Supplementary Data for BK5021

Systematic Prediction of New Ferroelectrics in Space Group *R*3. I

Contextual material

2. Predicted new inorganic ferroelectrics in space group *R*3

2.1. $Te(OH)_6 \cdot NaF$

Allmann (1976); Mo $K\alpha$, graphite monochromator; 231 unique F_{obs}; absorption corrections; final $R = 0.03$, unit weights, u_{iso}.

2.2. $MgSO_3 \cdot 6H_2O$ family

Andersen & Lindqvist (1984); monochromated neutrons, $\lambda = 1.21$ Å; 1,049 F_{obs}, 325 unique $I_{obs} \geq 3\sigma(I_{obs})$; absorption and secondary extinction corrections, u_{iso}; $wR = 0.049$ for all F_{obs}. Bats *et al*. (1986); 120 K; combined X-ray and neutron diffraction, Mo $K\alpha$, graphite monochromator; 3,245 F_{obs} including $F_{obs} = 0$ for $F^2_{obs} < 0$; absorption, unaveraged F_{obs} for extinction corrections, u_{iso}; $\lambda_{neutron} = 0.8977$ Å, 2,228 F_{obs}; absorption, unaveraged F_{obs} for extinction corrections, u_{iso}; final $R_{XRD} = 0.018$, $wR = 0.017$; $R_{ND} = 0.038, 0.042$; 9 independent atoms.

2.3. $Li_3P_3O_9 \cdot 3H_2O$

Masse *et al.* (1973); Mo $K\alpha$; no absorption correction; 540 independent F_{obs}, u_{iso}; final $R = 0.039$; 8 independent atoms, two of which are unreported H atoms.

2.4. $SeNbF_9$

Edwards & Jones (1970); Mo $K\alpha$; 724 independent F_{obs}, photometered film; no absorption correction, u_{iso}; R = 0.090; 16 independent atoms.

2.5. $Al_2(H_2PO_4)_3PO_4 \cdot 6H_2O$

Kniep & Wilms (1979); Cu Kα; no absorption corrections; 503 independent $F_{obs} > 3\sigma(F_{obs})$; u_{aniso} for Al and P, u_{iso} for the O atoms varied in refinement but not reported; final R = 0.081; 18 independent atoms including 6 unreported H atoms.

2.6. $[Cr(OCN_2H_4)_6] \cdot [(Co(NH_3)_2(NO_2)_4]_3 \cdot (CCl_4)_{0.5} \cdot (H_2O)_{1.5}$

Rau *et al.,* (1982); Mo $K\alpha$; 1,842 unique $I_{obs} > 1.96\sigma(I_{obs})$; final R = 0.059; 67 independent atoms, 15 H undetermined; $u_{iso/aniso}$ not reported.

2.7. $Mg_2Al_2SiO_5(OH)_4$ (Amesite - $6R_2$)

Steadman & Nuttal (1962); Cu $K\alpha$; 112 unique I_{obs}, visually estimates, Weissenberg films; final R = 0.18; neither uncertainties nor u determined; 16 independent atoms.

2.8. $NaZnBr_3 \cdot 5H_2O$

Brehler & Rott (1970); 475 F_{obs}; u_{aniso}, R = 0.063; 11 independent atoms including 5 H undetermined.

2.9. III-Ag_3SI

Perenthaler *et al.* (1981); Mo $K\alpha$, graphite monochromator; absorption, extinction corrections;

54 independent $I_{obs} > 3\sigma(I_{obs})$ at 135 K; u_{aniso}, site population varied, 16-domain scattering model; final $R_F = 0.08$; transition from phase II-($Pm3m$) to phase III-($R3$) Ag_3SI at $T_C = 155$ K; pyroelectric. Hull *et al.* (2001); $\lambda_{neutron}$ not stated, high-resolution powder diffraction; 4,063 data points at 10(1) K; u_{aniso}(Ag), u_{iso}(S, I), $R_{exp} = 0.0139$, $R_w = 0.0378$ for 35 parameters.

2.10. $(LiTaO_3)_9 \cdot Ta_2O_5$

Santoro *et al*., (1982); Cu(220) monochromatized $\lambda_{neutron} = 1.543$ Å; powder profile, Rietveld refinement, u_{iso}; $R_n = 0.0437$, $R_w = 0.0934$ for 9 independent atoms.

2.11. Tl_2S (carlinite)

Ketelaar & Gorter (1939); powder pattern; Cu $K\alpha$; initial investigation. Man (1970); single crystal electron diffraction, photometric intensities; single overall B parameter, $R_{hkl} = 0.258$; 11 independent atoms. Radke & Dickson (1975); perfect basal cleavage; no phase transition detected below $T_m = 722(5)$ K; powder pattern with Cu $K\alpha$, $a = 12.12(1)$, $c = 18.175(5)$ Å in agreement with Ketelaar & Gorter's (1939) values of 12.20(7) and 18.17(6) Å; characterized mineral carlinite as isostructural with synthetic Tl_2S. Giester *et al.* (2002); Mo $K\alpha$, graphite monochromator, CCD area detector; perfect cleavage parallel to (001); numerical absorption and extinction corrections; 2,449 independent $F^2_{obs} > 4\sigma F^2_{obs}$, $R_F = 0.055$, $wR_F^2 = 0.132$; 1,014 independent $F^2_{obs} > 4\sigma F^2_{obs}$ with $\theta < 24.5°$, $R_F = 0.039$.

2.12. $Ba_3Yb_4O_9$ family

Krüger & Müller-Buschbaum (1983); λ not stated; modified absorption correction; 384 unique $F_{obs} \geqslant 6\sigma(F_{obs})$, u_{iso}; final $R = 0.083$, $wR = 0.077$, 10 independent atoms.

2.13. $Fe_{12}As_5$ family

Maaref *et al.*, (1983); at ambient pressure, single crystals form only if 15 % of the Fe is substituted for by Ru; Ag $K\alpha$; no absorption correction; 424 independent $I_{obs} > 9\sigma(I_{obs})$; unit weights, u_{aniso}, $R = 0.039$.

2.14. $Sr_{17}Ta_{10}S_{42}$

Onoda *et al.*, (1993); electron diffraction and Cu $K\alpha$ powder diffraction; total profile Rietveld analysis; u_{iso}, $R_I = 0.024$, $R_F = 0.014$, $R_P = 0.064$; dark brown insulator; 26 independent atoms.

2.15. Pd_8Sb_3

Man & Imamov (1979); λ, unstated; overall $B = 0.75$ Å^2; 24 independent atoms; final $R = 0.187$. Wopersnow & Schubert (1976); Cu $K\alpha$, Weissenberg films, visual estimation; 552 F_{obs}, absorption corections, u_{iso}; $R = 0.14$ in space group $R3c$.

2.16. II-BaB_2O_4

Three determinations: Lu *et al.,* (1982); space group $R3$; λ, unstated; 693 independent reflections; block-diagonal least squares refinement, u_{aniso}, $R = 0.046$; uncertainties not given; 13 independent atoms. Fröhlich (1984); space group $R3c$; Mo $K\alpha$; ground spherical crystal; 531 independent reflections; extinction and spherical absorption corrections; u_{aniso}, $R = 0.027$, $wR = 0.025$. Ito *et al.,* (1990); space group $R3c$; Mo $K\alpha$; ground spherical crystal; 1,359 independent reflections with $F_{obs} > 3\sigma(F_{obs})$; extinction, spherical absorption corrections; u_{aniso}, final $R = 0.0116$, $wR = 0.0116$ following multipole refinement.

2.17. $CsCd(NO_2)_3$ family

Himmelreich (1998); Mo Kα, graphite monochromator; analytical absorption corrections; 2,066 unique F_{obs}; u_{aniso}, final R = 0.0125, wR = 0.0125; 5 independent atoms. Avdeev & Kharton (2002); Cu *K*α**,** graphite monochromator, powder diffraction; 4,501 data points, 36 parameters, u_{iso}, R_p = 0.0694, R_{wp} = 0.0892.

2.18. $Sc_7I_{12}C$ family

Dudis *et al.*, (1986); Mo *K*α, graphite monochromator; empirical absorption corrections; 1,209 unique $F_{obs} > 3\sigma(F_{obs})$; final R = 0.045, wR = 0.048 for $Sc_7I_{12}C$.

3. Structures reported in space group *R*3 that more likely are in crystal class 3*m*

3.1 $CsGeCl_3$ family

Christensen & Rasmussen (1965); Mo *K*α; Weissenberg film photometry; no absorption correction; 132 unique F_{obs} at 298 K; u_{iso}, final R = 0.087; 3 independent atoms. Thiele *et al.* (1987); Ag *K*α; 254 unique $I_{obs} > 3\sigma(I_{obs})$; absorption corrections; u_{aniso}, R = 0.0218, wR = 0.0196; space group *R*3*m*. Yamada *et al.* (1993); Cu *K*α; Rietveld powder profile refinement, 10-80° 2θ; R_p = 0.094, R_F = 0.080 in space group *R*3*m.*

3.2. $Sn_3PO_4F_3$

Berndt (1972); Cu *K*α; no absorption correction; 160 independent visually-estimated reflections, u_{iso}, R = 0.076; 5 independent atoms.

3.3. Ag_8GeTe_6

von Ünterrichter & Range, (1986); pseudocubic single crystals from the pseudobinary Ag_2Te–$GeTe_2$ system, rhombohedral angle $\alpha = 60.0^o$; Mo $K\alpha$; 1,042 unique F_{obs}, u_{aniso}, final $R = 0.0598$; full site occupancy only by the single Ge and four Te atoms; 18 independent atoms.

