*)	0.3818(5)	0.8666(5)	0.1034(3)	0.3710	0.8718	0.1024	0.14	-0.07	0.02	0.17
	6(*c*)										
O16	3(*a*)	0.1231(5)	0.6399(5)	0.2319(3)	0.1282	0.6290	0.2309	-0.06	0.14	0.02	0.17
O14	3(*a*)	0.3898(5)	0.8643(5)	0.2298(3)	0.3769	0.8714	0.2287	0.16	-0.09	0.02	0.17
	6(*c*)										
O17	3(*a*)	0.1216(5)	0.6361(5)	0.1058(3)	0.1286	0.6231	0.1046	-0.09	0.16	0.02	0.17
S4	3(*a*)	0.6840(2)	0.0308(2)	0.8300(1)	0.6704	0.0056	0.8332	0.17	0.32	-0.06	0.13
	6(*c*)										
S8	3(*b*)	0.6569(2)	0.6902(2)	0.1637(1)	0.6704	0.6649	0.1668	-0.17	0.32	-0.06	0.13
O18	3(*a*)	0.2645(5)	0.6002(5)	0.1695(3)	0.2502	0.5004	0.1698	0.18	1.27	-0.01	0.17
	6(*c*)										
O24	3(*a*)	0.5995(5)	0.7640(5)	0.1632(3)	0.4996	0.7498	0.1635	1.27	0.18	-0.01	0.17

Table S11

Atomic positions for $Cu_3Pb(TeO_6)(OH)_2$, parakhinite, at room temperature (Burns *et al.,* 1995) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 5.765(2), c = 18.001(9) Å with $z^* = z + 0.3103$ and $\Delta x = (x - x')c$, $\Delta y = (y - y')c$, $\Delta z = (z^* - z')c$

	Wyckoff position $P3_2$,$P3_212$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Pb	3(*a*),3(*b*)	0.3331(4)	0.1659(4)	0.4986	0.3327	0.1663	½	0.01	-0.01	-0.03	0.10
Te	3(*a*),3(*a*)	0.3296(8)	0.1661	0.2936(3)	0.1652	0.3305	⅓	0.95	-0.95	-0.71	0.02
Cu1	3(*a*),3(*a*)	0.833(2)	0.659(2)	0.0370(6)	0.783	-0.391	0	0.29	0.29	0.67	0.03
Cu2	3(*a*) 6(*c*)	0.326(2)	0.660(2)	0.3695(4)	0.082	0.660	0.3707	1.41	0.00	-0.02	0.02
Cu3	3(*a*) 6(*c*)	0.823(2)	0.660(2)	0.2948(4)	0.579	0.660	0.2960	1.41	0.00	-0.02	0.02
O1	3(*a*) 6(*c*)	0.575(6)	0.413(6)	0.229(3)	0.454	0.413	0.226	0.70	0.00	0.05	0.03
OH2	3(*a*) 6(*c*)	0.081(7)	0.413(7)	0.443(3)	-0.041	0.413	0.440	0.70	0.00	0.05	0.04
O2	3(*a*) 6(*c*)	1.080(7)	0.909(7)	0.227(4)	0.957	0.910	0.263	0.71	-0.01	-0.64	0.05
O6	3(*a*) 6(*c*)	0.076(6)	0.911(6)	0.369(3)	-0.047	0.910	0.404	0.71	0.01	-0.64	0.03
O3	3(*a*) 6(*c*)	0.497(8)	0.980(8)	0.299(4)	0.442	0.948	0.261	0.32	0.18	0.69	0.06
OH1	3(*a*) 6(*c*)	0.561(6)	0.916(6)	0.445(3)	0.506	0.948	0.406	0.32	-0.18	0.69	0.04
O4	3(*a*) 6(*c*)	0.576(5)	0.412(5)	0.370(2)	0.414	0.388	0.370	0.93	0.14	0.00	0.02
O5	3(*a*) 6(*c*)	0.118(6)	0.364(6)	0.296(3)	-0.044	0.388	0.296	0.93	-0.14	0.00	0.09

Table S12

Atomic positions for $ReH(CO)_4$ at room temperature (Masciocchi *et al*., 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 14.9733(7), c = 6.9984(4) Å with $z^* = z - 0.0084$ and $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Re1	3(*a*),3(*a*)	0.0851(7)	-0.0149(7)	0.8561(18)	0.0851	0	5/6	0	-0.22	0.16	0.19
C1	3(*a*)	0.1926(22)	-0.0083(29)	0.0231(63)	0.1792	0.0216	0.0237	0.20	-0.45	-0.01	0.25
	6(*c*)[A]										
C3	3(*a*)	0.1442(40)	-0.0515(14)	0.6423(49)	0.1576	-0.0216	0.6430	-0.20	-0.45	-0.01	0.25
C2	3(*a*)	0.1716(20)	0.1306(7)	0.7915(31)	0.1572	0.1455	0.7694	0.22	-0.22	0.15	0.25
	6(*c*)										
C4	3(*a*)	-0.0027(19)	-0.1603(9)	0.9195(52)	0.0117	-0.1455	0.8973	-0.22	-0.22	0.15	0.25
O1	3(*a*)	0.2493(33)	-0.0091(72)	0.134(12)	0.2270	0.0330	0.147	0.33	-0.63	-0.09	0.25
	6(*c*)										
O3	3(*a*)	0.1718(90)	-0.0750(89)	0.508(7)	0.1941	-0.0330	0.520	-0.33	-0.63	-0.09	0.25
O2	3(*a*)	0.2197(54)	0.2144(18)	0.739(8)	0.1945	0.2294	0.722	0.38	-0.22	0.12	0.25
	6(*c*)										
O4	3(*a*)	-0.0601(39)	-0.2444(19	0.961(14)	-0.0349	-0.2294	0.945	-0.38	-0.22	0.11	0.25
H1	3(*a*),3(*a*)	-0.003(4)	-0.0079(17)	0.036(8)	-0.006	-0.0055	0	0.04	-0.04	0.25	0.25
Re2	3(*a*)	0.7363(7)	0.2970(6)	0.5983(16)	0.7111	0.2723	0.6098	0.38	0.37	-0.08	0.19
	6(*c*)										
Re3	3(*a*)	0.2476(8)	0.6859(7)	0.3788(20)	0.2723	0.7111	0.3902	-0.37	-0.38	-0.08	0.19
C5	3(*a*)	0.8009(25)	0.2528(39)	0.4073(60)	0.7477	0.2108	0.4066	0.80	0.63	0.01	0.25
	6(*c*)										
C9	3(*a*)	0.1687(50)	0.6945(42)	0.594(11)	0.2108	0.7477	0.5934	-0.63	-0.80	0.01	0.25
C6	3(*a*)	0.8242(45)	0.2884(84)	0.7951(41)	0.7756	0.2302	0.7941	0.73	0.87	0.01	0.25
	6(*c*)										
C10	3(*a*)	0.172(5)	0.7269(38)	0.207(14)	0.2302	0.7756	0.206	-0.87	-0.73	0.01	0.25
C7	3(*a*)	0.8418(35)	0.4398(10)	0.550(14)	0.8361	0.3957	0.567	0.09	0.66	-0.12	0.25
	6(*c*)										
C11	3(*a*)	0.3516(30)	0.8304(13)	0.4162(62)	0.3957	0.8361	0.4331	-0.66	-0.09	-0.12	0.25
C8	3(*a*)	0.6347(36)	0.1525(10)	0.646(14)	0.5882	0.1478	0.652	0.70	0.07	-0.04	0.25
	6(*c*)										
C12	3(*a*)	0.1431(28)	0.5416(12)	0.3416(57)	0.1478	0.5882	0.3478	-0.07	-0.70	-0.04	0.25
O5	3(*a*)	0.8444(45)	0.2345(87)	0.293(11)	0.7759	0.1793	0.289	1.03	0.83	0.03	0.25
	6(*c*)										
O9	3(*a*)	0.1241(53)	0.7074(67)	0.714 (11)	0.1793	0.7759	0.711	-0.83	-1.03	0.02	0.25
O6	3(*a*)	0.8648(52)	0.2711(97)	0.918(7)	0.8037	0.1974	0.910	0.91	1.10	0.06	0.25
	6(*c*)										
O10	3(*a*)	0.1236(51)	0.7426(89)	0.098(11)	0.1974	0.8037	0.090	-1.10	-0.91	0.06	0.25
O7	3(*a*)	0.9132(61)	0.5201(20)	0.523(13)	0.9144	0.4656	0.539	-0.02	0.82	-0.11	0.25
	6(*c*)										
O11	3(*a*)	0.4110(67)	0.9155(19)	0.446(13)	0.4656	0.9144	0.461	-0.82	0.02	-0.11	0.25

O8	3(*a*) 6(*c*)	0.5803(37)	0.0644(14)	0.655(13)	0.5185	0.0753	0.672	0.93	-0.16	-0.12	0.25
O12	3(*a*)	0.0861(61)	0.4558(28)	0.312(13)	0.0753	0.5185	0.328	0.16	-0.93	-0.11	0.25
H2	3(*a*) 6(*c*)	0.666(4)	0.3182(18)	0.796(9)	0.666	0.3224	0.799	0.00	-0.06	-0.02	0.25
H3	3(*a*)	0.334(7)	0.6607(36)	0.531(13)	0.334	0.6564	0.534	0.00	0.06	-0.02	0.25

Table S13

Atomic positions in $Ni_2(NH_3)_9[Mo(CN)_8]\cdot 2H_2O$ at 153 K (Meske & Babel, 1999) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

$a = 9.551(1)$, $c = 23.267(7)$ Å, with $z^* = z - 0.12993$ and $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	$\Delta z^{\cong}$	u^{33}
Mo	3(*a*),3(*b*)	0.3600(1)	-0.00539(5)	-0.15278(3)	0.3600	0.0	$^5/_6$	0.00	-0.03	0.32	0.11
Ni1	3(*a*)	0.3624(2)	0.01080(9)	0.07484	0.36738	0.07177	0.09340	-0.05	-0.58	-0.43	0.11
	6(*c*)										
Ni2	3(*a*)	0.1327(2)	0.37234(8)	-0.11196(4)	0.07177	0.36738	-0.09340	0.58	0.05	-0.43	0.13
N1†	3(*a*)	0.617(3)	0.074(2)	-0.2577(5)	0.669	0.0665	-0.2450	-0.50	0.08	-0.29	0.19
N18	3(a)	0.619(4)	0.133(2)	-0.2629(7)	0.6847	0.0958	-0.2477	-0.63	0.36	-0.35	0.19
	6(*c*)										
N7	3(a)	0.655(2)	-0.0586(9)	-0.1009(6)	0.5889	-0.0958	-0.0856	0.63	0.36	-0.36	0.42
N7′	3(*a*)	0.655(2)	-0.0586(9)	-0.1009(6)	0.6025	-0.0665	-0.0883	0.50	0.08	-0.29	0.42
N2	3(*a*)	0.165(2)	-0.1134(8)	-0.2765(2)	0.1106	-0.1912	-0.2246	0.52	0.74	-1.21	0.14
	6(*c*)										
N5	3(*a*)	0.248(1)	0.2689(6)	-0.1606(2)	0.3018	0.1912	-0.1087	-0.52	0.74	-1.21	0.15
N3	3(*a*)	-0.033(1)	-0.2080(7)	-0.1215(2)	-0.0954	-0.4065	-0.1521	0.60	1.89	0.71	0.18
	6(*c*)										
N8	3(*a*)	0.249(1)	0.6050(6)	-0.1506(2)	0.3112	0.4065	-0.1812	-0.60	1.89	0.71	0.17
N4	3(*a*)	0.328(2)	0.0291(7)	-0.0019(2)	0.3407	0.8499	0.0584	-0.13	1.71	-1.40	0.14
	6(*c*)										
N6	3(*a*)	0.671(2)	0.3538(7)	-0.1186(3)	0.8499	0.3407	-0.0584	1.71	0.13	-1.40	0.26
NH9	3(*a*)	0.116(1)	-0.0626(6)	0.0908(2)	0.1319	-0.0262	0.0796	-0.16	-0.35	0.26	0.17
	6(*c*)										
NH16	3(*a*)	0.010(1)	0.1482(6)	-0.0682(2)	-0.0262	0.1319	-0.0796	0.35	0.16	0.26	0.17
NH10	3(*a*)	0.429(2)	0.2558(7)	0.0898(2)	0.4386	0.2885	0.0707	-0.09	-0.31	0.44	0.16
	6(*c*)										
NH14	3(*a*)	0.321(1)	0.4482(7)	-0.0515(2)	0.2885	0.4386	-0.0707	0.31	0.09	0.45	0.15
NH11	3(*a*)	0.390(1)	-0.0192(6)	0.1633(2)	0.3434	-0.0298	0.1708	0.44	0.10	-0.17	0.12
	6(*c*)										
NH15	3(*a*)	-0.040(1)	0.2972(7)	-0.1784(2)	-0.0298	0.3434	-0.1709	-0.10	-0.44	-0.17	0.17
NH12	3(*a*)	0.609(2)	0.0884(7)	0.0541(2)	0.5345	0.0490	0.0574	0.71	0.38	-0.08	0.16
	6(*c*)										
NH17	3(*a*)	0.010(1)	0.4600(7)	-0.0606(2)	0.0490	0.5345	-0.0574	-0.38	-0.71	-0.07	0.17
NH13‡	3(*a*),3(*a*)	0.308(1)	-0.2296(7)	0.0578(2)	0.2687	0.2687	0	0.37	-0.37	1.34	0.17
C1	3(*a*)	0.527(2)	0.060(1)	-0.2231(3)	0.563	0.0489	-0.2191	-0.34	0.11	-0.09	0.16
	6(*c*)										
C7	3(*a*)	0.550(2)	-0.0380(8)	-0.1182(4)	0.5140	-0.0489	-0.1142	0.34	0.10	-0.09	0.26