3.4. $(Na_2CaZr(Si_6O_{12}(OH, O)_6).H_2O$ (lovozerite)

Yamnova *et al.*, (2001); Mo$K\alpha$, graphite monochromator; 753 unique F_{obs}; u_{aniso}, $R = 0.077$; 11 independent atoms.

3.5. $BiCa_9(VO_4)_7$

Evans *et al.*, (2001); Mo$K\alpha$, CCD area detector; sample at 120 K; 3,375 independent $F^2_{obs} > 3\sigma(F^2_{obs})$; u_{aniso}, final $R = 0.0409$, $wR = 0.0423$; 36 unique atoms; second harmonic signal ~$3d_{1\mu}(KH_2PO_4)$. Kim *et al.* (2002); Mo$K\alpha$, graphite monochromator; 772 independent $F_{obs} > n(F_{obs})$, n not specified; u_{aniso}, final $R = 0.0539$, $wR^2 = 0.1283$; 17 unique atoms.

4. Structures reported in space group *R*3 that more likely are nonpolar

4.1. $Co_2Ge_3S_3$ skudderite family

Korenstein *et al.* (1977); Mo $K\alpha$; absorption corrections; 1,993 total F_{obs}, u_{iso}, final $R = 0.115$. Partik *et al.* (1996); Mo $K\alpha$, graphite monochromator; absorption corrections; multiple merohedral twinning; 6,404 total unique F_{obs}, u_{aniso}, final $R = 0.0374$; 12 independent atoms.

4.2. $K_2Sn_2O_3$

Braun & Hoppe (1978); Mo $K\alpha$; 348 unique F_{obs}; no absorption corrections; u_{aniso}, final $R =$

0.047; 5 independent atoms.

4.3. $[Cr(H_2O)_6]F_3 \cdot (H_2O)_3$

Epple & Massa, (1978); λ not stated; absorption correction; 521 unique $I_{obs} > 0$; u_{aniso}, final R = 0.047; 11 independent atoms.

4.4. $Cs[SbF_5OH]$

Nolte and de Beer (1979); Mo $K\alpha$, graphite monochromator; neither absorption nor extinction corrections; 328 $I_{obs} > 1.65\sigma(I_{obs})$, unit weights, u_{aniso}, final R = 0.051; 4 independent atoms. Space group $R3$ chosen rather than $R\bar{3}$ with its final R = 0.057.

4.5. $B_3N_3Cl_6$

Three determinations reported. Mueller (1971); Cu $K\alpha$ Weissenberg and Mo $K\alpha$ precession photometry; absorption corrections; 153 unique F_{obs}; u_{iso}, final R = 0.045; 4 independent atoms. Haasnoot *et al.*, (1972); Mo $K\alpha$, balanced filters; absorption and extinction corrections; 735 unique $F_{obs} > 2\sigma(F_{obs})$, 46 < $2\sigma(F_{obs})$; u_{aniso}, final R = 0.0269, wR = 0.0334. Gopinathan *et al.*, (1974); reinterpreted Haasnoot *et al.*'s (1972) diffraction data with all B-N bonds constrained equal based on molecular-orbital calculations; final R = 0.0254, wR = 0.0272.

4.6. Li_7SbO_6

Hauck (1969); brief report; Cu $K\alpha$; powder pattern; refinement with 27 reflections; R = 0.110 in $R3$, 0.159 in $R\bar{3}$ with $R3$ chosen**;** neither uncertainties nor u values provided; 6 independent atoms.

4.7. $Fe_2P_2Se_6$ and family

Klingen *et al.* (1973); Cu $K\alpha$; Weissenberg films, photometry; absorption corrections; *u* not reported, 138 unique F_{obs}, R = 0.140 in space group $R3$, 0.178 in $R\bar{3}$; 6 independent atoms. Wiedenmann *et al.* (1981); isomorphous $Fe_2P_2Se_6$ and $MnPSe_3$; $\lambda_{neutron} = 2.475$ Å; powder patterns between T = 4.2 and 170 K; paramagnetic-to-antiferromagnetic phase transition T_N = 119(1) K; *u* not reported, $R(FePSe_3)$ = 0.11 at 154 K, $R(MnPSe_3)$ = 0.02 at 100 K, both in space group $R\bar{3}$.

4.8. Ni_3TeO_6

Newnham & Meagher (1967); Cu $K\alpha$; 35 independent I_{obs} from powder pattern; neither *u* nor uncertainties reported, lowest R_I = 0.12, in space group $R3$; 6 independent atoms.

4.9. $2CeFCO_3 \cdot CaCO_3$ (parisite)

Donnay & Donnay, (1953); ionic packing considerations within a smaller pseudocell and the symmetry of space group $R3$ led to the coordinate set on which Table S29 with its 26 independent atoms is based. Ni *et al*. (2000) solved and refined the structure to R = 0.044 in monoclinic space group *Cc* with $\beta = 98.257°$.

4.10. $3CeFCO_3 \cdot 2CaCO_3$ (röntgenite)

Donnay & Donnay, (1953); approach used similar to that for parisite in §4.9; 18 independent atoms; space group $R3$.

4.11. $NiTiO_3$ and $CoTiO_3$

Sullivan & Pavlovic (1962); Abstract only, no experimental details.

4.12. $Er_{13}Ge_6O_{31}(OH)$

Genkina *et al.*, (1990); Mo $K\alpha$; empirical absorption correction; 2,406 $I_{obs} \geqslant 3\sigma(I_{obs})$; u_{aniso}, R = 0.041 in $R\bar{3}$, 0.037 in $R3$; 19 independent atoms.

4.13. II-$In_4(P_2Se_6)_3$

Voroshilov *et al.*, (1991): three phases with composition $In_4(P_2Se_6)_3$ identified in In_2Se_3–P_2Se_4 system. Phase III may be isostructural with monoclinic $In_4(P_2S_6)_3$. Phase I has not been fully determined. Phase II; Cu $K\alpha$, Ni-filter; powder pattern above 713 K, not presented; final R = 0.0795 for single overall u_{iso} = 0.06 Å; 6 independent atoms; unspecified test for piezoelectricity claimed positive.

4.14. $NaNi(AsO_4)$

Range & Meister, (1984); Mo $K\alpha$, graphite monochromator; 855 independent $F_{obs} > 5\sigma(F_{obs})$; absorption corrected; strong parameter correlations; u_{iso}, R = 0.045 in $R3$; 10 independent atoms.

4.15. Mg_3In

Schubert *et al.*, (1963); Cu $K\alpha$, Guinier pattern; 41 I_{obs}, many multiple *hkl* lines; idealized structure, coordinates estimated to nearest $^1/_{12}$; 8 independent atoms, overall B factor.

4.16. $AsTe_2I{\cdot}0.5H_2O$

Stergiou, (1994); Mo *K*α, graphite monochromator; 501 independent $F_{obs} > 3\sigma(F_{obs})$; absorption corrections; common scattering factor for Te and I, u_{aniso}; $R = 0.051$ in $R3$; 2 H undetermined, 5 independent atoms refined.

4.17. Au_5Sn

Osada *et al.*, (1974); Mo*K*α; 22 absorption-corrected $F(h0l)$; $R_{h0l} < 0.04$ in $R3$; neither uncertainties nor u reported; phase transition at $T_{PT} \approx 468$ K with entropy change ≈ 2.22 J mol^{-1} K^{-1} from heat capacity, $T_{PT} \approx 459$ K from resistivity measurements.

4.18. $InBrI_2$

Kniep & Blees, (1984); λ not stated; 487 unique reflections; u_{aniso}, $R = 0.046$ in $R3$, 0.050 in $R\bar{3}$; 4 independent atoms.

4.19. $H_3O^+{\cdot}Al_4SiP_3O_{16}^-{\cdot}nH_2O$

Ito *et al.*, (1985); Mo *K*α; neither absorption nor extinction corrections; 1,011 unique $F_{obs} > 3\sigma(F_{obs})$; u_{aniso}, final $R = 0.067$ in $R3$, H atoms not located; 20 independent non-H atoms. Refinement of this zeolite structure in $R\bar{3}$ led to $R = 0.08$, hence $R3$ was assumed.

5. Structures reported in space group *R*3 with lower predictability

5.1. $(NH_4)_3Sc(SeO_4)_3$

Valkonen & Niinistö (1978); Mo *K*α, graphite monochromator; ϕ-scan absorption correction; 1,028 $I_{obs} > 3\sigma(I_{obs})$; u_{aniso}, final $R = 0.063$; 14 independent atoms.

5.2. $Cu_7As_6Se_{13}$

Takeuchi & Horiuchi (1972); Cu $K\alpha$; Weissenberg films, photometry; cylindrical absorption corrections; 517 unique F_{obs}; u_{iso}, final $R = 0.148$; 10 independent atoms; semiconductor.

5.3. $MgHPO_3 \cdot 6H_2O$

Powell *et al.*, (1994); Cu $K\alpha$; 108 K; 352 independent $F_{obs} > 4\sigma(F_{obs})$; empirical absorption and extinction corrections, u_{aniso}; $R = 0.0209$, $wR = 0.0255$. Also, $\lambda_{neutrons} = 1.063(1)$ Å, 293 K; extinction corrected; 396 independent F_{obs} with 361 $F_{obs} > 2\sigma(F_{obs})$, u_{aniso}; $R = 0.041$, $wR = 0.023$; 10 independent atoms; structure first reported by Corbridge (1967).