C2	3(*a*)	0.231(1)	-0.0759(7)	-0.2337(2)	0.2607	-0.0452	-0.2528	-0.28	-0.29	0.44	0.14
	6(*c*)										
C4	3(*a*)	0.335(2)	0.0145(8)	-0.0614(3)	0.3059	0.0452	-0.0805	0.28	-0.29	0.44	0.11
C3	3(*a*)	0.103(1)	-0.1382(7)	-0.1321(2)	0.1167	-0.1558	-0.1519	-0.13	0.17	0.46	0.13
	6(*c*)										
C5	3(*a*)	0.286(1)	0.1734(6)	-0.1617(2)	0.2725	0.1558	-0.1815	0.13	0.17	0.46	0.12
C8	3(*a*)	0.290(1)	0.7421(7)	-0.1540(2)	0.3035	0.7554	-0.1785	-0.13	-0.13	0.57	0.14
	6(*c*)										
C6	3(*a*)	0.561(1)	0.2312(7)	-0.1303(3)	0.5481	0.2446	-0.1548	0.13	-0.13	0.57	0.16
O1[††]	3(*a*)	0.599(2)	0.786(2)	-0.0030(7)	0.551	0.731	-0.0019	0.46	0.53	0.03	0.24
	6(*c*)										
O3	3(*a*)	0.675(1)	0.503(1)	0.0007(4)	0.731	0.551	0.0019	-0.53	-0.46	-0.03	0.19
O2	3(*a*)	0.630(2)	0.767(2)	0.0195(7)	0.674	0.808	0.0101	-0.42	-0.39	0.22	0.24
	6(*c*)										
O4	3(*a*)	0.848(2)	0.718(2)	-0.0006(5)	0.808	0.674	-0.0101	0.38	0.42	0.22	0.19

[†] Occupancy of N1 reported as 0.59(1); that of N18 at a distance of about 0.56 Å, as 0.41(1). Atoms N18 and N7, N1 and N7′ pair in the supergroup as indicated by the bracket.

[‡] The reported *y*(NH13) value of -0.2296 is replaced by 0.2296.

[††] Occupancy of O1 and O2 both reported as 0.50(1); that of O3 as 0.59(1) and O4 as 0.41(1). The occupancy of N1 reported as 0.41(1).

Table S14(*a*)
Atomic positions for the 6T polytype of $Ca_{1.89}Ta_{1.80}Sm_{0.16}Ti_{0.10}O_7$ at room temperature (Grey & Roth, 2000) with hypothetical *x´*, *y´*, *z´* coordinates and Δx, Δy, Δz and u_{iso} displacements in Å
a = 7.353(1)(6), c = 36.264(1) Å
$z^* = z - 0.0006$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')b$ and $\Delta z = (z - z')c$.

Atom	Wyckoff position $P3_1$,$P3_121$	*x*	*y*	*z*	*x´*	*y´*	*z´*	Δx	Δy	Δz	u_{iso}
Ca1	3(*a*)	0.1812(8)	0.1813(8)	-0.0042(1)	0.1812	0.1812	0	0.00	0.00	-0.15	0.09
Ta11	3(*a*)	0.6676(3)	0.6679(2)	0.0004(1)	0.6677	0.6677	0	0.00	0.00	0.01	0.05
Ca12	3(*a*)	0.1771(9)	0.6797(9)	-0.0024(2)	0.1767	0.6741	0.0006	0.00	0.04	-0.11	0.09
	6(*c*)										
Ca13	3(*a*)	0.6685(9)	0.1762(7)	-0.0036(2)	0.6741	0.1761	-0.0006	-0.04	0.00	-0.11	0.12
Ca2	3(*a*)	-0.0036(13)	0.8371(12)	0.9196(3)	0.0033	0.8306	0.9181	-0.05	0.05	0.05	0.13
	6(*c*)										
Ta4	3(*a*)	0.1796(3)	0.1759(3)	0.7501(1)	0.1727	0.1694	0.7486	0.05	0.05	0.05	0.09
Ta22	3(*a*)	0.5113(3)	0.8470(2)	0.9168(1)	0.5119	0.8358	0.9152	-0.01	0.08	0.06	0.10
	6(*c*)										
Ta43	3(*a*)	0.6768(3)	0.1755(9)	0.7531(1)	0.6761	0.1642	0.7515	0.01	0.08	0.06	0.08
Ca31	3(*a*),3(*b*)	0.8569(9)	0.0341(9)	0.8358(2)	0.8569	0	$^5/_6$	0	0.25	0.09	0.11
Ta21	3(*a*)	0.0132(2)	0.3477(2)	0.9167(1)	0.0145	0.3338	0.9165	-0.01	0.10	0.01	0.07
	6(*c*)										
Ta41	3(*a*)	0.6820(2)	0.6801(2)	0.7504(1)	0.6807	0.6662	0.7502	0.01	0.10	0.01	0.05
Ta23	3(*a*)	0.5106(2)	0.3436(3)	0.9141(1)	0.5128	0.3401	0.9167	-0.02	0.03	-0.09	0.08
	6(*c*)										
Ca42	3(*a*)	0.1750(11)	0.6635(12)	0.7474(2)	0.1727	0.6599	0.7500	0.02	-0.03	-0.09	0.13
Ta3	3(*a*),3(*b*)	0.3167(2)	0.0169(2)	0.8338(1)	0.3167	0	$^5/_6$	0	0.12	0.02	0.05
Ca32	3(*a*)	0.3648(7)	0.5207(7)	0.8297(2)	0.3609	0.5000	0.8320	0.03	0.15	-0.08	0.08
	6(*c*)										
Ca33	3(*a*)	0.8569(8)	0.5207(9)	0.8325(2)	0.8609	0.5000	0.8347	-0.03	0.15	-0.08	0.08
O1	3(*a*)	0.0585(27)	0.8723(25)	0.8596(5)	0.0702	0.8651	0.8613	-0.09	0.05	-0.06	0.12
	6(*c*)										
O12	3(*a*)	0.2168(21)	0.1421(23)	0.8038(4)	0.2051	0.1349	0.8054	0.09	0.05	-0.06	0.06
O2	3(*a*)	0.4593(27)	0.2687(28)	0.8633(6)	0.4666	0.2718	0.8611	-0.05	-0.02	0.08	0.13
	6(*c*)										
O8	3(*a*)	0.2021(24)	0.7251(26)	0.8079(5)	0.1948	0.7282	0.8056	0.05	-0.02	0.08	0.11
O3	3(*a*)	0.9525(24)	0.8171(20)	0.9795(5)	0.9510	0.7906	0.9736	0.01	0.19	0.21	0.09
	6(*c*)										
O5	3(*a*)	0.1588(22)	0.2359(23)	0.6989(4)	0.1604	0.2094	0.6931	-0.01	0.19	0.21	0.13
O4	3(*a*)	0.3783(23)	0.5327(20)	0.0201(4)	0.4038	0.5522	0.0264	-0.19	-0.14	-0.23	0.08
	6(*c*)										
O20	3(*a*)	0.5716(20)	0.4293(21)	0.9673(4)	0.5522	0.4038	0.9736	0.14	0.19	-0.23	0.10
O6	3(*a*)	0.6040(26)	0.1289(23)	0.8058(4)	0.6000	0.1211	0.8043	0.03	0.06	0.06	0.08
	6(*c*)										
O7	3(*a*)	0.4749(24)	0.8867(23)	0.8640(4)	0.4789	0.8789	0.8624	-0.03	0.06	0.06	0.09

O9	3(*a*)	0.9742(26)	0.3267(20)	0.9726(7)	0.9896	0.3407	0.9708	-0.11	-0.10	0.07	0.14
	6(*c*)										
O18	3(*a*)	0.6644(17)	0.6454(21)	0.6977(6)	0.6489	0.6593	0.6959	0.11	-0.10	0.07	0.08
O10	3(*a*)	0.763(2)	0.5229(19)	0.0325(4)	0.7948	0.5464	0.0320	-0.23	-0.17	0.02	0.09
	6(*c*)										
O11	3(*a*)	0.5698(21)	0.8266(20)	0.9685(4)	0.5464	0.7948	0.9680	0.17	0.23	-0.02	0.10
O13	3(*a*)	0.7032(23)	0.7235(28)	0.8048(5)	0.7171	0.6772	0.8045	-0.10	0.34	0.01	0.13
	6(*c*)										
O28	3(*a*)	0.0537(24)	0.369(2)	0.8625(5)	0.0399	0.3228	0.8622	0.10	0.34	0.01	0.07
O14	3(*a*)	0.8079(21)	0.4463(21)	0.9072(4)	0.8358	0.4824	0.9072	-0.21	-0.27	-0.01	0.11
	6(*c*)										
O26	3(*a*)	0.3813(19)	0.4815(21)	0.7594(4)	0.3534	0.5176	0.7595	0.21	-0.27	-0.01	0.09
O15	3(*a*)	0.7807(21)	0.4766(21)	0.7595(4)	0.7046	0.4118	0.7505	0.56	0.48	0.33	0.10
	6(*c*)										
O27	3(*a*)	0.2166(20)	0.6531(19)	0.9253(4)	0.2927	0.5882	0.9162	-0.56	0.48	0.33	0.11
O16	3(*a*)	0.5763(21)	0.8777(19)	0.7424(4)	0.6513	0.9155	0.7508	-0.55	-0.28	-0.30	0.10
	6(*c*)										
O25	3(*a*)	0.8109(20)	0.0468(19)	0.9075(4)	0.7358	0.0845	0.9159	0.55	-0.28	-0.30	0.09
O17	3(*a*)	0.2133(19)	0.2474(20)	0.9254(4)	0.1925	0.1838	0.9252	0.15	0.47	0.01	0.08
	6(*c*)										
O19	3(*a*)	0.9878(18)	0.8799(19)	0.7416(4)	0.0087	0.8162	0.7415	-0.15	0.47	0.01	0.10
O21	3(*a*)	0.9594(17)	0.2377(21)	0.7668(4)	0.9160	0.3047	0.7664	0.32	-0.49	0.02	0.12
	6(*c*)										
O23	3(*a*)	0.5677(20)	0.6283(17)	0.9008(4)	0.6112	0.6953	0.9003	-0.32	-0.49	0.02	0.10
O22	3(*a*)	0.4519(20)	0.0658(18)	0.9318(4)	0.4134	-0.0276	0.9312	0.28	0.69	0.02	0.12
	6(*c*)										
O24	3(*a*)	0.4024(18)	0.1210(19)	0.7362(3)	0.4410	0.0276	0.7355	-0.28	0.69	0.03	0.10

Table S14(*b*)
As in Table S14(*a*) but with origin shifted +(⅓, ⅔, 1/6).

Atom	Wyckoff position $P3_1$,$P3_121$	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	u_{iso}
Ta11	3(*a*), 3(*b*)	0.0009(3)	0.3346(2)	0.1671(1)	0	0.3346	1/6	0.007	0	0.015	0.05
Ca13	3(*a*), 3(*b*)	0.0018(9)	0.8429(7)	0.1631(2)	0	0.8429	1/6	0.013	0	-0.130	0.12
Ta3	3(*a*), 3(*a*)	0.6500(2)	0.6836(2)	0.0005(1)	0.6668	0.6668	0	-0.124	0.124	0.018	0.05
Ca33	3(*a*), 3(*a*)	0.1902(8)	0.1874(9)	0.9992(2)	0.1888	0.1888	0	0.010	-0.010	-0.029	0.08
Ca1	3(*a*)	0.5145(8)	0.8480(8)	0.1625(1)	0.5021	0.8482	0.1658	0.091	-0.001	-0.120	0.09
	6(*c*)										
Ca12	3(*a*)	0.5104(9)	0.3464(9)	0.1643(2)	0.4979	0.3461	0.1676	0.092	0.002	-0.120	0.09
Ca2	3(*a*)	0.3297(13)	0.5038(12)	0.0863(3)	0.3299	0.5061	0.0861	-0.001	-0.017	0.007	0.13
	6(*c*)										
Ca42	3(*a*)	0.5083(11)	0.3302(12)	0.9141(2)	0.5061	0.3299	0.9139	0.016	0.002	0.007	0.13
Ta4	3(*a*)	0.5129(3)	0.8426(3)	0.9168(1)	0.5133	0.8436	0.9167	-0.003	-0.007	0.004	0.09
	6(*c*)										
Ta22	3(*a*)	0.8446(3)	0.5137(2)	0.0835(1)	0.8436	0.5133	0.0833	0.007	0.003	0.007	0.10
Ta43	3(*a*)	0.0101(3)	0.8422(9)	0.9198(1)	0.0102	0.8431	0.9195	-0.001	-0.007	0.011	0.08
	6(*c*)										
Ta23	3(*a*)	0.8439(2)	0.0103(3)	0.0808(1)	0.8431	0.0102	0.0805	0.006	0.001	0.011	0.08
Ca31	3(*a*)	0.1902(9)	0.7008(93)	0.0025(2)	0.1888	0.6994	0.0030	0.010	0.010	-0.018	0.11
	6(*c*)										
Ca32	3(*a*)	0.6981(7)	0.1874(7)	0.9964(2)	0.6994	0.1888	0.9970	-0.010	-0.010	-0.021	0.08
Ta21	3(*a*)	0.3465(2)	0.0144(2)	0.0834(1)	0.3467	0.0148	0.0832	-0.001	-0.003	0.007	0.07
	6(*c*)										
Ta41	3(*a*)	0.0153(2)	0.3468(2)	0.9171(1)	0.0148	0.3467	0.9168	0.004	0.001	0.011	0.05
O1	3(*a*)	0.3918(27)	0.5390(25)	0.0263(5)	0.3918	0.5372	0.0259	0.00	0.013	0.016	0.12
	6(*c*)										
O8	3(*a*)	0.5354(24)	0.3918(26)	0.9746(5)	0.5372	0.3918	0.9741	-0.013	0.00	0.017	0.11
O12	3(*a*)	0.5501(21)	0.8088(23)	0.9705(4)	0.5517	0.8085	0.9699	-0.012	0.002	0.022	0.06
	6(*c*)										
O7	3(*a*)	0.8082(24)	0.5534(23)	0.0307(4)	0.8085	0.5517	0.0301	-0.002	0.013	0.022	0.09
O2	3(*a*)	0.7926(27)	0.9354(28)	0.0300(6)	0.7941	0.9364	0.0288	-0.011	-0.006	0.045	0.13
	6(*c*)										
O6	3(*a*)	0.9373(26)	0.7956(23)	0.9725(4)	0.9364	0.7941	0.9712	0.006	0.011	0.046	0.08
O3	3(*a*)	0.2858(24)	0.4838(20)	0.1462(5)	0.2871	0.4852	0.1463	-0.010	-0.010	0.005	0.09
	6(*c*)										
O4	3(*a*)	0.7116(23)	0.1994(20)	0.1868(4)	0.7129	0.1981	0.1870	0.010	0.010	-0.006	0.08
O5	3(*a*)	0.4921(22)	0.9026(23)	0.8656)4)	0.4927	0.9028	0.8652	-0.004	-0.002	0.018	0.13
	6(*c*)										
O11	3(*a*)	0.9031(21)	0.4933(20)	0.1352(4)	0.9029	0.4926	0.1348	0.002	0.005	0.019	0.10

O20	3(*a*)	0.9049(20)	0.0960(21)	0.1340(4)	0.9043	0.0950	0.1341	0.004	0.007	0.001	0.20
	6(*c*)										
O10	3(*a*)	0.0963(20)	0.1896(19)	0.1992(4)	0.0957	0.1907	0.1992	0.004	-0.008	0.001	0.09
O9	3(*a*)	0.3075(26)	0.9934(20)	0.1393(7)	0.3098	0.9956	0.1375	-0.017	-0.016	0.067	0.14
	6(*c*)										
O18	3(*a*)	0.9977(17)	0.3121(21)	0.8644(6)	0.9956	0.3098	0.8625	0.015	0.017	0.067	0.08
O13	3(*a*)	0.0365(23)	0.3902(28)	0.9715(5)	0.0361	0.3886	0.9712	0.003	0.012	0.013	0.13
	6(*c*)										
O28	3(*a*)	0.3870(24)	0.0357(20)	0.0292(5)	0.3886	0.0361	0.0288	-0.012	-0.003	0.013	0.07
O14	3(*a*)	0.1412(21)	0.1130(21)	0.0739(4)	0.1422	0.1135	0.0738	-0.007	-0.004	0.002	0.11
	6(*c*)										
O15	3(*a*)	0.1140(21)	0.1433(21)	0.9262(4)	0.1135	0.1422	0.9262	0.004	0.008	0.002	0.10
O26	3(*a*)	0.7146(19)	0.1482(21)	0.9261(4)	0.7141	0.1462	0.9260	0.004	0.015	0.005	0.09
	6(*c*)										
O25	3(*a*)	0.1442(20)	0.7135(19)	0.0742(4)	0.1462	0.7141	0.0740	-0.015	-0.004	0.006	0.09
O27	3(*a*)	0.5499(20)	0.3198(19)	0.0920(4)	0.5482	0.3204	0.0919	0.013	-0.004	0.005	0.11
	6(*c*)										
O19	3(*a*)	0.3211(18)	0.5466(19)	0.9083(4)	0.3204	0.5482	0.9081	0.005	-0.012	0.006	0.10
O16	3(*a*)	0.9096(21)	0.5444(19)	0.9091(4)	0.9119	0.5455	0.9085	-0.017	-0.008	0.022	0.10
	6(*c*)										
O17	3(*a*)	0.5466(19)	0.9141(20)	0.0921(4)	0.5455	0.9119	0.0915	0.008	0.016	0.022	0.08
O21	3(*a*)	0.2927(17)	0.9044(21)	0.9335(4)	0.2939	0.9027	0.9330	-0.009	0.013	0.018	0.12
	6(*c*)										
O23	3(*a*)	0.9010(20)	0.2950(17)	0.0675(4)	0.9027	0.2939	0.0670	-0.013	0.008	0.018	0.10
O22	3(*a*)	0.7852(20)	0.7325(18)	0.0985(4)	0.7864	0.7341	0.0978	-0.009	-0.012	0.025	0.12
	6(*c*)										
O24	3(*a*)	0.7357(18)	0.7877(19)	0.9029(3)	0.7341	0.7864	0.9022	0.012	0.010	0.025	0.10

Table S15(*a*)
Atomic positions for (Ce,La)$BSiO_5$ at room temperature (Callegari *et al.,* 1992) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 6.844(3), c = 6.700(4) Å. $z^* = z + 0.0096$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Ce,La†	3(*a*),3(*b*)	0.5869(1)	-0.0018(1)	0.8429	0.5869	0	5/6	0.000	-0.012	0.064	0.08
Si	3(*a*),3(*a*)	0.5823(4)	-0.0026(7)	0.344(1)	0.5823	0	⅓	0.000	-0.018	0.074	0.07
B	3(*a*),3(*b*)	0.116(1)	0.018(2)	0.821(2)	0.116	0	5/6	0.000	0.123	-0.080	0.09
O1	3(*a*)	0.3532(7)	0.1978(8)	0.8696(6)	0.3413	0.1936	0.856	0.081	0.029	0.085	0.10
	6(*c*)										
O2	3(*a*)	0.1893(7)	0.3294(8)	0.1559(6)	0.1936	0.3413	0.1431	-0.029	-0.081	0.086	0.09
O3	3(*a*)	0.6140(7)	0.4768(8)	0.1679(6)	0.6057	0.4649	0.1622	0.057	0.081	0.038	0.09
	6(*c*)										
O4	3(*a*)	0.4530(7)	0.5974(8)	0.8436(6)	0.4649	0.6057	0.8378	-0.081	-0.057	0.039	0.09
O5	3(*a*),3(*a*)	0.0589(7)	0.0571(7)	0.6229(6)	0	0.0571	⅔	0.403	0	-0.293	0.16

† Ce, 0.56; La, 0.34; Th, 0.04; Ca, 0.02 atoms per formula unit.

Table S15(*b*)
Atomic positions for (Ce,La)$BSiO_5$ at room temperature (Burns *et al.,* 1993) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 6.841(2), c = 6.702(2) Å with $z^* = z + 0.8326$ and $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.
The sense of the a and b axes as reported is reversed below.

	Wyckoff position $P3_1$,$P3_121$	$-x$	$-y$	z^*	x'	y'	z'	Δx	Δy	$\Delta z^{\cong}$	u^{33}
Ce,La[†]	3(*a*),3(*b*)	0.58816(6)	0.00016(7)	0.8326	0.5869	0	5/6	0.008	0.001	-0.005	0.06
Si	3(*a*),3(*a*)	0.5833(3)	-0.0001(4)	0.332(2)	0.5823	0	⅓	0.007	-0.018	-0.007	0.03
B	3(*a*),3(*b*)	0.1104(18)	-0.001(2)	0.8386(3)	0.110	0	5/6	0.000	-0.007	0.034	0.18
O4-1[‡]	3(*a*)	0.3429(12)	0.1945(12)	0.854(1)	0.3436	0.1941	0.856	-0.005	0.003	-0.014	0.07
	6(*c*)										
O5-2	3(*a*)	0.1936(12)	0.3443(11)	0.1417(11)	0.1941	0.3436	0.1439	0.003	0.005	0.014	0.09
O1-3	3(*a*)	0.6039(13)	0.4623(12)	0.1617(9)	0.6045	0.4636	0.1626	-0.003	-0.012	-0.006	0.07
	6(*c*)										
O2-4	3(*a*)	0.4650(14)	0.6051(12)	0.8364(9)	0.4636	0.6045	0.8374	0.013	0.004	-0.006	0.07
O3A-5	3(*a*),3(*a*)	0.004(2)	-0.056(2)	0.050(2)	-0.026	-0.026	0	0.205	-0.205	0.335	0.05
O3B-5′	3(*a*),3(*a*)	-0.054(3)	0.001(2)	0.952(2)	-0.027	-0.027	0	-0.188	0.189	-0.322	0.05

[†] Atom occupancy: Ce, 0.50; La, 0.32; Nd, 0.08; Th, 0.05; Pr, 0.03; Ca, 0.01 and Sm, 0.01.
O5, 0.55; O5′, 0.45.

[‡] First atom numbering as in Burns *et al* (1993), second as in Tables S15(*a, c–f*).

Table S15(*c*)
Atomic positions for $LaBGeO_5$ at room temperature [Kaminskii *et al.*, (1990) and Belokoneva *et al.*, (1991)] with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 7.020(5), c = 6.879(4) Å. $z^* = z + 0.8505$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
La	3(*a*),3(*b*)	0.58933(6)	0.00074(5)	0.8505	0.58933	0	5/6	0	0.005	0.118	0.07
Ge	3(*a*),3(*a*)	0.5800(1)	-0.0033(1)	0.3517(4)	0.5800	0	⅓	0	-0.023	0.126	0.05
B	3(*a*),3(*b*)	0.114(1)	0.010(1)	0.830(1)	0.114	0	5/6	0	0.070	-0.022	0.14
O1	3(*a*) 6(*c*)	0.3438(8)	0.1900(8)	0.8621(7)	0.3379	0.1885	0.8436	0.041	0.011	0.127	0.08
O2	3(*a*)	0.1870(9)	0.3320(8)	0.1750(8)	0.1885	0.3379	0.1564	-0.011	-0.041	0.128	0.10
O3	3(*a*) 6(*c*)	0.6125(8)	0.4685(9)	0.1264(7)	0.6113	0.4628	0.1434	0.008	0.040	-0.117	0.08
O4	3(*a*)	0.457(1)	0.6101(8)	0.8397(8)	0.4628	0.6113	0.8566	-0.041	-0.008	-0.116	0.09
O5	3(*a*),3(*a*)	0.057(1)	0.0436(9)	0.6312(8)	0	0.0436	⅔	0.400	0	-0.244	0.11

Table S16(*a*)
Atomic positions for $PrBGeO_5$ phase II at 923 K (Belokoneva *et al.,* 1998) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 6.9436(1), c = 6.8688(2) Å. $z^* = z + 0.842$ with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Pr	3(*a*),3(*b*)	0.589(2)	0.000(3)	0.842	0.589(2)	0	5/6	0	0	0.06	0.12
Ge†	3(*a*),3(*a*)	0.5761(9)	-0.001(2)	0.340(3)	0.5761	0	⅓	0	-0.01	0.05	0.12
B	3(*a*),3(*b*)	0.111(1)	0.005(2)	0.815(2)	0.111	0	5/6	0	0.04	-0.12	0.10
O1	3(*a*) 6(*c*)	0.346(2)	0.191(2)	0.862(2)	0.342	0.191	0.848	0.02	0.01	0.10	0.14
O2	3(*a*)	0.192(2)	0.339(2)	0.166(3)	0.191	0.342	0.152	0.01	-0.02	0.10	0.13
O3	3(*a*),3(*a*) 6(*c*)	0.619(2)	0.485(2)	0.182(3)	0.612	0.464	0.176	0.05	0.15	0.04	0.14
O4	3(*a*)	0.443(2)	0.606(2)	0.830(3)	0.464	0.612	0.824	-0.15	-0.05	0.04	0.18
O5	3(*a*),3(*a*)	0.054(1)	0.046(1)	0.625(2)	0	0.046	⅔	0.38	0	-0.28	0.13

† First atom numbering as in Chi *et al.* (1997), second as in Park & Bluhm (1996*b*).