5.4. Cronstedtite-6R

Steadman & Nuttal (1963); Co $K\alpha$, Mo $K\alpha$; visual intensity estimates; projections along [010] and $[1\bar{1}0]$, u not determined, final $R = 0.15$; 16 independent atoms.

5.5. $Cu_6Hg_3As_4S_{12}$ (aktashite) and $Cu_6Zn_3As_4S_{12}$ (nowackiite)

Aktashite (A) (Kaplunnik *et al.,* 1980), nowackiite (N) (Marumo, 1967), Nowacki (1982); A; Mo $K\alpha$, graphite monochromator; 758 unique I_{obs}, u_{iso}, $R = 0.081$; 9 independent atoms. N; Cu $K\alpha$, Weissenberg films, photometry; absorption corrections; 637 unique F_{obs}, u_{iso}, final $R = 0.078$; 9 independent atomic sites.

5.6. $Na_{0.55}TiS_2$

Rouxel *et al.,* (1971); X-ray powder pattern, λ not stated; $Na_{1-x}TiS_2$ phase with $0.4 < x < 0.7$;

neither uncertainties nor *u* reported; 15 I_{obs}, $R_{(undefined)}$ = 0.10; 4 (or 5) independent atoms.

5.7. $H_6As_{6.3}Cu_{0.84}FeMg_{0.1}Mn_{13.9}O_{33}Si_{17}$ (dixenite)

Araki & Moore (1981); Mo *K*α, graphite monochromator; 2,507 $F_{obs} > 1.4\ \sigma(F_{obs})$ including Bijvoet pairs; u_{aniso}, R = 0.064, wR = 0.065; 28 independent atom sites.

5.8. $[C(NH_2)_3]_6As_2Mo_{18}O_{62}{\cdot}9H_2O$

Ichida & Sasawaki (1983); Mo*K*α; absorption corrections; 3,560 unique $F_{obs}^2 > 3\sigma(F_{obs}^2)$; u_{iso}, R = 0.041, wR = 0.040.

5.9. $H_{0.8}Ca_{1.77}Ce_{2.1}Cl_{0.73}Fe_{1.41}K_{0.19}Mn_{3.7}Na_{13.61}Nb_{0.92}O_{76}Si_{25}Y_{0.25}Zr_{3.17}$ (oneillite)

Johnsen & Grice (1999); Mo*K*α; ground spherical crystal, absorption corrections; 3,803 $I_{obs} > 2\sigma(I_{obs})$; u_{aniso}, R =0.032, wR^2 = 0.072; 49 independent atoms reported.

5.10. $AlCa_3Cd_{17}$

Cordier *et al.*, (1999); Mo*K*α, graphite monochromator; absorption corrections; 1,027 independent F^2_{obs}; u_{iso}, final R = 0.061; 60 independent atoms.

Supplementary Data for BK5021

Systematic Prediction of New Ferroelectrics in Space Group *R*3. I

Tables S1 – S48

Table S1.
Atomic positions for $MgSO_3 \cdot 6H_2O$ at room temperature (Anderson & Lindqvist, 1984). The original rhombohedral atomic coordinates are transformed to hexagonal axes.
$a_H = 8.838(3)$, $c_H = 9.083(3)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
Mg	3(*a*),3(*a*)	0	0	0	0	0	0.	0	0	0.	0.0	0.13
S	3(*a*),3(*b*)	0	0	0.5021(6)	0	0	0.5	0	0	0.19	0.19	0.14
O1	9(*b*),9(*e*)	0.1268(3)	0.1765(3)	0.4330(3)	0.1517	0.1517	0.5	-0.61	0.61	-0.57	0.83	0.15
Ow1†	9(*b*)	0.0046(3)	-0.1869(3)	0.1915(3)	-0.0214	-0.1653	0.1822	0.23	-0.19	0.08	0.23	0.17
Ow2	18(*f*) 9(*b*)	0.0474(3)	0.1437(3)	-0.1728(3)	0.0214	0.1653	-0.1822	0.23	-0.19	0.08	0.23	0.15
H1	9(*b*)	0.0713(5)	-0.2458(5)	0.1215(5)	0.0865	-0.2235	0.1417	-0.13	-0.20	-0.18	0.34	0.20
H2	18(*f*) 9(*b*)	-0.1016(5)	0.2012(5)	-0.1620(5)	-0.0864	0.2235	-0.1418	-0.13	-0.20	-0.18	0.34	0.26
H3	9(*b*)	0.0262(5)	-0.1561(5)	0.2475(5)	-0.0372	-0.2227	0.2052	0.56	0.59	0.38	1.07	0.27
H4	18(*f*) 9(*b*)	0.1005(5)	0.2893(5)	-0.1630(5)	0.0372	0.2227	-0.2052	0.56	0.59	-0.38	1.07	0.22

† Reported values replaced by $\bar{y}$, *x*-*y*, *z* or *y*-*x*, $\bar{x}$, *z* with Ow1 and Ow2 designations interchanged.

Table S2

Atomic positions[‡] for $SeNbF_9$ at room temperature (Edwards & Jones, 1970) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and U_{iso} displacements in Å

$a = 13.03(2)$ Å, $c = 14.76(3)$. $z^* = z + 0.1291$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Se1[†]	9(*b*)	0.0921(8)	-0.2999(8)	0.5826(9)	0.0839	-0.2936	0.5803	0.11	-0.08	0.04	0.11	0.17(3)
	18(*f*)											
Nb1	9(*b*)	0.3711(7)	0.0757	0.4221(9)	0.3775	0.0839	0.4197	-0.08	-0.11	0.04	0.16	0.18(4)
Se2	9(*b*)	0.0001(7)	0.0001(7)	0.2486(9)	0.0001	0.0001	0.2594	0.00	0.00	-0.16	0.16	0.18(4)
	18(*f*)											
Nb2	9(*b*)	0.0001(7)	0.0001(7)	0.7298(11)	0.0001	0.0001	0.7406	0.00	0.00	-0.16	0.16	0.17(4)
F1	9(*b*)	0.022(9)	0.121(9)	0.659(11)	0.0171	0.1187	0.6738	0.07	0.03	-0.23	0.25	0.33(14)
	18(*f*)											
F9	9(*b*)	0.116 (6)	0.1068(6)	0.311(7)	0.1187	0.1015	0.3262	-0.03	0.07	-0.23	0.24	0.24(9)
F3	9(*b*)	-0.167 (4)	-0.269 (4)	0.490(5)	-0.1670	-0.2859	0.4872	0.00	0.22	0.05	0.13	0.19(8)
	18(*f*)											
F12	9(*b*)	-0.303(6)	-0.119 (6)	0.516(7)	-0.2859	-0.1189	0.5128	-0.22	0.00	0.05	0.12	0.26(10)
F4	9(*b*)	-0.403(4)	-0.363 (4)	0.495(5)	-0.4036	-0.3717	0.4911	0.01	0.11	0.06	0.13	0.19(8)
	18(*f*)											
F6	9(*b*)	-0.024(6)	-0.4057(5)	0.513 (7)	-0.0319	-0.4036	0.5089	0.11	-0.01	0.06	0.12	0.25(10)
F5	9(*b*)	-0.004(4)	-0.291(5)	0.657(5)	-0.0869	-0.2395	0.6564	1.08	-0.66	0.01	0.94	0.20(8)
	18(*f*)											
F8	9(*b*)	-0.189(11)	-0.403(11)	0.345(14)	-0.2395	-0.3192	0.3436	0.66	-1.08	0.01	0.94	0.37(15)
F2	9(*b*)	0.413(5)	-0.174(5)	0.519(6)	0.4586	-0.1812	0.5166	-0.59	0.09	0.03	0.55	0.23(9)
	18(*f*)											
F11	9(*b*)	-0.500(5)	0.189(5)	0.48667)	-0.4586	0.1812	0.4834	-0.596	0.09	0.02	0.56	0.21(8)
F7	9(*b*)	-0.266(6)	-0.256(6)	0.352(8)	-0.2128	-0.3209	0.3389	-0.68	0.85	0.19	0.80	0.27(10)
	18(*f*)											
F10	9(*b*)	0.160(8)	0.386(8)	0.6742(61)	0.2128	0.3209	0.6611	-0.68	0.85	0.19	0.80	0.30(13)

[†] Assuming the 18(*f*) site for Se and Nb is equally occupied by both atoms above T_c.