Table S16(*b*)
Atomic positions in $PrBGeO_5$ phase III at 293 K (Belonkeva *et al*., 1998) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 12.0202(1), c = 6.7999(2) Å. $z^* = z + 0.6807$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')$, $z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Pr1	3(*a*) 6(*c*)	0.2763(3)	0.1378(3)	-0.3193	0.3339	0.1669	-0.3310	-0.69	-0.35	0.08	0.08
Pr3	3(*a*)	0.1959(3)	0.3914(3)	0.3427(5)	0.1669	0.3339	0.3310	0.35	0.69	0.08	0.07
Pr2	3(*a*),3(*a*)	0.5284(3)	0.4710(3)	0.0170(5)	0.4997	0.4997	0	0.34	-0.34	0.12	0.08
Ge1	3(*a*) 6(*c*)	0.2805(5)	0.1386(5)	0.1811(9)	0.3336	0.1667	0.1686	-0.64	-0.34	0.08	0.07
Ge3	3(*a*)	0.1948(6)	0.3866(6)	-0.1561(7)	0.1667	0.3336	-0.1686	0.64	0.33	0.08	0.07
Ge2	3(*a*),3(*b*)	0.5268(5)	0.4744(5)	0.5145(8)	0.5006	0.5006	½	0.31	-0.31	0.10	0.07
B1	3(*a*),3(*a*)	0.0710	-0.0419	0.6527	0	-0.0419	⅔	0.85	0	-0.10	0.09
B2	3(*a*) 6(*c*)	0.2629	0.6380	0.7107	0.3333	0.6380	0.6667	-0.85	0	0.30	0.09
B3	3(*a*)	0.5962	0.3047	0.7107	0.6667	0.3047	0.6667	-0.85	0	0.30	0.09
O1	3(*a*) 6(*c*)	0.653(3)	0.496(3)	0.354(3)	0.732	0.659	0.332	-0.95.	1.96	0.15	0.09
O2	3(*a*)	0.822(2)	0.810(2)	-0.309(3)	0.659	0.732	-0.332	1.96	0.94	0.16	0.11
O3	3(*a*),3(*a*)	0.504(3)	0.684(3)	0.021(3)	0.594	0.594	0	-1.08	1.08	0.14	0.09
O4	3(*a*) 6(*c*)	0.172(3)	0.155(2)	0.341(3)	0.244	0.331	0.333	-0.86	-2.12	0.05	0.11
O5	3(*a*)	0.506(3)	0.315(3)	0.674(4)	0.331	0.244	0.667	2.10	0.86	0.05	0.11
O6	3(*a*),3(*a*)	0.326(3)	0.482(3)	0.000(3)	0.404	0.404	0	-0.94	0.94	0.00	0.11
O7	3(*a*) 6(*c*)	0.561(3)	0.590(3)	0.688(3)	0.660	0.637	0.665	-1.19	-0.56	0.16	0.11
O9	3(*a*)	0.683(2)	0.759(2)	0.358(3)	0.637	0.660	0.335	0.55	1.19	0.16	0.11
O8	3(*a*),3(*a*)	0.748(2)	0.635(2)	0.026(3)	0.692	0.692	0	0.68	-0.68	0.18	0.11
O10	3(*a*) 6(*c*)	0.221(2)	0.302(2)	0.664(2)	0.330	0.359	0.661	-1.31	-0.69	0.02	0.11
O12	3(*a*)	0.416(3)	0.438(3)	0.341(4)	0.359	0.330	0.339	0.69	1.30	0.01	0.11
O11	3(*a*),3(*a*)	0.356(2)	0.260(1)	0.007(2)	0.308	0.308	0	0.58	-0.58	0.05	0.11
$O13_{NPD}$†	3(*a*),3(*b*)	-0.029(1)	-0.038(1)	0.475(1)	-0.034	-0.034	½	0.14	0.09	-0.17	0.08
$O14_{NPD}$	3(*a*) 6(*c*)	0.305(1)	0.630(1)	0.443(1)	0.301	0.646	0.596	0.06	-0.19	-1.04	0.09
$O15_{NPD}$	3(*a*)	0.661(1)	0.296(1)	0.252(1)	0.646	0.301	0.404	0.18	-0.06	-1.03	0.09

† Neutron powder diffraction result; all other coordinates from single crystal X-ray diffraction.

Table S17(*a*)
Atomic positions for $LaBSiO_5$ at 293 K (Ono *et al*., 1996) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 6.876(2), c = 6.747(1) Å. $z^* = z + 0.0008$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
La	3(*a*),3(*b*)	0.59872(9)	-0.00004(4)	0.8341	0.59872	0	5/6	0	-0.000	0.005	0.09
Si	3(*a*),3(*a*)	0.5826(5)	-0.0003(5)	0.332(2)	0.5826	0	⅓	0	-0.002	-0.007	0.08
B	3(*a*),3(*b*)	0.111(2)	-0.001(2)	0.834(2)	0.111	0	5/6	0	-0.007	0.007	0.10
O1	3(*a*) 6(*c*)	0.344(2)	0.192(2)	0.863(1)	0.344	0.192	0.862	0.000	0.000	0.004	0.12
O2	3(*a*)	0.192(2)	0.344(2)	0.138(1)	0.192	0.344	0.138	0.000	0.000	0.003	0.10
O3	3(*a*) 6(*c*)	0.602(2)	0.467(2)	0.164(1)	0.603	0.467	0.164	0.007	0.000	0.003	0.12
O4	3(*a*)	0.468(2)	0.605(2)	0.837(1)	0.467	0.603	0.836	0.007	0.014	0.004	0.10
O5	3(*a*),3(*a*)	0.039(2)	-0.001(2)	0.333(2)	0.039	0	⅓	0	-0.007	0.000	0.14

Table S17(*b*)
Atomic positions for $LaBSiO_5$ at room temperature (Samygina *et al.,* 1993) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

$a = 6.815(1)$, $c = 6.758(1)$ Å. $z^* = z + 0.8361$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
La	3(*a*),3(*b*)	0.5987(1)	0.0000(1)	0.8361	0.5987	0	5/6	0	-0.000	0.019	0.08
Si	3(*a*),3(*a*)	0.5833(4)	0.0001(5)	0.332(2)	0.5833	0	⅓	0.005	0.000	-0.007	0.08
B	3(*a*),3(*b*)	0.106(2)	-0.001(2)	0.833(1)	0.106	0	5/6	0.000	-0.007	0.000	0.07
O1	3(*a*) 6(*c*)	0.3453(9)	0.1924(9)	0.8605(9)	0.3449	0.1926	0.8605	0.003	-0.001	0.000	0.09
O2	3(*a*)	0.1928(9)	0.3444(9)	0.1396(1)	0.1926	0.3449	0.1395	0.000	-0.003	0.001	0.09
O3	3(*a*) 6(*c*)	0.6029(9)	0.4670(10)	0.1630(9)	0.6031	0.4669	0.1631	0.007	-0.001	0.001	0.09
O4	3(*a*)	0.4667(2)	0.6033(2)	0.8368(8)	0.4668	0.6031	0.8369	-0.001	-0.001	0.001	0.09
O5	3(*a*),3(*a*)	-0.0002(2)	0.039(1)	0.666(1)	0	0.039	⅔	-0.001	0.000	0.000	0.14

Table S17(*c*)
Atomic positions for $LaBSiO_5$ at 273 K (Belokonova *et al.,* 1996) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

$a = 6.838(2)$, $c = 6.773(2)$. $z^* = z + 0.834$, with $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
La	3(*a*),3(*b*)	0.59784(8)	0.00000(8)	0.834	0.59784	0	5/6	0	0.000	0.007	0.08
Si	3(*a*),3(*a*)	0.5825(4)	0.0000(5)	0.332(2)	0.5825	0	⅓	0.000	0.000	-0.007	0.07
B	3(*a*),3(*b*)	0.111(2)	0.001(2)	0.834(2)	0.111	0	5/6	0.000	0.007	0.007	0.09
O1	3(*a*)	0.343(1)	0.191(1)	0.861(1)	0.343	0.191	0.860	0.000	0.000	0.007	0.10
	6(*c*)										
O2	3(*a*)	0.191(1)	0.343(1)	0.141(1)	0.191	0.343	0.140	0.000	0.000	0.007	0.09
O3	3(*a*)	0.603(1)	0.466(1)	0.163(1)	0.603	0.466	0.164	0.007	0.000	-0.007	0.09
	6(*c*)										
O4	3(*a*)	0.466(1)	0.603(1)	0.835(1)	0.466	0.603	0.836	0.000	0.001	-0.007	0.09
O5	3(*a*),3(*a*)	0.000(2)	0.037(2)	0.666(2)	0	0.037	⅔	0.000	0.000	-0.007	0.16

Table S17(*d*)

Atomic positions for $LaBSiO_5$ at 473 K (Belokonova *et al.,* 1996) determined in space group $P3_121$ with u^{33} displacements in Å

a = 6.827(2), c = 6.779(2) Å with $z^* = z + ½$.

	Wyckoff position $P3_121$	x	y	z^*	u^{33}
La	3(*b*)	0.5988(1)	0	$^5/_6$	0.10
Si	3(*a*)	0.5826(3)	0	⅓	0.09
B	3(*b*)	0.109(2)	0	$^5/_6$	0.09
O1	6(*c*)	0.3436(7)	0.1933(8)	0.8615(7)	0.13
O2		0.1933(8)	0.3436(7)	0.1385(7)	0.13
O3	6(*c*)	0.6039(8)	0.4693(9)	0.1708(7)	0.11
O4		0.4693(9)	0.6039(8)	0.835(1)	0.11
O5	3(*a*)	0	0.037(1)	⅔	0.15

Table S18(*a*)
Atomic positions for β-$LaBSiO_5$ at 296 K (Chi *et al*., 1997) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

a = 6.874(1), c = 6.717(3) Å. $z^* = z$ -0.0064, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_112$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
La	3(*a*),3(*b*)	1.66655(3)	0.74270(2)	0.4936	1.60616	0.80308	½	0.42	-0.42	-0.04	0.07
Si	3(*a*),3(*a*)	1.6667(1)	0.7487(1)	-0.0012(5)	1.6103	0.8051	0	0.39	-0.39	0.01	0.07
B	3(*a*),3(*b*)	0.5573(6)	1.3327(5)	0.163(1)	0.6300	1.2600	1/6	-0.50	0.50	-0.03	0.12
O1	3(*a*)	0.3248(4)	0.1405(4)	0.1882(4)	0.4218	0.2384	0.1185	-0.67	-0.67	0.47	0.09
O1	3(*a*) 6(*c*)	0.3248(4)	0.1405(4)	0.1882(4)	0.4218	0.2358	0.2395	-0.67	-0.66	-0.34	0.09
O5†	3(*a*)	0.7196(7)	0.3363(7)	0.2846(7)	0.8166	0.2384	0.2149	-0.67	0.67	0.47	0.09
O5'	3(*a*)	0.717(1)	0.331(1)	0.0425(9)	0.814	0.2358	0.0938	-0.67	0.65	-0.34	0.09
O2	3(*a*),3(*b*)	0.5188(4)	1.5261(4)	0.1398(5)	0.6816	1.3633	1/6	-1.12	1.12	-0.18	0.09
O3	3(*a*) 6(*c*)	0.8068(5)	-0.0638(5)	0.1595(5)	0.7178	0.8333	0.1619	0.61	0.71	-0.02	0.11
O4	3(*a*)	0.2046(5)	0.7303(4)	0.1691(5)	0.1156	0.8333	0.1715	0.61	-0.71	- 0.02	0.10

† Occupancy of O5 site 58%, O5' site 42%; x' y' z'(O1) coordinates corresponding to those for O5′ are also given.

Table S18(*b*)

Atomic positions for $PbBAsO_5$ at room temperature (Park & Bluhm, 1996*a*) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å

$a = 7.122(1)$, $c = 6.935(2)$ Å. $z^* = z + 0.3019$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_112$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Pb	3(*a*),3(*b*)	1.6674(1)	0.7316(1)	0.5137	1.5993	0.7997	½	0.49	-0.49	0.09	0.09
As†	3(*a*),3(*a*)	1.6690(3)	0.7392(3)	0.0136(5)	1.6055	0.8027	0	0.45	-0.45	0.09	0.08
B	3(*a*),3(*b*)	0.573(4)	1.347(4)	0.198(3)	0.640	1.280	1/6	-0.48	0.48	0.21	0.10
O3-1	3(*a*) 6(*c*)	0.343(3)	0.148(3)	0.196(2)	0.433	0.243	0.234	-0.64	-0.68	-0.26	0.12
O5-5	3(*a*)	0.720(2)	0.337(3)	0.061(2)	0.810	0.243	0.099	-0.64	0.67	-0.26	0.14
O1-2	3(*a*),3(*b*)	0.514(3)	1.514(2)	0.158(2)	0.676	1.352	1/6	1.15	1.15	-0.06	0.12
O2-4	3(*a*) 6(*c*)	0.206(3)	0.733(3)	0.196(3)	0.107	0.828	0.179	0.71	-0.68	0.12	0.10
O4-3	3(*a*)	0.820(3)	0.923(3)	0.171(2)	0.721	0.828	0.154	0.71	0.68	0.12	0.10

† First atom numbering as in Park & Bluhm (1996*a*), second as in Chi *et al.* (1996).

Table S18(*c*)
Atomic positions for $BaBAsO_5$ at room temperature (Park & Bluhm, 1996*b*) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

$a = 7.267(1)$, $c = 7.106(1)$ Å. $z^* = z' - 0.0030$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Ba	3(*a*),3(*b*)	1.6666(3)	0.9415(3)	0.5003(1)	1.7387	0.8693	½	-0.52	0.52	0.01	0.10
As	3(*a*),3(*a*)	1.6669(5)	0.9361(4)	0.0020(1)	1.7353	0.8677	0	-0.50	0.50	0.01	0.09
B	3(*a*),3(*b*)	0.668(4)	0.423(4)	0.497(4)	0.727	0.364	½	-0.43	0.43	-0.02	0.08
O1-2	3(*a*) 6(*c*)	0.815(3)	0.895(3)	0.847(3)	0.812	0.777	0.851	0.02	0.86	-0.03	0.22
O3-1†	3(*a*)	0.810(3)	0.154(3)	0.145(2)	0.812	0.036	0.149	-0.02	0.86	-0.03	0.15
O2-4	3(*a*) 6(*c*)	0.519(3)	0.750(3)	0.149(2)	0.519	0.629	0.146	0.00	0.88	0.02	0.20
O4-3	3(*a*)	0.492(3)	0.480(3)	0.524(2)	0.371	0.480	0.521	0.88	0	0.02	0.15
O5-5	3(*a*),3(*a*)	0.637(3)	0.301(3)	0.336(2)	0.625	0.313	⅓	0.09	-0.09	0.02	0.16

† First atom numbering as in Park & Bluhm (1996*b*), second as in Chi *et al.* (1997); coordinates transformed under $P3_1$ symmetry as necessary for direct comparison with Table S18(*a*, *b*).

Table S19

Atomic positions for $KTlF_4$ at room temperature (Hebecker, 1975) with hypothetical z' x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 8.025, c = 10.160 Å; uncertainties not reported.
$z^* = z + 0.139$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Tl1	3(*a*),3(*b*)	0.0005(5)	0.3604(5)	0.155(1)	0	0.3604	1/6	0.00	0	-0.12	0.10
Tl2	3(*a*),3(*b*)	0.1758(5)	0.1761(5)	0.489(1)	0.1760	0.1760	½	0.00	0.00	-0.11	0.09
K1	3(*a*)	0.479(4)	0.305(4)	0.150(3)	0.478	0.313	0.155	0.01	-0.06	-0.05	0.12
K2	6(*c*) 3(*a*)	0.321(4)	0.477(4)	-0.159(4)	0.313	0.478	-0.155	0.06	-0.01	-0.04	0.15
F1	3(*a*)	0.05(1)	0.32(1)	0.39(1)	0.065	0.335	0.39	-0.12	-0.12	0.00	0.14
F3	6(*c*) 3(*a*)	0.35(1)	0.08(1)	-0.39(1)	0.335	0.065	-0.39	0.12	0.12	0.00	0.14
F2	3(*a*)	0.47(1)	0.34(1)	0.39(1)	0.465	0.345	0.395	0.04	-0.04	-0.05	0.17
F4	6(*c*) 3(*a*)	0.35(1)	0.46(1)	-0.40(1)	0.345	0.465	-0.395	0.04	-0.04	-0.05	0.19
F5	3(*a*)	0.28(1)	0.47(1)	0.10(1)	0.285	0.48	0.099	0.04	-0.06	0.00	0.18
F6	6(*c*) 3(*a*)	-0.19(1)	0.51(1)	0.57(1)	-0.195	0.52	0.569	-0.04	-0.06	0.00	0.14
F7	3(*a*),3(*a*)	0.20(1)	0.01(1)	0.32(1)	0.20	0	1/3	0	0.08	-0.13	0.22
F8	3(*a*),3(*b*)	-0.07(2)	0.04(2)	0.23(1)	0	0.04	1/6	-0.56	0	0.64	0.23

Table S20(*a*)
Atomic positions for Fe_7Se_8 at room temperature (Andresen & Leciejewicz, 1964) with hypothetical x', y', z' coordinates and Δx, Δy, Δz displacements in Å

a = 7.2613(9), c = 17.675(5) Å [see ACBCA35 1210], with $\Delta x = (x - x')a$; $\Delta y = (y - y')b$; $\Delta z = (z - z')c$

	Wyckoff position $P3_1$,$P3_121$	x	y	z	x'	y'	z'	Δx	Δy	Δz
Fe1	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0
Fe4	3(*a*),3(*b*)	0	0	1/6	0	0	1/6	0	0	0
Fe2	3(*a*)	½	0	0	½	0	0	0	0	0
	6(*c*)									
Fe3	3(*a*)	0	½	0	0	½	0	0	0	0
Fe5	3(*a*),3(*b*)	½	½	½	½	½	½	0	0	0
Fe6	3(*a*)	½	0	0.182	½	0	0.182	0	0	0
	6(*c*)									
Fe7	3(*a*)	½	0	0.485	½	0	0.485	0	0	0
Se1	3(*a*)	1/6	⅓	0.083	1/6	⅓	0.083	0	0	0
	6(*c*)									
Se6	3(*a*)	⅓	1/6	0.917	⅓	1/6	0.917	0	0	0
Se2	3(*a*)	1/6	⅓	0.417	1/6	⅓	0.417	0	0	0
	6(*c*)									
Se5	3(*a*)	⅓	1/6	0.583	⅓	1/6	0.583	0	0	0
Se3	3(*a*)	1/6	⅓	¾	1/6	⅓	¾	0	0	0
	6(*c*)									
Se4	3(*a*)	⅓	1/6	¼	⅓	1/6	¼	0	0	0
Se7	3(*a*)	⅔	⅓	0.083	⅔	⅓	0.083	0	0	0
	6(*c*)									
Se8	3(*a*)	⅓	⅔	¼	⅓	⅔	0.250	0	0	0

Table S20(*b*)
Atomic positions for Fe_7S_8 at room temperature (Fleet, 1971) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 6.8673(9), c = 17.062(2) Å with $z^* = z + 0.3364$, $\Delta x = (x - x')a$; $\Delta y = (y - y')b$; $\Delta z = (z - z')c$

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Fe1	3(*a*),3(*b*)	0.5	0.5	0.5123(8)	0.5	0.5	½	0	0	0.21	0.10
Fe3	3(*a*),3(*b*)	0.0146(5)	0.9855(5)	0.4960(5)	0	0	½	0.10	-0.10	-0.07	0.10
Fe2	3(*a*)	0.4708(10)	0.9855(5)	0.4960(5)	0.4708	0	0.5000	0	-0.10	-0.07	0.10
	6(*c*)										
Fe4	3(*a*)	0.0146(5)	0.5292(10)	0.4960(5)	0	0.5293	0.5000	0.10	020	-0.07	0.10
Fe6	3(*a*),3(*a*)	0.9836(4)	0.0164(4)	0.6646(5)	0	0.0164	⅔	-0.11	0.11	-0.04	0.10
Fe5	3(*a*)	0.5328(9)	0.0164(4)	0.6646(5)	0.5000	0	0.6646	0.23	0.11	0.00	0.10
	6(*c*)										
Fe7	3(*a*)	0.9836(4)	0.4672(9)	0.3354(5)	0.0000	0.5000	0.3354	-0.11	-0.23	0.00	0.10
S1†	3(*a*)	0.1667	0.3333	-0.0819†	⅙	⅓	-0.0840	0.00	0.00	0.04	0.09
	6(*c*)										
S5	3(*a*)	0.3333	0.1667	0.0860(5)	⅓	⅙	0.0840	0.00	0.00	0.03	0.09
S4	3(*a*)	0.6667	0.8333	-0.0819	⅔	⅚	-0.0840	0.00	0.00	0.04	0.09
	6(*c*)										
S7	3(*a*)	0.8333	0.6667	0.0860(5)	⅚	⅔	0.0840	0.00	0.00	0.03	0.09
S2	3(*a*)	0.1667	0.8333	-0.0819	⅙	⅚	-0.0758	0.00	0.00	-0.10	0.09
	6(*c*)										
S8	3(*a*)	0.8333	0.1667	0.0697(12)	⅚	⅙	0.0758	0.00	0.00	-0.10	0.09
S3	3(*a*)	0.6667	0.3333	-0.0819	⅔	⅓	-0.0840	0.00	0.00	0.04	0.09
	6(*c*)										
S6	3(*a*)	0.3333	0.6667	0.0860(5)	⅓	⅔	0.0840	0.00	0.00	0.03	0.09

† All z(S) coordinates replaced by z - 0.1712; z(Fe7) replaced by $\bar{z}$ (Fe7)

Table S21
Atomic positions for B_2O_3 at room temperature (Gurr *et al.*, 1970) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 4.336(1), c = 8.430(2) Å, with $z^* = z + 0.7972$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
O1	3(a) 6(c)†	0.547(3)	0.397(3)	0.797	0.546	0.398	0.794	0.01	-0.01	0.03	0.10
O2	3(a)	0.149(2)	0.600(3)	0.8747(9)	0.148	0.601	0.872	0.01	-0.01	0.03	0.10
O3	3(a),3(a)	0.005(2)	0.161(4)	0.668(2)	0	0.161	⅔	0.02	0.00	0.01	0.09
B1	3(a)	0.223(5)	0.393(5)	0.777(3)	0.223	0.395	0.777	0.00	-0.02	0.00	0.13
B2	3(a) 6(c)	0.828(4)	0.603(5)	0.889(2)	0.828	0.605	0.889	0.00	-0.02	0.00	0.10

† See footnote 1 for equivalent positions.