Table S3

Atomic positions for $Al_2(H_2PO_4)_3PO_4 \cdot 6H_2O$ at room temperature (Kniep & Wilms, 1979) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

$a = 9.066(4)$, $c = 17.45(1)$ Å. $z^* = z + 0.0079$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position *R*3, *R*32	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	u_{aniso} †
Al1	3(*a*) 6(*c*)	0	0	-0.1257(5)	0	0	-0.1290	0	0	0.06	0.06	n/r
Al2	3(*a*)	0	0	0.1322(5)	0	0	0.1290	0	0	0.06	0.06	n/r
P1	9(*b*),9(*d*)	0.2575(4)	0.0107(5)	0.0045(3)	0.2575	0	0	0	0.10	0.08	0.13	n/r
P2	3(*a*),3(*b*)	0	0	0.5079	0	0	½	0	0	0.14	0.14	n/r
O1	9(*b*) 18(*f*)	0.1530(13)	-0.0359(13)	-0.0686(7)	0.1375	-0.0029	-0.0734	0.14	-0.30	0.08	0.27	n/r
O2	9(*b*)	0.1580(13)	-0.0300(13)	0.0782(6)	0.1735	0.0029	0.0734	0.14	-0.30	0.08	0.27	n/r
O3	9(*b*) 18(*f*)	0.3594(16)	-0.0818(19)	0.0029(8)	0.3037	-0.1436	-0.0004	0.50	0.56	0.06	0.92	n/r
O4	9(*b*)	0.3916(13)	0.2053(11)	0.0037(6)	0.4473	0.1435	0.0004	-0.50	0.56	0.06	0.54	n/r
O5	3(*a*), 3(*b*)	0	0	0.4208(11)	0	0	½	0	0	-1.38	1.38	n/r
O6	9(*b*),9(*e*)	0.1525(11)	0.1705(12)	0.5379(6)	0.1615	0.1615	½	-0.08	0.08	0.66	0.66	n/r
O7	9(*b*) 18(*f*)	0.1858(11)	0.1341(11)	-0.1944(6)	0.1739	0.1523	-0.1976	0.11	-0.17	0.06	0.16	n/r
O8	9(*b*)	0.1705(12)	0.1620(11)	0.2007(7)	0.1523	0.1739	0.1976	0.17	-0.11	0.06	0.16	n/r

† Thermal parameters refined but not reported (n/r).

Table S4

Atomic positions for $[Cr(OCN_2H_4)_6]\cdot[(Co(NH_3)_2(NO_2)_4]_3\cdot(CCl_4)_{0.5}\cdot(H_2O)_{1.5}$ at room temperature (Rau *et al.,* 1982) with hypothetical $x'y'z'$ coordinates and Δx, Δy, Δz displacements in Å.
$a = 21.0070(80)$, $c = 18.810(7))$ Å, $z^* = z + 0.0090$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$u_{iso/aniso}$ [†]
	$R3,R\bar{3}$											
Co1	9(*b*)	0.2970(1)	0.3356(1)	0.6563(1)	0.2937	0.3418	0.6559	0.07	-0.13	0.01	0.11	n/r
	18(*f*)											
Co2	9(*b*)	0.3480(1)	0.0514(1)	0.3444(1)	0.3418	0.0481	0.3441	0.13	0.07	0.01	0.18	n/r
Cr1	3(*a*)	0	0	0.3047(1)	0	0	0.3073	0	0	-0.05	0.05	n/r
	6(*c*)											
Cr2	3(*a*)	0	0	0.6901(1)	0	0	0.6927	0	0	-0.05	0.05	n/r
Cl1[‡]	3(*a*), 3(*a*)	0	0	0.0801(2)	0	0	0.0856	0	0	-0.10	0.10	n/r
Cl2´		0	0	-0.0912	0	0	-0.0856	0	0	-0.10	0.10	n/r
Cl2,Cl1´	9(*b*), 9(*b*)	0.0869(2)	0.0542(2)	-0.0389(2)	0.0826	0 .0515	-0.0409	0.09	0.06	0.04	0.14	n/r
C1	3(*a*), 3(*a*)	0	0	0.9889(5)	0	0	0.0111	0.00	0.00	-0.21	0.21	n/r
O1[††]	9(*b*)	0.1295(3)	0.3039(3)	0.4635(2)	0.1295	0.3039	0.4635	0	0	0	0	n/r
	18(*f*)											
O22	*9(b)*	*0.8705*	*0.6961*	*0.5364*	*0.8705*	*0.6961*	*0.5364*	*0*	*0*	*0*	*0*	-
O2	9(*b*)	0.0892(3)	0.0571(3)	0.3648(2)	0.0580	0.0737	0.3663	0.66	-0.35	-0.03	0.57	n/r
	18(*f*)											
O4	9(*b*)	0.0903(3)	0.0468(3)	0.6322(3)	0.0737	0.0156	0.6337	0.35	0.66	-0.03	0.89	n/r
O3	9(*b*)	0.0301(3)	0.0879(3)	0.2464(2)	0.0057	0.0686	0.2480	0.51	0.41	-0.03	0.80	n/r
	18(*f*)											
O5	9(*b*)	0.0492(3)	0.0873(3)	0.7504(2)	0.0686	0.0629	0.7520	-0.41	0.51	-0.03	0.47	n/r
O6	9(*b*)	0.2499(4)	0.4140(4)	0.5769(3)	0.2790	0.3746	0.5517	-0.61	0.83	0.47	0.88	n/r
	18(*f*)											
O20	9(*b*)	0.3351(4)	0.1059(4)	0.4736(4)	0.3746	0.1350	0.4483	-0.83	-0.61	0.47	1.34	n/r
O7	9(*b*)	0.3623(4)	0.4546(4)	0.5668(3)	0.3758	0.4633	0.5749	-0.28	-0.18	-0.15	0.43	n/r
	18(*f*)											
O18	9(*b*)	0.4720(4)	0.0740(4)	0.4170(3)	0.4633	0.0875	0.4251	0.18	-0.28	-0.15	0.29	n/r
O8	9(*b*)	0.1984(4)	0.2394(4)	0.5479(3)	0.2010	0.2360	0.5585	-0.05	0.07	-0.20	0.22	n/r
	18(*f*)											
O21	9(*b*)	0.2326(4)	0.0325(4)	0.4310(4)	0.2360	0.0351	0.4415	-0.07	-0.05	-0.20	0.21	n/r
O9	9(*b*)	0.2996(4)	0.2406(4)	0.5554(3)	0.3192	0.3113	0.5590	-0.41	1.49	-0.07	1.36	n/r
	18(*f*)											
O19	9(*b*)	0.3820(4)	0.9725(4)	0.4375(3)	0.3113	0.9921	0.4410	1.49	-0.41	-0.07	1.36	n/r
O10	9(*b*)	0.2317(4)	0.2008(4)	0.7223(4)	0.2095	0.2140	0.7307	0.47	-0.28	-0.16	0.44	n/r
	18(*f*)											
O15	9(*b*)	0.2272(4)	0.0268(4)	0.2610(4)	0.2140	0.0046	0.2693	0.28	0.47	-0.16	0.68	n/r
O11	9(*b*)	0.3416(4)	0.2691(4)	0.7563(4)	0.3473	0.3288	0.7516	-0.12	-1.25	0.09	1.32	n/r
	18(*f*)											
O17	9(*b*)	0.3885(4)	0.9758(4)	0.2532(3)	0.3288	0.9815	0.2484	1.25	-0.12	0.09	1.20	n/r
O12	9(*b*)	0.2935(4)	0.3974(4)	0.7879(3)	0.2553	0.3552	0.7633	0.80	0.89	0.46	1.53	n/r
	18(*f*)											

O14	9(*b*)	0.3129(4)	0.1380(4)	0.2614(4)	0.3552	0.0998	0.2367	-0.89	0.80	0.46	0.97	n/r
O13	9(*b*)	0.3963(4)	0.4336(4)	0.7397(3)	0.3736	0.4370	0.7552	0.48	-0.07	-0.29	0.53	n/r
	18(*f*)											
O16	9(*b*)	0.4404(4)	0.0860(4)	0.2293(3)	0.4370	0.0634	0.2448	0.47	-0.41	-0.29	0.53	n/r
C2	9(*b*)	0.1170(5)	0.1198(5)	0.3935(5)	0.1086	0.1243	0.3972	0.18	-0.09	-0.07	0.17	n/r
	18(*f*)											
C4	9(*b*)	0.1288(6)	0.0241(6)	0.5991(5)	0.1243	0.0157	0.6028	0.09	0.18	-0.07	0.25	n/r
C3	9(*b*)	0.0913(6)	0.1331(6)	0.2151(5)	0.1110	0.1070	0.2178	-0.41	0.55	-0.05	0.50	n/r
	18(*f*)											
C5	9(*b*)	0.0301(6)	0.1306(6)	0.7795(6)	0.0040	0.1110	0.7822	0.55	0.41	-0.05	0.84	n/r
N1	9(*b*)	0.3043(5)	0.4130(5)	0.5912(5)	0.3422	0.4105	0.5912	-0.80	0.05	0.00	0.78	n/r
	18(*f*)											
N7	9(*b*)	0.4081(6)	0.0305(6)	0.4087(5)	0.4105	0.0684	0.4088	-0.05	-0.80	0.00	0.83	n/r
N2	9(*b*)	0.2593(5)	0.2828(5)	0.5805(5)	0.2419	0.2916	0.5772	0.37	-0.18	0.06	0.33	n/r
	18(*f*)											
N8	9(*b*)	0.3003(5)	0.0672(5)	0.4261(5)	0.2916	0.0498	0.4228	0.18	0.37	0.06	0.49	n/r
N3	9(*b*)	0.2889(5)	0.2582(5)	0.7224(5)	0.2443	0.2723	0.7202	0.94	-0.30	0.04	0.83	n/r
	18(*f*)											
N5	9(*b*)	0.2863(5)	0.0727(5)	0.2821(5)	0.2723	0.0281	0.2798	0.29	0.94	0.04	1.14	n/r
N4	9(*b*)	0.3329(5)	0.4051(5)	0.7371(5)	0.3482	0.4012	0.7355	-0.32	0.08	0.03	0.29	n/r
	18(*f*)											
N6	9(*b*)	0.3973(5)	0.0377(5)	0.2662(5)	0.4012	0.0530	0.2646	-0.08	-0.32	0.03	0.37	n/r
N9	9(*b*)	0.1961(5)	0.3083(5)	0.6804(5)	0.2026	0.3661	0.6666	-0.14	-1.21	0.26	1.31	n/r
	18(*f*)											
N11	9(*b*)	0.4239(5)	0.1569(5)	0.3473(5)	0.3661	0.1634	0.3334	1.21	-0.14	0.26	1.18	n/r
N10	9(*b*)	0.3983(5)	0.3598(5)	0.6333(5)	0.3833	0.3155	0.6462	0.32	0.93	-0.24	1.15	n/r
	18(*f*)											
N12	9(*b*)	0.2712(5)	-0.0528(5)	0.3410(5)	0.3155	-0.0678	0.3538	-0.93	0.32	-0.24	0.85	n/r
N13	9(*b*)	0.1832(5)	0.1457(5)	0.4247(5)	0.1770	0.1248	0.4191	0.13	0.44	0.11	0.53	n/r
	18(*f*)											n/r
N18	9(*b*)	0.1038(6)	0.9540(6)	0.5865(6)	0.1248	0.9478	0.5809	-0.44	0.13	0.11	0.41	
N14	9(*b*)	0.0859(5)	0.1611(5)	0.3973(5)	0.0962	0.1805	0.4079	-0.22	-0.41	-0.20	0.59	n/r
	18(*f*)											
N17	9(*b*)	0.1998(6)	0.0739(6)	0.5816(6)	0.1805	0.0842	0.5921	0.41	-0.22	-0.20	0.41	n/r
N15	9(*b*)	0.1458(5)	0.1197(5)	0.2102(5)	0.1671	0.1014	0.1973	-0.45	0.38	0.24	0.48	n/r
	18(*f*)											
N20	9(*b*)	0.0839(6)	0.1884(6)	0.8157(6)	0.0656	0.1671	0.8027	0.38	0.45	0.24	0.75	n/r
N16	9(*b*)	0.0957(5)	0.1934(5)	0.1872(5)	0.1085	0.1692	0.2065	-0.27	0.51	-0.36	0.57	n/r
	18(*f*)											
N19	9(*b*)	0.9637(6)	0.1213(6)	0.7742(6)	0.9394	0.1085	0.7935	0.51	0.27	-0.36	0.77	n/r