Table S22

Atomic positions for mineral low-combeite $Na_2Ca_2Si_3O_9$ (Fischer & Tillmanns, 1983) at room temperature with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 10.464(2), c = 13.176(3) Å, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Si1	3(*a*)	0.4710(4)	0.1811(4)	0.5623	0.4765	0.1858	0.5632	-0.06	-0.05	-0.01	0.10
	6(*c*)										
Si2	3(*a*)	0.1904(4)	0.4819(4)	0.4358(4)	0.1858	0.4765	0.4368	0.05	0.06	-0.01	0.06
Si3	3(*a*)	0.6207(4)	0.4840(4)	0.4472(3)	0.6380	0.4868	0.4399	-0.18	-0.03	0.10	0.08
	6(*c*)										
Si4	3(*a*)	0.4896(4)	0.6553(4)	0.5675(4)	0.4868	0.6380	0.5601	0.03	0.18	0.10	0.08
Si5	3(*a*)	0.8176(5)	0.8564(5)	0.2405(4)	0.8243	0.8509	0.2322	-0.07	0.06	0.11	0.09
	6(*c*)										
Si6	3(*a*)	0.8455(4)	0.8310(4)	0.7762(4)	0.8509	0.8243	0.7678	-0.06	0.07	0.11	0.09
O1	3(*a*),3(*a*)	0.6015(9)	0.6131(9)	0.5077(8)	0.6073	0.6073	½	-0.06	0.06	0.10	0.12
O3	3(*a*)	0.347(1)	0.599(1)	0.4929(9)	0.364	0.714	0.4939	-0.18	-1.20	-0.01	0.12
	6(*c*)										
O2	3(*a*)	0.666(1)	0.1709(9)	0.1718(9)	0.649	0.286	0.1728	0.18	-1.20	-0.01	0.16
O4	3(*a*)	0.778(1)	0.8907(9)	0.3498(9)	0.791	0.8924	0.3386	-0.13	-0.02	0.15	0.13
	6(*c*)										
O5	3(*a*)	0.894(1)	0.804(1)	0.6726(9)	0.892	0.791	0.6614	0.02	0.14	0.15	0.13
O6	3(*a*)	0.4773(9)	0.2659(9)	0.1305(7)	0.4552	0.2635	0.1183	0.23	0.03	0.16	0.11
	6(*c*)										
O7	3(*a*)	0.261(1)	0.4331(9)	0.8940(8)	0.264	0.4552	0.8817	-0.02	-0.23	0.16	0.13
O8	3(*a*)	0.162(1)	0.235(1)	0.1162(9)	0.138	0.063	0.1109	0.25	1.80	0.07	0.14
	6(*c*)										
O9	3(*a*)	0.8866(9)	0.752(1)	0.2277(8)	0.8623	0.925	0.2224	0.25	1.81	0.07	0.12
O10	3(*a*)	0.5168(9	0.088(1)	0.0009(8)	0.5379	0.101	-0.0042	-0.22	-0.14	0.07	0.13
	6(*c*)										
O11	3(*a*)	0.4410(9)	0.5765(9)	0.6760(8)	0.4621	0.5633	0.6709	-0.22	0.14	0.07	0.12
O12	3(*a*)	0.7613(9)	0.5766(9)	0.0128(8)	0.7707	0.5653	0.0089	-0.10	0.12	0.05	0.13
	6(*c*)										
O13	3(*a*)	0.554(1)	0.780(1)	0.9949(9)	0.5653	0.7707	0.9911	-0.12	0.10	0.05	0.13
O14	3(*a*),3(*b*)	0.931(1)	0.011(1)	0.1832(9)	0.931	0	1/6	0.00	0.12	0.22	0.13
O15	3(*a*)	0.733(1)	0.6766(9)	0.8368(8)	0.754	0.6713	0.8321	-0.22	0.06	0.06	0.13
	6(*c*)										
O16	3(*a*)	0.666(1)	0.775(1)	0.1727(9)	0.6713	0.7540	0.1679	-0.06	0.22	0.06	0.16
O17	3(*a*)	0.8546(8)	0.4533(8)	0.2125(7)	0.7033	0.3438	0.2155	1.58	1.15	-0.04	0.09
	6(*c*)										
O18	3(*a*)	0.448(1)	0.531(1)	0.1148(9)	0.2967	0.6405	0.1178	1.58	-1.15	-0.04	0.14

Ca1	3(*a*)	0.9751(2)	0.6421(2)	0.3395(4)	0.8184	0.8125	0.3740	1.64	-1.78	-0.45	0.09
	6(*c*)										
Ca4	3(*a*)	0.9828(4)	0.6617(4)	0.5915(5)	0.8125	0.8184	0.6260	1.78	-1.63	-0.45	0.12
Ca2	3(*a*)	0.8438(3)	0.3332(4)	0.5055(4)	0.8281	0.3182	0.5045	0.16	0.16	0.01	0.09
	6(*c*)										
Ca3	3(*a*)	0.3033(4)	0.8123(4)	0.4965(5)	0.3182	0.8281	0.4955	-0.16	-0.17	0.01	0.13
Na1	3(*a*)	0.6503(6)	0.0067(5)	0.4144(6)	0.6503	0	⅓	0.00	0.07	1.07	0.13
Na5	3(*a*)	0.1468(4)	0.9723(4)	0.1807(5)	0.0228	0.9052	0.2516	1.30	0.70	-0.93	0.13
	6(*c*)										
Na2	3(*a*)	0.9935(7)	0.1618(8)	0.3442(6)	0.1176	0.0948	0.4151	-1.30	0.70	-0.93	0.12
Na3	3(*a*)	0.5042(7)	0.6784(7)	0.3389(6)	0.5066	0.6652	0.3299	-0.03	0.14	0.12	0.13
	6(*c*)										
Na4	3(*a*)	0.652(2)	0.509(2)	0.679(2)	0.665	0.5066	0.6701	-0.14	0.03	0.12	0.12

Table S23

Atomic positions for $Ti_6C_{3+\delta}$ at room temperature (Kukol' *et al.*, 1995) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

$a = 3.060$, $c = 14.91$ Å (uncertainties not reported); $\Delta x = (x - x')a$; $\Delta y = (y - y')b$; $\Delta z = (z - z')c$

	Wyckoff position $P3_1$,$P3_121$	site occupancy	x	y	z	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Ti1[†]	3(*a*) 6(*c*)	0.911(9)	0	⅔	-0.0879(3)	0	⅔	-0.08805	0.00	0.00	0.002	0.13
Ti2	3(*a*)	1.00(2)	⅔	0	0.0882(3)	⅔	0	0.08805	0.00	0.00	0.002	0.05
C1	3(*a*),3(*b*)	1.00(4)	⅔	0	⅚	⅔	0	⅚	0.00	0.00	0.00	0.13
C2	3(*a*),3(*a*)	0.24(5)	⅔	0	⅓	⅔	0	⅓	0.00	0.00	0.00	0.20

[†] Reported occupancies Ti1, 0.911(9); Ti2, 1.00(2); C1, 1.00(4) and C2, 0.24(5).

Table S24
Atomic positions for $IrGe_4$ at room temperature (Panday & Schubert, 1969) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 6.215, c = 7.784 Å; uncertainties not reported.
$z^{*} = z + 0.0086$ and $\Delta x = (x - x')a$, $\Delta y = (y - y')b$, $\Delta z = (z - z')c$

	Wyckoff position $P3_1$,$P3_121$	x	y	z^{*}	x'	y'	z'	Δx	Δy	$\Delta z^{\cong}$	u_{iso}
Ir	3(a),3(a)	0.318	0.001	0.342	0.318	0	⅓	0.00	0.01	0.13	0.08
Ge1	3(a) 6(c)	0.491	0.22	0.056	0.489	0.22	0.056	0.01	0.00	0.00	0.07
Ge2	3(a)	0.222	0.487	0.943	0.222	0.489	0.944	0.00	-0.01	-0.02	0.06
Ge3	3(a),3(b)	0.077	0.002	0.830	0.077	0	⅚	0.00	0.01	-0.05	0.03
Ge4	3(a),3(b)	0.61	0.002	0.830	0.61	0	⅚	0.00	0.01	-0.05	0.12

Table S25
Atomic positions for Nb_6C_5 at room temperature (Christensen, 1985) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å

a = 5.464(5), c = 15.422(5) Å; $z^* = z + 0.168$ and $\Delta x = (x - x')a$, $\Delta y = (y - y')b$ and $\Delta z = (z - z')c$.

	Wyckoff position $P3_1$,$P3_112$	x	y	z	x'	y'	z'	Δx	Δy	Δz	site occupancy
Nb1	3(*a*) 6(*c*)	0.421(5)	-0.122(5)	0.422(5)	0.436	-0.119	0.422	-0.08	-0.02	0.00	1
Nb6	3(*a*)	0.116(5)	-0.451(5)	0.244(5)	0.119	-0.436	0.244	-0.02	-0.08	0.00	1
Nb2	3(*a*) 6(*c*)	-0.242(5)	-0.460(5)	0.415(5)	-0.224	-0.454	0.415	-0.10	-0.03	0.00	1
Nb5	3(*a*)	0.449(5)	0.207(5)	0.252(5)	0.454	0.224	0.252	-0.03	-0.09	0.00	1
Nb3	3(*a*) 6(*c*)	0.089(5)	0.227(5)	0.419(5)	0.106	0.234	0.417	-0.09	-0.04	0.03	1
Nb4	3(*a*)	-0.241(5)	-0.124(5)	0.251(5)	-0.234	-0.106	0.250	-0.04	-0.10	0.02	1
C1	3(*a*),3(*b*)	0.101(5)	0.540(5)	0.493(5)	0.094	0.547	½	0.04	-0.04	-0.06	0.93(6)
C2	3(*a*),3(*b*)	-0.229(5)	-0.124(5)	0.503(5)	-0.235	-0.118	½	0.03	-0.03	0.05	0.75(6)
C3	3(*a*),3(*b*)	0.430(5)	0.219(5)	0.499(5)	0.433	0.216	½	-0.02	-0.02	0.02	1.00(6)
C4	3(*a*),3(*a*)	-0.216(5)	0.229(5)	0.327(5)	-0.222	0.222	⅓	0.03	0.04	-0.09	0.82(6)
C5	3(*a*),3(*a*)	0.463(5)	0.569(5)	0.335(5)	0.447	0.553	⅓	0.09	0.09	0.03	0.71(6)
C6	3(*a*),3(*a*)	0.111(5)	-0.111(5)	0.335(5)	0.111	-0.111	⅓	0.00	0.00	0.03	0.52(6)

Table S26
Atomic positions in mineral sheldrickite $NaCa_3(CO_3)_2F_3 \cdot H_2O$ at room temperature (Grice *et al*., 1997) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 6.726(2), c = 15.044(4) Å with $\Delta x = (x - x')a$, $\Delta y = (y - y')b$ and $\Delta z = (z - z')c$.
a and b axes as reported are reversed in table.

	Wyckoff position $P3_2$,$P3_221$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Na1	3(*a*), 3(*b*)	0.297(1)	0.001(1)	0.165(1)	0.297	0	1/6	0	0.01	-0.03	0.15
Ca1	3(*a*)	-0.0009(7)	0.6161(4)	0	-0.0010	0.6223	-0.0022	0.01	-0.04	0.03	0.10
	6(*c*)										
Ca2	3(*a*)	0.6284(4)	-0.0011(5)	0.0045(4)	0.6223	-0.0010	0.0022	0.04	-0.01	0.03	0.09
Ca3	3(*a*),3(*a*)	0.3710(5)	0.3706(5)	-0.0043(4)	0.3707	0.3708	0	0.01	-0.01	-0.06	0.13
C1	3(*a*)	0.317(2)	0.567(2)	0.168(1)	0.318	0.567	0.166	-0.01	001	0.03	0.11
	6(*c*)										
C2	3(*a*)	0.752(2)	0.432(2)	0.169(1)	0.751	0.433	0.167	0.01	-0.01	0.03	0.11
O1	3(*a*)	0.348(2)	0.664(2)	0.090(1)	0.335	0.659	0.091	0.09	0.03	-0.02	0.13
	6(*c*)										
O4	3(*a*)	0.654(2)	0.321(2)	-0.092(2)	0.659	0.335	-0.091	-0.03	-0.09	-0.02	0.12
O2	3(*a*)	0.333(1)	0.668(2)	0.238(2)	0.335	0.667	0.239	-0.01	0.01	-0.02	0.11
	6(*c*)										
O5	3(*a*)	0.666(1)	0.336(2)	0.761(2)	0.667	0.335	0.761	-0.01	0.01	-0.01	0.12
O3	3(*a*)	0.273(2)	0.353(2)	0.167(1)	0.274	0.354	0.167	-0.01	-0.01	0.00	0.13
	6(*c*)										
O6	3(*a*)	0.921(2)	0.646(2)	0.165(1)	0.922	0.646	0.166	-0.01	0.00	0.00	0.16
O*W*	3(*a*), 3(*b*)	0.202(2)	0.203(2)	0.831(1)	0	0.202	5/6	1.37	0	-0.03	0.15
F1	3(*a*)	0.266(2)	0.997(1)	0.010(1)	0.2685	0.999	0.0075	-0.02	-0.01	0.04	0.15
	6(*c*)										
F2	3(*a*)	0.002(2)	0.271(1)	-0.005(1)	-0.001	0.2685	-0.0075	0.02	0.02	0.04	0.13
F3	3(*a*),3(*a*)	0.734(2)	0.730(2)	-0.020(1)	0.732	0.732	0	0.01	-0.01	-0.30	0.12

Table S27
Atomic positions for high pressure phase I of ZnTe at room temperature (Kusaba & Weidner, 1994) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 4.045(1), c = 9.342(4) Å with $z^* = z + 0.015$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')b$ and $\Delta z = (z - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Zn	3(*a*),3(*a*)	0.35	0.20	0.015	0.275	0.275	0	0.30	-0.30	0.14	0.10
Te	3(*a*),3(*b*)	0.49	0.49	0.485	0.49	0.49	½	0.00	0.00	-0.14	0.10

Table S28

Atomic positions in $CaCO_3 \cdot H_2O$ at room temperature (Effenberger, 1981) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 10.5536(10), c = 7.545(2) Å with $z^* = z - 0.3333$ and $\Delta x = (x - x')a$, $\Delta y = (y - y')b$ and $\Delta z = (z - z')c$.

	Wyckoff position $P3_1$, $P3_112$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
Ca1	3(*a*)	0.1853(7)	0.0879(7)	0.	0.1821	0.0911	0.	0.03	-0.03	0.	0.12
Ca2	3(*a*)	0.8413(7)	0.4235(7)	-0.0062(10)	0.8432	0.4216	0.	-0.02	0.02	-0.05	0.12
Ca3	3(*a*)	1.5259(5)	0.7641(5)	0.0065(12)	1.5267	0.7633	0.	-0.01	0.01	0.05	0.06
O*W*1	3(*b*)	0.392(2)	0.191(2)	0.502(3)	0.389	0.194	½	0.03	-0.03	0.01	0.09
O*W*2	3(*b*)	1.066(2)	0.541(2)	0.491(3)	1.071	0.536	½	-0.05	0.05	-0.07	0.14
O*W*3	3(*b*)	1.748(2)	0.877(2)	0.516(3)	1.750	0.875	½	-0.02	0.02	0.12	0.13
O1	3(*a*) 6(*c*)	0.206(2)	0.240(2)	0.731(3)	0.214	0.242	0.737	-0.08	-0.02	0.05	0.14
O2	3(*a*)	0.020(2)	0.245(2)	0.603(3)	0.028	0.242	0.597	-0.08	0.03	-0.05	0.14
O3	3(*a*) 6(*c*)	0.885(2)	0.587(2)	0.755(3)	0.883	0.583	0.736	0.02	0.04	-0.05	0.11
O4	3(*a*)	0.701(2)	0.579(2)	0.603(3)	0.699	0.583	0.597	0.02	-0.04	0.05	0.11
O5	3(*a*) 6(*c*)	0.547(2)	0.899(2)	0.733(3)	0.542	0.907	0.736	0.05	-0.08	-0.03	0.16
O6	3(*a*)	0.370(2)	0.912(2)	0.594(3)	0.365	0.906	0.597	0.05	0.06	-0.03	0.16
O7	3(*a*),3(*b*)	0.060(2)	0.062(2)	0.546(3)	0.082	0.041	½	-0.23	0.22	0.35	0.14
O8	3(*a*),3(*b*)	0.660(2)	0.400(2)	0.790(3)	0.630	0.370	⅚	0.32	0.32	-0.32	0.11
O9	3(*a*),3(*b*)	1.401(2)	0.723(2)	0.546(3)	1.416	0.708	½	-0.16	0.16	0.35	0.16
C1	3(*a*),3(*a*)	0.092(2)	0.179(2)	0.643(3)	0.090	0.181	⅔	0.02	-0.02	-0.18	0.14
C2	3(*a*),3(*a*)	0.750(2)	1.516(2)	0.705(3)	0.755	1.511	⅔	- 0.05	0.05	0.29	0.11

⅔.

Table S29

Atomic positions for $Li_7Cu_7Si_5$ at room temperature (Pavlyuk *et al*., 1995) with *B* parameter in $Å^2$

a = 14.144(6), *c* = 13.527(3) Å

	x	*y*	*z*	*B*
Cu1/Si1	0.4819(7)	0.2941(6)	0.0000(8)	0.9(2)
Cu2	0.1390(5)	0.2935(5)	0.9398(8)	0.66(14)
Cu3	0.4239(6)	0.2959(6)	0.8240(8)	0.43(12)
Cu4	0.0331(6)	0.2393(6)	0.3954(8)	0.65(13)
Cu5/Si2	0.3588(7)	0.2973(7)	0.1327(8)	1.1(2)
Cu6	0.5433(6)	0.2969(6)	0.1765(8)	0.79(13)
Cu7/Si3	0.2508(7)	0.2960(7)	0.7955(9)	1.0(2)
Cu8	0.3838(6)	0.0854(6)	0.4275(8)	0.62(14)
Cu9/Si4	0.4763(7)	0.5141(7)	0.6105(9)	0.87(13)
Cu10	0.3593(6)	0.4073(6)	0.4571(8)	1.0(2)
Cu11	0.5385(6)	0.4089(6)	0.4958(8)	0.71(12)
Cu12	0237(6)	0.4045(6)	0.4161(8)	0.64(14)
Cu13	0.0232(6)	0.2964(6)	0.0815(8)	0.67(14)
Cu14/Si5	0.2070(6)	0.5808(7)	0.3840(8)	0.56(14)
Cu15/Si6	0.3718(8)	0.1914(8)	0.2776(10)	1.04(13)
Cu16/Si7	0.5361(8)	0.6238(7)	0.0579(9)	1.1(2)
Cu17/Si8	0.0335(6)	0.1247(6)	0.0455(7)	0.49(13)
Cu18/Si9	0.4741(7)	0.6208(7)	0.8875(8)	0.82(15)
Cu19/Si10	0.0337(7)	0.1812(7)	0.2181(9)	0.8(2)
Cu20/Si11	0.2011(7)	0.4625(7)	0.0537(8)	0.59(14)
Cu21/Si12	0.2042(6)	0.0780(6)	0.3917(8)	0.91(14)
Si 13/Cu22	0.3722(13)	0.2476(12)	0.4336(13)	0.5(3)
Si 14	0.375(2)	0.138(2)	0.100(2)	1.5(3)
Si 15	0.4227(13)	0.4605(14)	0.7828(14)	0.4(3)
Si 16	0.5345(13)	0.4572(13)	0.1175(14)	0.5(3)
Si 17/Cu23	0.0393(12)	0.4687(11)	0.1190(12)	0.7(2)
Si 18	0.3696(13	0.6267(13)	0.0225(12)	0.7(2)
Si 19	0.0384(14)	0.0777(13)	0.3543(13)	0.8(3)
Si 20/Cu24	0.3643(10)	0.4724(10)	0.1399(11)	0.7(2)
Si 21	0.1933(13)	0.2921(13)	0.1039(13)	0.7(3)
Si 22/Cu25	0.2563(10)	0.1306(10)	0.7627(11)	0.2(2)
Si 23/Cu26	0.4437(10)	0.1453(11)	0.7416(11)	1.1(2)
Si 24	0.1946(12)	0.4103(12)	0.4487(14)	0.6(3)
Si 25	0.5894(15)	0.2924(14)	0.862(2)	1.4(3)
Si 26	0.0811(14)	0.2952(14)	0.7722(14)	1.3(3)
Li 1/Cu27	0.519(4)	0.221(4)	0.540(4)	2.101(3)
Li 2/Cu28	0.184(3)	0.226(3)	0.485(3)	2.101(3)
Li 3/Cu29	0.111(3)	0.155(3)	0.669(3)	2.101(3)
Li 4/Cu30	0.363(3)	0.544(3)	0.345(3)	2.101(3)
Li 5/Cu31	0.597(5)	0.070(5)	0.639(5)	2.101(3)
Li 6/Cu32	0.262(4)	0.080(4)	0.580(4)	2.101(3)
Cu33	0.571(4)	0.162(4)	0.949(4)	2.101(3)

Li8	0.031(11)	0.406(11)	0.916(13)	2.101(3)
Li9	0.500(11)	0.091(10)	0.233(10)	2.101(3)
Li10	0.037(11)	0.303(11)	0.582(13)	2.101(3)
Li11	0.383(11)	0.084(11)	0.912(14)	2.101(3)
Li12	0.368(10)	0.607(10)	0.517(11)	2.101(3)
Li13	0.139(10)	0.408(11)	0.244(11)	2.101(3)
Li14	0.250(12)	0.291(11)	0.304(12)	2.101(3)
Li15	0.256(10)	0.486(10)	0.849(10)	2.101(3)
Li16	0.584(11)	0.292(10)	0.368(11)	2.101(3)
Li17	0.362(11)	0.298(11)	0.628(12)	2.101(3)
Li18	0.057(10)	0.092(10)	0.846(11)	2.101(3)
Li19	0.228(10)	0.15(1)	0.99(1)	2.101(3)
Li20	0.257(10)	0.418(11)	0.638(11)	2.101(3)
Li21	0.169(10)	0.101(9)	0.178(10)	2.101(3)
Li22	0.367(12)	0.415(12)	0.965(12)	2.101(3)

Table S30
Atomic positions proposed by Pauling & Kamb (1982) for lithiophorite, $Li_6Al_{14}(OH)_{42}Mn_{21}O_{42}$, at room temperature.

a = 13.370, c = 28.200 Å; uncertainties not reported.

Li1	0.318	0.254	0	O3	-0.444	-0.222	-0.034	O45	-0.492	-0.127	0.034
Li2	0.175	0.54	0	O4	0.032	0.159	-0.034	O46	-0.016	0.254	0.034
Li3	-0.254	0.397	0	O5	-0.413	0.064	-0.034	O47	0.365	0.159	0.034
Li4	0.46	-0.032	0	O6	0.603	0.016	-0.034	O48	0.555	0.111	0.034
Li5	-0.397	-0.318	0	O7	-0.206	-0.031	-0.034	O49	-0.254	0.064	0.034
Li6	0.032	-0.175	0	O8	0.08	0.397	-0.034	O50	0.032	0.492	0.034
Al1	0.079	0.063	0	O9	0.27	0.349	-0.034	O51	0.222	0.444	0.034
Al2	-0.063	0.349	0	O10	0.461	0.302	-0.034	O52	0.413	0.397	0.034
Al3	0.127	0.301	0	O11	-0.349	0.254	-0.034	O53	-0.397	0.349	0.034
Al4	-0.301	0.159	0	O12	-0.158	0.207	-0.034	O54	-0.206	0.302	0.034
Al5	-0.349	-0.079	0	O13	0.127	0.635	-0.034	O55	0.079	0.73	0.034
Al6	-0.159	-0.127	0	O14	0.318	0.588	-0.034	O56	0.27	0.683	0.034
Al7	0.508	0.206	0	O15	0.508	0.54	-0.034	O57	-0.54	0.635	0.034
Al9	0.365	0.492	0	O16	-0.301	0.492	-0.034	O58	-0.349	0.587	0.034
Al10	0.413	-0.27	0	O17	-0.016	-0.079	-0.034	O59	-0.064	0.016	0.034
Al11	0.222	-0.222	0	O18	0.175	-0.127	-0.034	O60	0.127	-0.032	0.034
Al12	-0.016	0.587	0	O19	0.365	-0.174	-0.034	O61	0.317	-0.079	0.034
Al13	0.27	0.016	0	O20	-0.254	-0.27	-0.034	O62	-0.302	-0.175	0.034
Al14	-0.206	-0.365	0	O21	-0.063	-0.317	-0.034	O63	-0.111	-0.222	0.034
Mn1	0.222	0.111	0.1667	O22	0.222	0.111	-0.132	O64	0.174	0.206	0.132
Mn2	-0.111	0.444	0.1667	O23	-0.111	0.444	-0.132	O65	-0.159	0.539	0.132
Mn3	0.444	0.222	0.1667	O24	-0.444	-0.222	-0.132	O66	-0.492	-0.127	0.132
Mn4	0.032	0.159	0.1667	O25	0.032	0.159	-0.132	O67	-0.016	0.254	0.132
Mn5	0.413	0.064	0.1667	O26	0.413	0.064	-0.132	O68	0.365	0.159	0.132
Mn6	0.603	0.016	0.1667	O27	0.603	0.016	-0.132	O69	0.555	0.111	0.132
Mn7	-0.206	-0.031	0.1667	O28	-0.206	-0.031	-0.132	O70	-0.254	0.064	0.132
Mn8	0.08	0.397	0.1667	O29	0.08	0.397	-0.132	O71	0.032	0.492	0.132
Mn9	0.27	0.349	0.1667	O30	0.27	0.349	-0.132	O72	0.222	0.444	0.132
Mn10	0.461	0.302	0.1667	O31	0.461	0.302	-0.132	O73	0.413	0.397	0.132
Mn11	-0.349	0.254	0.1667	O32	-0.349	0.254	-0.132	O74	-0.397	0.349	0.132
Mn12	-0.158	0.207	0.1667	O33	-0.158	0.207	-0.132	O75	-0.206	0.302	0.132
Mn13	0.127	0.635	0.1667	O34	0.127	0.635	-0.132	O76	0.079	0.73	0.132
Mn14	0.318	0.588	0.1667	O35	0.318	0.588	-0.132	O77	0.27	0.683	0.132
Mn15	0.508	0.54	0.1667	O36	0.508	0.54	-0.132	O78	-0.54	0.635	0.132
Mn16	-0.301	0.492	0.1667	O37	-0.301	0.492	-0.132	O79	-0.349	0.587	0.132
Mn17	-0.016	-0.079	0.1667	O38	-0.016	-0.079	-0.132	O80	-0.064	0.016	0.132
Mn18	0.175	-0.127	0.1667	O39	0.175	-0.127	-0.132	O81	0.127	-0.032	0.132
Mn19	0.365	-0.174	0.1667	O40	0.365	-0.174	-0.132	O82	0.317	-0.079	0.132
Mn20	-0.254	-0.27	0.1667	O41	-0.254	-0.27	-0.132	O83	-0.302	-0.175	0.132
Mn21	-0.063	-0.317	0.1667	O42	-0.063	-0.317	-0.132	O84	-.0111	-0.222	0.132
O1	-0.222	0.111	-0.034	O43	0.174	0.206	0.034				
O2	-0.111	0.444	-0 .034	O44	–0.159	0.539	0.034				

Table S31

Atomic positions in $K_5CoW_{12}O_{40}\cdot 20H_2O$ at room temperature (Muncaster *et al.*, 2000) with hypothetical x', y', z' coordinates and Δx, Δy, Δz and u_{iso} displacements in Å

a = 18.937(3), c = 12.484(2) Å with $z^* = z + 0.4572$; $\Delta x = (x - x')a$; $\Delta y = (y - y')b$; $\Delta z = (z - z')c$.