† $u_{iso/aniso}$ not reported (n/r).

‡ Assuming a 1.63 Å displacement by one of the three Cl2 atoms to the location 00*z*, thereby transforming it to Cl1′ and effectively rotating the CCl_4 solvate as that C-Cl1′ bond becomes oriented with sense opposite that of the original C-Cl1 bond.

†† At 3.05 Å from O8 and less than 3.00 Å from O11,O17, O21, N12 and N14, O1 is assumed to be the water O in the postulated 1.5 H_2O. If this location and stoichiometry is confirmable, a second water *O22* atom is likely located close to the inversion-related position $-x_{O1}$, $-y_{O1}$,$-z_{O1}$ with both locations only half-occupied.[4]

Table S5

Atomic positions for amesite-6R_2 $Mg_2Al_2SiO_5(OH)_4$ at room temperature (Steadman *et al.,* 1962), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.
$a = 5.31$, $c = 42.1$ Å. $z^* = z - 0.130$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u[†]
	$R3,R\bar{3}$											
Mg1,Al1[††]	9(b)	0.333	0.0	0.115	0.333	0.	0.083	0.	-0.	1.32	1.32	n/d
	18(f)											
Mg2,Al2	9(b)	0.667	0.	-0.052	0.667	0.	-0.083	0.	0.	1.32	1.32	n/d
Al3,Si1[‡]	3(a)	0	0	0.384	0	0	0.417	0	0	-1.37	-1.37	n/d
	6(c)											
Al6,Si4	3(a)	0.	0.	0.551	0	0	0.583	0.	0.	-1.37	-1.37	n/d
Al4, Si2	3(a)	0	0.	0.717	0	0	0.750	0.	0.	-1.39	-1.39	n/d
	6(c)											
Al5,Si3	3(a)	0.	0.	0.217	0	0	0.250	0	0	-1.39	-1.39	n/d
O1	3(a)	0.	0.	0.424	0.	0.	0.416	0.	0.	0.32	0.32	n/d
	6(c)											
O4	3(a)	0.	0.	0.591	0.	0.	0.584	0.	0.	0.31	0.31	n/d
O2	3(a)	0.	0.	0.757	0.	0.	0.750	0.	0.	0.29	0.29	n/d
	6(c)											
O3	3(a)	0.	0.	0.257	0.	0.	0.250	0.	0.	0.29	0.29	n/d
O10	3(a)	0.	0.	-0.076	0.	0.	-0.083	0.	0.	0.31	0.31	n/d
	6(c)											
O9	3(a)	0.	0.	0.091	0.	0.	0.083	0.	0.	0.31	0.31	n/d
O5	9(b)	0.525(25)	0.	0.037	0.596	0.	0.033	-0.38	0.	0.19	0.42	n/d
	18(f)											
8	9(b)	0.333	0.	-0.028	0.404	0.	-0.033	-0.38	0.	0.19	0.42	n/d
O6	9(b)	0.475(25)	0.	-0.130	0.404	0.	-0.135	0.38	0.	0.19	0.42	n/d
	18(f)											
O7	9(b)	0.667	0.	0.139	0.596	0.	0.135	0.38	0.	0.19	0.42	n/d

[†] u not determined (n/d).
[††] Mg, Al site occupancy 67, 33% respectively.
[‡] Al, Si site occupancy 50, 50% respectively.

Table S6

Atomic positions for III-Ag_3IS at room temperature (Perenthaler *et al.,* 1981), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

$a_R = 4.882(5)$ Å, $\alpha = 90.0°$. $z^* = z - 0.004$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position $R3$, $Pm\bar{3}m$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ag†	3(*b*),12(*h*)	0.015(1)	0.899(1)	0.5016(1)	0	0.899	0.5	0.07	0	0.01	0.07	0.23
I	1(*a*),3(*a*)	0.5	0.5	0.5	0.5	0.5	0.5	0	0	0	0	0.13
S	1(*a*),3(*b*)	0.036(1)	0.036(1)	0.036(1)	0.0	0.0	0.0	0.18	0.18	0.18	0.31	0.13

† Origin displaced ½,½,½ for direct comparison with Table 6, see §2.9.

Table S7

Atomic positions for $(LiTaO_3)_9{\cdot}Ta_2O_5$ in space group $R3$ (Santoro *et al.,* 1982).

$a = 5.1576(1)$, $c = 13.77842(2)$ Å. $z^* = z + 0.0152$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occ.
	$R3$, $R\bar{3}$												
Li1†	3(*a*)	0	0	0.2917(5)	0	0	0.2500	0	0	0.57	0.37	0.16	0.83
	6(*c*)												
Li2	3(*a*)	0	0	0.7917	0	0	0.75	0	0	0.57	0.37	0.16	0.83
Ta1	3(*a*),3(*a*)	0	0	0.0152	0	0	0.	0	0	0.21	0	0.08	1.0
Ta2	3(*a*),3(*b*)	0	0	0.5152	0	0	0.5	0	0	0.21	0	0.08	1.0
Ta3	3(*a*)	0	0	0.2882	0	0	0.25	0	0	0.53	0.32	0.08	0.03
	6(*a*)												
Ta4	3(*a*)	0	0	0.7882	0	0	0.75	0	0	0.53	0.32	0.08	0.03
O1	9(*b*)	0.0498(2)	0.3407(4)	0.0872(2)	0.	0.3407	0.25	0.26	0	-2.24	2.46	0.08	1.0
	18(*b*)												
O2	9(*b*)	0.6593	0.9502	0.5872	0.6593	0.	0.75	0	-0.26	-2.24	2.46	0.08	1.0
Li3	3(*a*),3(*b*)	0	0	0.64(1)	0	0	0.5	0	0	1.93	1.93	0.16	0.03

† Occupancy of Li1 and Li2 sites, each 83 %; Li3, Ta3 and Ta4 sites, each 3 %; all other sites, 100 %. u_{iso}(Li), u_{iso}(Ta), u_{iso}(O1) and u_{iso}(O2) varied but set at same value for different sites.

Table S8(*a*)

Atomic positions for Tl_2S at room temperature (Giester, 2002), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 12.20(7), c = 18.17(6)Å. $z^* = z + 0.0007$; $\Delta x = (x\text{-}x')a$, $\Delta y = (y\text{-}y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
	$R3$, $R\bar{3}$											
Tl1†	9(*b*)	0.1257(1)	0.2030(1)	0.9219(1)	0.1208	0.2219	0.9086	0.06	-0.23	0.24	0.32	0.21
	18(*f*)											
Tl4	9(*b*)	0.2407(1)	0.1060(1)	0.1046(1)	0.2219	0.1010	0.0914	0.23	0.06	0.24	0.36	0.21
Tl2	9(*b*)	0.1352(1)	0.2396(1)	0.2364(1)	0.1391	0.2221	0.2424	-0.05	0.21	-0.11	0.22	0.21
	18(*f*)											
Tl6	9(*b*)	0.2045(1)	0.0791(1)	0.7517(1)	0.2221	0.0830	0.7576	-0.21	-0.05	-0.11	0.26	0.21
Tl3	9(*b*)	0.1398(1)	0.2386(1)	0.5675(1)	0.1402	0.2226	0.5748	-0.00	0.20	-0.13	0.24	0.21
	18(*f*)											
Tl5	9(*b*)	0.2066(1)	0.0821(1)	0.4179(1)	0.2226	0.0824	0.4252	-0.20	-0.00	-0.13	0.24	0.21
S1	3(*a*),	0.	0.	0.037(1)	0.	0	0.	0.	0.	0.67	0.67	0.22
S2	3(*a*)	0.	0.	0.308(1)	0.	0.	0.334	0.	0.	-0.46	0.46	0.22
	6(*c*)											
S3	3(*a*)	0.	0.	0.641(1)	0.	0.	0.666	0.	0.	-0.46	0.46	0.22
S4	9(*b*)	0.666(1)	0.657(1)	0.313(1)	0.665	0.664	0.310	0.01	-0.08	0.06	0.10	0.20
	18(*c*)											
S5	9(*b*)	0.336(1)	0.330(1)	0.694(1)	0.335	0.336	0.690	0.01	-0.08	0.06	0.10	0.22

† Some coordinates in table are symmetry equivalents of reported values.