	Wyckoff position $P3_1$,$P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{iso}
K1	3(*a*) 6(*c*)	0.6292(3)	0.2581(3)	0.3324(4)	0.6291	0.2584	0.3330	0.01	-0.01	-0.01	0.19
K2	3(*a*)	0.3706(3)	0.7413(3)	0.3332(4)	0.3707	0.7416	0.3337	-0.01	-0.01	-0.01	0.19
W1	3(*a*) 6(*c*)	0.58239(6)	0.14952(5)	0.63296(7)	0.58240	0.14956	0.63300	-0.01	-0.01	-0.01	0.18
W3	3(*a*)	0.43285(6)	0.85040(5)	0.03363(7)	0.43286	0.85044	0.03367	-0.01	-0.01	-0.01	0.18
W2	3(*a*) 6(*c*)	0.56723(6)	0.14953(5)	0.03355(7)	0.56718	0.14957	0.03367	0.01	-0.01	-0.01	0.18
W4	3(*a*)	0.41755(6)	0.85039(5)	0.63288(7)	0.41761	0.85043	0.63300	-0.01	-0.01	-0.01	0.18
W5	3(*a*) 6(*c*)	0.62811(6)	0.99127(6)	0.03078(8)	0.62813	0.99124	0.03096	-0.01	0.01	-0.01	0.19
W8	3(*a*)	0.63684(6)	0.00879(6)	0.63554(8)	0.63686	0.00876	0.63571	-0.01	0.01	-0.01	0.19
W6	3(*a*) 6(*c*)	0.37191(6)	0.00870(6)	0.03085(8)	0.37191	0.00874	0.03096	0.00	-0.01	-0.01	0.19
W7	3(*a*)	0.36317(6)	0.99122(6)	0.63560(8)	0.36317	0.99126	0.63571	0.00	-0.01	-0.01	0.19
W9	3(*a*) 6(*c*)	0.55323(6)	0.84685(5)	0.84395(8)	0.55323	0.84689	0.84408	0.00	-0.01	-0.01	0.18
W12	3(*a*)	0.70634(5)	0.15308(5)	0.82246(8)	0.70634	0.15311	0.82259	0.00	-0.01	-0.01	0.18
W10	3(*a*) 6(*c*)	0.29367(5)	0.84687(5)	0.82233(8)	0.29367	0.84692	0.82250	0.00	-0.01	-0.01	0.18
W11	3(*a*)	0.44676(6)	0.15304(5)	0.84400(8)	0.44676	0.15308	0.84417	0.00	-0.01	-0.01	0.18
Co1	3(*a*),3(*b*)	0.5001 (2)	0.0000(2)	0.8333(3)	0.5001	0	5/6	0.00	0.00	0.00	0.16
O1	3(*a*) 6(*c*)	0.4199(10)	0.2239(9)	0.8115(13)	0.4203	0.2244	0.8117	-0.01	-0.01	-0.01	0.19
O13	3(*a*)	0.1963(9)	0.7750(9)	0.8548(14)	0.1960	0.7756	0.8550	0.01	-0.01	-0.01	0.20
O2	3(*a*) 6(*c*)	0.4093(9)	-0.0657(8)	0.0699(11)	0.4089	-0.0658	0.0697	0.01	0.01	0.01	0.19
O5	3(*a*)	0.4743(9)	0.0659 (9)	0.5972(12)	0.4747	0.0658	0.5970	-0.01	0.01	0.01	0.18
O3	3(*a*) 6(*c*)	0.5912(10)	0.0661(9)	0.0695(12)	0.5921	0.0666	0.0695	-0.02	-0.01	0.00	0.19
O4	3(*a*)	0.5264(10)	-0.0671(9)	0.5971 (11)	0.5255	-0.0666	0.5971	0.02	-0.01	0.00	0.18
O6	3(*a*) 6(*c*)	0.6861(9)	0.0660(8)	0.9238(12)	0.6860	0.0664	0.9234	0.01	-0.01	0.01	0.18
O18	3(*a*)	0.6195(8)	-0.0668(8)	0.7436(11)	0.6196	-0.0664	0.7433	-0.01	-0.01	0.01	0.17

O7	3(*a*)	0.5773(10)	0.7738(9)	0.8136(13)	0.5784	0.7744	0.8131	-0.02	-0.01	0.01	0.16
	6(*c*)										
O10	3(*a*)	0.8052(9)	0.2250(9)	0.8540(14)	0.8041	0.2256	0.8535	0.02	-0.01	0.01	0.20
O8	3(*a*)	0.3152(9)	0.7901(8)	0.7103(12)	0.3146	0.7913	0.7125	0.01	-0.02	-0.03	0.23
	6(*c*)										
O11	3(*a*)	0.5228(9)	0.2076(8)	0.9520(11)	0.5234	0.2087	0.9542	-0.01	-0.02	-0.03	0.17
O9	3(*a*)	0.4755(8)	0.7915(8)	0.9555(11)	0.4755	0.7911	0.9556	0.00	0.01	-0.01	0.17
	6(*c*)										
O12	3(*a*)	0.6844(10)	0.2093(8)	0.7109(11)	0.6844	0.2089	0.7110	0.00	0.01	-0.01	0.18
O14	3(*a*)	0.4658(9)	0.0924(9)	0.1117(12)	0.4657	0.0931	0.1102	0.01	-0.01	0.02	0.18
	6(*c*)										
O26	3(*a*)	0.3725(9)	-0.0938(8)	0.5579(12)	0.3726	-0.0931	0.5564	-0.01	-0.01	0.02	0.18
O15	3(*a*)	0.7287(8)	0.0929(8)	0.7129(13)	0.7278	0.0937	0.7130	0.02	-0.02	-0.01	0.19
	6(*c*)										
O19	3(*a*)	0.6333(9)	-0.0945(9)	0.9536(11)	0.6341	-0.0937	0.9537	-0.02	-0.02	-0.01	0.17
O16	3(*a*)	0.6456(9)	0.1788(9)	0.9226(11)	0.6456	0.1780	0.9225	0.00	0.02	0.01	0.17
	6(*c*)										
O20	3(*a*)	0.4676(9)	0.8228(8)	0.7443(12)	0.4676	0.8220	0.7442	0.00	0.02	0.01	0.18
O17	3(*a*)	0.5333(9)	0.1784(9)	0.7454(11)	0.5323	0.1784	0.7451	0.02	0.00	0.01	0.17
	6(*c*)										
O25	3(*a*)	0.3529(9)	0.8216(9)	0.9220(12)	0.3539	0.8216	0.9216	-0.02	0.00	0.01	0.18
O21	3(*a*)	0.6219(10)	0.2246(8)	0.1239(10)	0.6218	0.2247	0.1250	0.01	-0.01	-0.01	0.18
	6(*c*)										
O24	3(*a*)	0.3969(10)	0.7753(9)	0.5406(12)	0.3971	0.7753	0.5417	-0.01	0.00	-0.01	0.20
O22	3(*a*)	0.6032(10)	0.2235(9)	0.5402(12)	0.6030	0.2237	0.5408	0.01	-0.01	-0.01	0.20
	6(*c*)										
O28	3(*a*)	0.3792(11)	0.7760(9)	0.1252(12)	0.3793	0.7763	0.1259	-0.01	-0.01	-0.01	0.20
O23	3(*a*)	0.5329(9)	-0.0939(8)	0.1077(12)	0.5335	-0.0934	0.1080	-0.01	-0.01	-0.01	0.18
	6(*c*)										
O36	3(*a*)	0.6275(10)	0.0929(10)	0.5583(11)	0.6269	0.0934	0.5587	0.01	-0.01	-0.01	0.19
O27	3(*a*)	0.3108(10)	0.0120(11)	0.5408(13)	0.3110	0.0127	0.5419	-0.01	-0.01	-0.01	0.21
	6(*c*)										
O33	3(*a*)	0.2986(11)	-0.0114(11)	0.1237(14)	0.2983	-0.0117	0.1248	0.01	0.01	-0.01	0.22
O29	3(*a*)	0.2723(9)	-0.0934(9)	0.7124(13)	0.2725	-0.0927	0.7122	-0.01	-0.01	0.01	0.19
	6(*c*)										
O39	3(*a*)	0.3654(9)	0.0920(9)	0.9546(13)	0.3652	0.0927	0.9544	0.01	-0.01	0.01	0.20
O30	3(*a*)	0.3790(10)	0.0652(9)	0.7448(12)	0.3783	0.0656	0.7443	0.01	-0.01	0.01	0.19
	6(*c*)										
O37	3(*a*)	0.3121(9)	-0.0661(8)	0.9228(12)	0.3127	-0.0656	0.9224	-0.01	-0.01	-0.01	0.18
O31	3(*a*)	0.4157(9)	-0.0596(9)	0.7471(12)	0.4155	-0.0606	0.7485	0.01	0.02	-0.02	0.18
	6(*c*)										
O40	3(*a*)	0.4760(9)	0.0616(9)	0.9169(13)	0.4759	0.0606	0.9182	0.01	0.02	-0.02	0.19

O32	3(*a*)	0.7005(11)	0.0123(11)	0.1240(15)	0.7003	0.0124	0.1251	0.01	-0.01	-0.01	0.22
O35	6(*c*) 3(*a*)	0.6878(11)	-0.0125(11)	0.5404(15)	0.6879	-0.0124	0.5415	-0.01	-0.01	-0.01	0.23
O34	3(*a*)	0.5853(8)	0.0628(8)	0.7475(8)	0.5855	0.0628	0.7484	0.01	0.00	-0.01	0.19
O38	6(*c*) 3(*a*)	0.5228(9)	-0.0627(9)	0.9174(12)	0.5227	-0.0628	0.9183	0.01	0.01	0.01	0.18
O*W*1	3(*a*)	0.4984(8)	-0.0012(9)	0.2741(10)	0.4989	-0.0003	0.2746	-0.01	-0.02	-0.01	0.16
O*W*2	6(*c*) 3(*a*)	0.4997(10)	-0.0007(9)	0.3917(11)	0.4992	0.0003	0.3921	0.01	-0.02	-0.01	0.18
O*W*3	3(*a*)	0.3480(12)	0.8812(12)	0.3186(15)	0.3470	0.8817	0.3186	0.02	-0.01	0.00	0.23
O*W*6	6(*c*) 3(*a*)	0.4644(12)	0.1177(12)	0.3481(15)	0.4654	0.1183	0.3481	-0.02	-0.01	0.00	0.24
O*W*4	3(*a*)	0.5340(12)	0.8835(12)	0.3496(14)	0.5344	0.8829	0.3505	-0.01	0.01	-0.01	0.23
O*W*5	6(*c*) 3(*a*)	0.6520(12)	0.1176(12)	0.3154(15)	0.6515	0.1171	0.3162	0.01	0.01	-0.01	0.23
O*W*7	3(*a*)	0.8684(16)	0.1317(16)	0.997(2)	0.8681	0.1322	0.997	0.01	-0.01	0.00	0.29
O*W*8	6(*c*) 3(*a*)	0.7357(15)	0.8674(16)	0.669(2)	0.7359	0.8678	0.669	-0.01	-0.01	0.00	0.29
O*W*9	3(*a*),3(*a*)	0.742(3)	0.000(3)	0.334(4)	0.742	0	⅓	0.00	0.00	0.01	0.39
O*W*10	3(*a*),3(*b*)	0.805(3)	0.804(3)	0.500(4)	0.8045	0.8045	½	0.01	-0.01	0.00	0.42
O*W*11	3(*a*),3(*b*)	0.801(2)	-0.004(3)	0.836(4)	0.801	0	⅚	0.00	-0.08	0.04	0.40
O*W*12	3(*a*),3(*a*)	0.259(4)	-0.003(4)	0.337(5)	0.259	0	⅓	0.00	-0.06	0.05	0.48