Table S8(*b*)

Atomic positions for Tl_2S at room temperature (Man, 1970), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

a = 12.20(7), c = 18.17(6)Å. $z^* = z - 0.031$; $\Delta x = (x\text{-}x')a$, $\Delta y = (y\text{-}y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*3*m*	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
Tl1	9(*b*),9(*b*)	0.119	0.191	0.926	0.103	0.207	0.926	0.19	-0.19	0	0.19	0.10
Tl2	9(*b*),9(*b*)	0.122	0.201	0.290	0.108	0.215	0.290	0.17	-0.17	0	0.17	0.10
Tl3	9(*b*),9(*b*)	0.118	0.209	0.625	0.109	0.218	0.625	0.11	-0.11	0	0.11	0.10
Tl5	9(*b*),9(*b*)	0.227	0.093	0.443	0.213	0.107	0.443	0.17	-0.17	0	0.17	0.10
Tl4	9(*b*)	0.233	0.103	0.109	0.224	0.112	0.109	0.11	-0.11	0	0.11	0.10
Tl6	9(*b*)	0.233	0.096	0.777	0.219	0.110	0.777	0.17	-0.17	0	0.17	0.10
S1	3(*a*)	0.	0.	0.164	0.	0	0.164	0.	0.	0	0	0.10
S3	3(*a*)	0.	0.	0.822	0.	0.	0.822	0.	0.	0	0	0.10
S2	3(*a*),3(*b*),	0.	0.	0.488	0.	0.	0.488	0.	0.	0	0	0.10
S4	9(*b*) 18(*c*) †	0.665	0.657	0.195	0.664	0.662	0.1795	0.01	-0.06	0.28	0.29	0.10
S5	9(*b*)	0.333	0.337	0.164	0.338	0.336	0.1795	-0.06	0.01	-0.28	0.29	0.10

† The z' coordinates in position 18(*c*) are the only z values in *R*3*m* contrained by symmmetry.

Table S8(*c*)

Atomic positions for Tl_2S at room temperature (Man, 1970), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 12.20(7), c = 18.17(6)Å. $z^* = z - 0.047$; $\Delta x = (x\text{-}x')a$, $\Delta y = (y\text{-}y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, $R\bar{3}m$	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
Tl1	9(*b*) 18(*h*)	0.119	0.191	0.926	0.108	0.216	0.9085	-0.06	-0.11	0.04	0.15	0.10
Tl4	9(*b*)	0.233	0.103	0.109	0.216	0.108	0.0915	0.10	0.05	0.02	0.13	0.10
Tl2	9(*b*) 18(*h*)	0.122	0.201	0.290	0.109	0.217	0.2565	-0.01	-0.02	0.31	0.31	0.10
Tl6	9(*b*)	0.233	0.096	0.777	0.217	0.109	0.7435	0.02	0.01	0.33	0.33	0.10
Tl3	9(*b*) 18(*h*)	0.118	0.209	0.625	0.108	0.216	0.591	0.01	0.02	0.33	0.33	0.10
Tl5	9(*b*)	0.227	0.093	0.443	0.216	0.108	0.409	0.	0.	0.33	0.33	0.10
S1	3(*a*) 6(*c*)	0.	0	0.164	0.	0.	0.171	0.	0.	-0.42	0.42	0.10
S3	3(*a*)	0.	0.	0.822	0.	0.	0.829	0.	0.	-0.42	0.42	0.10
S2	3(*a*),3(*b*)	0.	0.	0.488	0.	0.	0.5	0.	0.	-0.51	0.51	0.10
S4	9(*b*) 36(*i*)†	0.665	0.657	0.195	0.664	0.662	0.1795	0.01	0.04	0.28	0.28	0.10
S5	9(*b*)	0.333	0.337	0.164	0.338	0.336	0.1795	0.01	0.04	-0.28	0.28	0.10

† The 36(*i*) position is necessarily only 50 % occupied.

Table S9(*a*)

Atomic positions for $Ba_3Yb_4O_9$ at room temperature (Krueger & Mueller-Buschbaum, 1983), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

$a = 6.042$, $c = 24.859$ Å.† $z^* = z - 0.1059$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ba1	3(*a*)	0.	0.	-0.1059	0.	0.	-0.0846	0.	0.	-0.53	-0.53	0.10
	6(*c*)											
Ba2	3(*a*)	0.	0.	0.0632(4)	0.	0.	0.0846	0.	0.	-0.53	-0.53	0.11
Ba3	3(*a*),3(*b*)	0.	0.	0.4559(5)	0.	0.	0.5	0.	0.	-1.10	-1.10	0.14
Yb1	3(*a*)	0.	0.	0.3345(4)	0.	0.	0.3481	0.	0.	-0.34	-0.34	0.10
	6(*c*)											
Yb3	3(*a*)	0.	0.	0.6384(3)	0.	0.	0.6519	0.	0.	-0.34	-0.34	0.14
Yb2	3(*a*)	0.	0.	0.7701(5)	0.	0.	0.7803	0.	0.	-0.25	-0.25	0.10
	6(*c*)											
Yb4	9(*b*)	0.	0.	0.2095(3)	0.	0.	0.2197	0.	0.	-0.25	-0.25	0.10
O1	9(*b*)	0.918(9)	0.692(10)	0.154(1)	0.941	0.641	0.109	-0.14	0.31	1.11	1.14	0.11
	18(*f*)											
O3	9(*b*)	0.036(8)	0.410(8)	-0.065(2)	0.059	0.359	-0.109	0.14	0.31	1.10	1.13	0.11
O2	9(*b*),9(*e*)	0.969(9)	0.439(9)	0.044(2)	0.	0.439	0.	-0.19	0.	1.09	1.11	0.12

† Uncertainties in lattice constants not reported.

Table S9(*b*)

Atomic positions for $Ba_3Ho_4O_9$ at room temperature (Mueller-Buschbaum & Scheikowski, 1990), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

$a = 6.098(6)$, $c = 25.14(2)$ Å. $z^* = z - 0.0974$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ba1	3(*a*)	0.	0.	-0.0974	0.	0.	-0.0809	0.	0.	-0.41	-0.01	0.14
	6(*c*)											
Ba2	3(*a*)	0.	0.	0.0643(3)	0.	0.	0.0809	0.	0.	-0.42	-0.01	0.06
Ba3	3(*a*),3(*b*)	0.	0.	0.4775(3)	0.	0.	0.5	0.	0.	-0.57	-0.42	0.09
Ho1	3(*a*)	0.	0.	0.3271(2)	0.	0.	0.3437	0.	0.	-0.42	-0.14	0.08
	6(*c*)											
Ho3	3(*a*)	0.	0.	0.6397(3)	0.	0.	0.6563	0.	0.	-0.42	-0.14	0.04
Ho2	3(*a*)	0.	0.	0.7675(4)	0.	0.	0.7846	0.	0.	-0.43	-0.11	0.08
	6(*c*)											
Ho4	9(*b*)	0.	0.	0.1984(3)	0.	0.	0.2154	0.	0.	-0.43	-0.11	0.04
O1	9(*b*)	0.887(6)	0.621(7)	0.158(1)	0.941	0.611	0.119	-0.33	0.06	0.98	1.05	0.13
	18(*f*)											
O3	9(*b*)	0.005(7)	0.399(7)	-0.080(1)	0.059	0.389	-0.119	-0.33	0.06	0.98	1.05	0.14
O2	9(*b*),9(*e*)	0.020(6)	0.466(7)	0.046(1)	0.	0.466	0.	0.12	0.	1.16	1.17	0.14

Table S9(*c*)

Atomic positions for $Ba_3Tm_4O_9$ at room temperature (Mueller-Buschbaum & Scheikowski, 1990), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.
$a = 6.0556(4)$, $c = 24.957(2)$ Å. $z^* = z - 0.0984$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ba1	3(*a*)	0.	0.	-0.0984	0.	0.	-0.0815	0.	0.	-0.42	-0.42	0.13
	6(*c*)											
Ba2	3(*a*)	0.	0.	0.0645(3)	0.	0.	0.0815	0.	0.	-0.42	-0.42	0.07
Ba3	3(*a*),3(*b*)	0.	0.	0.4788(4)	0.	0.	0.5	0.	0.	-0.53	-0.53	0.11
Tm1	3(*a*)	0.	0.	0.3268(5)	0.	0.	0.3434	0.	0.	-0.41	-0.41	0.09
	6(*c*)											
Tm3	3(*a*)	0.	0.	0.6399(3)	0.	0.	0.6566	0.	0.	-0.42	-0.42	0.05
Tm2	3(*a*)	0.	0.	0.7675(6)	0.	0.	0.7822	0.	0.	-0.37	-0.37	0.07
	6(*c*)											
Tm4	9(*b*)	0.	0.	0.2032(5)	0.	0.	0.2178	0.	0.	-0.36	-0.36	0.04
O1	9(*b*)	0.894(6)	0.665(7)	0.150(1)	0.942	0.624	0.110	-0.29	0.25	1.00	1.04	0.11
	18(*f*)											
O3	9(*b*)	0.010(7)	0.417(7)	-0.070(1)	0.058	0.376	-0.110	-0.29	0.25	1.00	1.04	0.14
O2	9(*b*),9(*e*)	0.988(6)	0.424(7)	0.039(1)	0.	0.424	0.	-0.07	0.	0.97	0.97	0.12

Table S9(*d*)

Atomic positions for $Ba_3Lu_4O_9$ at room temperature (Krueger & Mueller-Buschbaum, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.
$a = 6.03$, $c = 24.753$ Å. $z^* = z - 0.1050$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ba1	3(*a*)	0.	0.	-0.1050	0.	0.	-0.0873	0.	0.	-0.44	-0.44	0.03
	6(*c*)											
Ba2	3(*a*)	0.	0.	0.0697(5)	0.	0.	0.0873	0.	0.	-0.44	-0.44	0.15
Ba3	3(*a*),3(*b*)	0.	0.	0.4818(9)	0.	0.	0.5	0.	0.	-0.45	-0.45	0.12
Lu1	3(*a*)	0.	0.	0.3323(6)	0.	0.	0.3521	0.	0.	-0.49	-0.49	0.12
	6(*c*)											
Lu3	3(*a*)	0.	0.	0.6281(5)	0.	0.	0.6479	0.	0.	-0.49	-0.49	0.15
Lu2	3(*a*)	0.	0.	0.7630(4)	0.	0.	0.7751	0.	0.	-0.30	-0.30	0.03
	6(*c*)											
Lu4	9(*b*)	0.	0.	0.2128(4)	0.	0.	0.2249	0.	0.	-0.30	-0.30	0.12
O1	9(*b*)	0.889(9)	0.664(11)	0.152(2)	0.935	0.602	0.111	-0.28	0.37	1.01	1.05	0.12
	18(*f*)											
O3	9(*b*)	0.020(11)	0.460(9)	-0.069(2)	0.066	0.398	-0.111	-0.28	0.37	1.04	1.07	0.13
O2	9(*b*),9(*e*)	0.973(12)	0.426(12)	0.034(3)	0.	0.426	0.	-0.16	0.	0.85	0.86	0.15

Table S9(*e*)

Atomic positions for $Ba_3Y_4O_9$ at room temperature (Szymanik *et al.*, 1998), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.[†]

$a = 6.11$, $c = 25.187$ Å. $z^* = z - 0.098$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
	$R3$, $R\bar{3}$										
Ba1	3(*a*)	0.	0.	-0.098	0.	0.	-0.082	0.	0.	-0.40	0.40
	6(*c*)										
Ba2	3(*a*)	0.	0.	0.066(6)	0.	0.	0.082	0.	0.	-0.40	0.40
Ba3	3(*a*),3(*b*)	0.	0.	0.481(9)	0.	0.	0.5	0.	0.	-0.48	0.48
Y1	3(*a*)	0.	0.	0.329(5)	0.	0.	0.346	0.	0.	-0.43	0.43
	6(*c*)										
Y3	3(*a*)	0.	0.	0.637(6)	0.	0.	0.654	0.	0.	-0.43	0.43
Y2	3(*a*)	0.	0.	0.760(6)	0.	0.	0.779	0.	0.	-0.47	0.47
	6(*c*)										
Y4	9(*b*)	0.	0.	0.203(7)	0.	0.	0.221	0.	0.	-0.46	0.46
O1	9(*b*)	0.81(1)	0.66(2)	0.152(5)	0.89	0.61	0.112	-0.53	0.31	1.01	1.10
	18(*f*)										
O3	9(*b*)	0.02(2)	0.44(1)	-0.073(2)	0.11	0.39	-0.112	-0.53	0.31	0.99	1.10
O2	9(*b*),9(*e*)	0.98(1)	0.39(1)	0.040(5)	0.	0.39	0.	-0.12	0.	1.01	1.02

[†] Thermal parameters not reported.

Table S10

Atomic positions for $Sr_{17}Ta_{10}S_{42}$ at room temperature (Onoda *et al.*, 1993), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.

$a = 18.1525\ (4)$, $c = 18.6574\ (4)$ Å; $z^* = z + 0.0122$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3,\ R\bar{3}$											
Sr1	9(*b*), 18(*f*)	-0.023(2)	0.177(2)	0.075(3)	-0.025	0.175	0.078	0.04	0.03	-0.06	0.08	0.13
Sr6	9(*b*)	0.027(2)	0.826(2)	0.919(3)	0.025	0.825	0.922	0.04	0.03	-0.06	0.08	0.13
Sr2	9(*b*) 18(f)	0.023(2)	0.826(2)	0.262(2)	0.029	0.832	0.253	-0.11	-0.11	0.17	0.23	0.13
Sr5	9(*b*)	-0.035(2)	0.162(3)	0.756(3)	-0.029	0.168	0.747	-0.11	-0.11	0.17	0.23	0.13
Sr3	9(*b*) 18(*f*)	-0.045(2)	0.161(2)	0.432(3)	-0.039	0.164	0.427	-0.11	-0.05	0.09	0.15	0.13
Sr4	9(*b*)	0.033(2)	0.833(3)	0.578(2)	0.039	0.836	0.573	-0.11	-0.05	0.09	0.15	0.13
Ta1	3(*a*) 6(*c*)	0.	0.	0.1679	0.	0.	0.1520	0.	0.	0.30	0.30	0.11
Ta5	3(*a*)	0.	0.	0.864(2)	0.	0.	0.848	0.	0.	0.30	0.30	0.11
Ta2	3(*a*) 6(*c*)	0.	0.	0.366(3)	0.	0.	0.347	0.	0.	0.35	0.35	0.11
Ta4	3(*a*)	0.	0.	0.672(3)	0.	0.	0.653	0.	0.	0.35	0.35	0.11
Ta3	9(*b*) 18(*f*)	0.001(1)	0.331(1)	0.289(2)	0.001	0.331	0.281	0.	0.	0.15	0.15	0.11
Ta6	9(*b*)	0.001(1)	0.669(1)	0.727(2)	0.001	0.669	0.719	0.	0.	0.15	0.15	0.11
S1	9(*b*) 18(*f*)	0.015(5)	0.900(6)	0.116(4)	0.018	0.902	0.094	-0.06	-0.04	0.42	0.43	0.05
S10	9(*b*)	-0.022(5)	0.095(6)	0.929(4)	-0.018	0.098	0.906	-0.03	-0.05	0.43	0.43	0.05
S2	9(*b*) 18(*f*)	-0.020(6)	0.089(5)	0.274(5)	-0.020	0.092	0.253	0.	-0.05	0.39	0.39	0.05
S9	9(*b*)	0.019(6)	-0.095(5)	0.768(5)	0.019	-0.092	0.747	0.	-0.05	0.39	0.39	0.05
S3	9(*b*) 18(*f*)	0.008(4)	0.887(5)	0.418(4)	0.018	0.886	0.402	-0.18	0.02	0.30	0.35	0.05
S8	9(*b*)	-0.028(4)	0.115(4)	0.614(4)	-0.018	0.114	0.598	-0.18	0.02	0.30	0.35	0.05
S4	9(*b*) 18(*f*)	-0.012(5)	0.326(6)	0.359(3)	0.039	0.322	0.332	-0.93	0.08	0.51	1.06	0.05
S12	9(*b*)	0.910(6)	0.683(5)	0.696(4)	0.961	0.678	0.668	-0.93	0.08	0.51	1.06	0.05
S5	9(*b*) 18(*f*)	0.099(4)	0.300(4)	0.177(4)	0.051	0.311	0.166	0.87	0.20	0.21	0.93	0.05
S11	9(*b*)	-0.002(5)	0.678(4)	0.845(3)	-0.051	0.689	0.834	0.89	-0.20	0.21	0.93	0.05
S6	9(*b*) 18(*f*)	0.101(5)	0.297(4)	0.520(4)	0.102	0.314	0.588	-0.02	-0.31	-1.27	1.31	0.05
S14	9(*b*)	0.896(4)	0.669(4)	0.344(4)	0.897	0.686	0.412	-0.02	-0.31	-1.27	1.31	0.05
S7	9(*b*) 18(*f*)	0.100(5)	0.306(5)	0.849(4)	0.116	0.321	0.911	-0.29	-0.26-	-1.16	1.22	0.05
S13	9(*b*)	0.868(3)	0.665(4)	0.027(4)	0.884	0.679	0.089	-0.29	-0.26	-1.16	1.22	0.05

Table S10(*a*)

Atomic positions for $Sr_{17}Ta_{10}S_{42}$ at ambient temperature (Onoda, *et al.,* 1993) with hypothetical *x´y´ z´* coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [73870]
a = 18.1525(4), c = 18.6574(4) Å. $z^* = z + 0.0100$; $\Delta x = (x - x´)a$,$\Delta y = (y - y´)a$, $\Delta z = (z^* - z´)c$.

	Wyckoff position $R3$,$P6_3$†	x	y	z	$x´$	$y´$	$z´$	Δx	Δy	Δz	Δxyz	u_{iso}
Sr1	9(*b*)	-0.024(1)	0.177(1)	0.0797(9)	-0.024	0.172	0.0797	0.	0.	0.	0.	0.13
	18(*f*)											
Sr4	9(*b*)	0.024(1)	0.833(1)	0.5797(9)	0.024	0.828	0.5797	0.	0.	0.	0.	0.13
Sr6	9(*b*)	0.0425(8)	0.835(1)	0.930(1)	0.0425	0.835	0.930	0.	0.	0.	0.	0.13
	18(*f*)											
Sr3	9(*b*)	-0.0425(8)	0.165(1)	0.430(1)	-0.0425	0.165	0.430	0.	0.	0.	0.	0.13
Sr2	9(*b*)	0.028(1)	0.8323(9)	0.253(1)	0.028	0.8323	0.253	0.	0.	0.	0.	0.13
	18(*f*)											
Sr5	9(*b*)	-0.028(1)	0.1677(9)	0.753(1)	-0.028	0.1677	0.753	0.	0.	0.	0.	0.13
Ta1	3(*a*)	0	0	0.177	0	0	0.1768	0.	0.	0.	0.	0.12
	6(*c*)											
Ta4	3(*a*)	0	0	0.6767	0	0	0.6768	0.	0.	0.	0.	0.12
Ta5	3(*a*)	0	0	0.8637(6)	0	0	0.8637	0.	0.	0.	0.	0.12
	6(*c*)											
Ta2	3(*a*)	0	0	0.3637(6)	0	0	0.3637	0.	0.	0.	0.	0.12
Ta3	9(*b*)	0	0.3333	0.2277(5)	0	0.3333	0.2277	0.	0.	0.	0.	0.12
	18(*f*)											
Ta6	9(*b*)	0	0.6667	0.7277(5)	0	0.6667	0.7277	0.	0.	0.	0.	0.12
S1	9(*b*)	0.022(3)	0.894(3)	0.116(2)	0.022	0.894	0.116	0.	0.	0.	0.	0.13
	18(*f*)											
S8	9(*b*)	-0.022(3)	0.106(3)	0.616(2)	-0.022	0.106	0.616	0.	0.	0.	0.	0.13
S10	9(*b*)	-0.010(3)	0.112(3)	0.926(2)	-0.010	0.112	0.926	0.	0.	0.	0.	0.13
	18(*f*)											
S3	9(*b*)	0.010(3)	0.888(3)	0.426(2)	0.010	0.888	0.426	0.	0.	0.	0.	0.13
S2	9(*b*)	-0.025(2)	0.084(2)	0.270(3)	-0.025	0.084	0.270	0.	0.	0.	0.	0.13
	18(*f*)											
S9	9(*b*)	0.025(2)	-0.084(2)	0.770(3)	0.025	-0.084	0.770	0.	0.	0.	0.	0.13
S4	9(*b*)	0	0.3333	0.349(1)	0	0.3333	0.349	0.	0.	0.	0.	0.13
	18(*f*)											
S11	9(*b*)	0	0.6667	0.849(1)	0	0.6667	0.849	0.	0.	0.	0.	0.13
S5	9(*b*)	0.1052(6)	0.3125(7)	0.1859(7)	0.1052	0.3125	0.1859	0.	0.	0.	0.	0.13
	18(*f*)											
S12	9(*b*)	0.8948(6)	0.6875(7)	0.6859(7)	0.8948	0.6875	0.6859	0.	0.	0.	0.	0.13
S6	9(*b*)	0.1052(6)	0.3125(7)	0.5193	0.1052	0.3125	0.5193	0.	0.	0.	0.	0.13
	18(*f*)											
S13	9(*b*)	0.8948(6)	0.6875(7)	0.0193	0.8948	0.6875	0.0193	0.	0.	0.	0.	0.13
S14	9(*b*)	0.8948(6)	0.6875(7)	0.3526	0.8948	0.6875	0.3526	0.	0.	0.	0.	0.13
	18(*f*)											
S7	9(*b*)	0.1052(6)	0.3125(7)	0.8526	0.1052	0.3125	0.8526	0.	0.	0.	0.	0.13

† Space groups $P6_1$, $P6_3/m$, $P6_122$, $P6_522$, $P6cc$, $P6_3mc$, $P6_3mc$, $P6_3/mcm$ and $P6_3/mmc$ also satisfy the symmetry condition transformation $\bar{x}$, $\bar{y}$, ½+z.

Table 10(*b*)

Atomic positions for $Sr_{17}Ta_{10}S_{42}$ in space group $P6_1$ (Onoda, *et al.,* 1993) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [73870]
a = 18.1525(4), c = 18.6574(4) Å. $z^* = z + 0.0100$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $P6_3$,$P6_3/m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	Δxyz	u_{iso}
Sr1	9(*b*) 12(*i*)	-0.024	0.172	0.0797	-0.033	0.168	0.0749	0.16	0.06	0.09	0.23	0.13
Sr6	9(*b*)	0.0425	0.835	0.930	0.033	0.832	0.9251	0.17	0.06	0.09	0.23	0.13
Sr2	9(*b*),6(*h*)	0.028	0.8323	0.253	0.028	0.8323	0.25	0.	0.	0.06	0.06	0.13
Ta1	3(*a*) 4(*e*)	0	0	0.1768	0	0	0.1565	0.	0.	0.38	0.38	0.12
Ta5	3(*a*)	0	0	0.8637	0	0	0.8435	0.	0.	0.38	0.38	0.12
Ta3	9(*b*),6(*h*)	0	0.3333	0.2277	0	0.3333	0.25	0.	0.	-0.42	0.42	0.12
S1	9(*b*) 12(*i*)	0.022	0.894	0.116	0.016	0.891	0.095	0.11	0.05	0.39	0.41	0.13
S10	9(*b*)	-0.010	0.112	0.926	-0.016	0.109	0.905	0.11	0.05	0.39	0.41	0.13
S2	9(*b*),6(*h*)	-0.025	0.084	0.270	-0.025	0.084	0.25	0.	0.	0.37	0.37	0.13
S4	9(*b*),6(*h*)	0	0.3333	0.349	0	0.3333	0.25	0.	0.	1.85	1.85	0.13
S5	9(*b*),6(*h*)	0.1052	0.3125	0.1859	0.1052	0.3125	0.25	0.	0.	-1.20	1.20	0.13
S6	9(*b*) 12(*i*)	0.1052	0.3125	0.5193	0.1052	0.3125	0.5834	0.	0.	-1.20	1.20	0.13
S14	9(*b*)	0.8948	0.6875	0.3526	0.8948	0.6875	0.4166	0.	0.	-1.19	1.19	0.13

Table S11(*a*)

Atomic positions for Pd_8Sb_3 at room temperature (Man & Imamov, 1979), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 7. 59 (5), c = 43.2 (1) Å; $z^* = z + 0.180$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*3*c*	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso} †
Pd1	9(*b*)	0.25	0.01	0.218	0.262	0.009	0.217	-0.09	0.01	0.04	0.09	0.10
	18(*f*)											
Pd2	9(*b*)	0.735	0.008	0.716	0.747	0.009	0.717	-0.09	0.01	0.04	0.09	0.10
Pd3	9(*b*)	0.651	0.004	0.254	0.646	0.000	0.251	0.04	0	0.02	0.04	0.10
	18(f)											
Pd4	9(*b*)	0.358	0.997	0.747	0.354	0.990	0.751	0.03	0	0.02	0.04	0.10
Pd5	9(*b*)	0.306	0.001	0.285	0.306	-0.001	0.287	0	0.01	-0.09	0.09	0.10
	18(*f*)											
Pd6	9(*b*)	0.694	0.002	0.789	0.694	0.001	0.787	0	0.01	0.09	0.09	0.10
Pd7	9(*b*)	0.64	0.017	0.321	0.64	0.013	0.318	0	0.03	0.13	0.13	0.10
	18(*f*)											
Sb2	9(*b*)	0.36	0.01	0.685	0.36	0.013	0.682	0	-0.02	0.13	0.13	0.10
Pd9	3(*a*)	0	0	0.322	0.	0.	0.324	0	0	-0.09	0.09	0.10
	6(*c*)											
Pd13	3(*a*)	0	0	0.826	0.	0.	0.824	0	0	0.09	0.09	0.10
Pd12	3(*a*)	0	0	0.67	0.	0.	0.669	0	0	0.02	0.02	0.10
	6(*c*)											
Pd16	3(*a*)	0	0	0.169	0.	0.	0.169	0	0	0.02	0.02	0.10
Pd10	3(*a*)	0	0	0.382	0.	0.	0.385	0	0	-0.09	0.09	0.10
	6(*c*)											
Pd14	3(*a*)	0	0	0.887	0.	0.	0.885	0	0	0.09	0.09	0.10
Pd11	3(*a*)	0	0	0.545	0.	0.	0.543	0	0	0.09	0.09	0.10
	6(*c*)											
Pd15	3(*a*)	0	0	0.04	0.	0.	0.042	0	0	-0.09	0.09	0.10
Sb1	9(*b*)	0.657	0.006	0.186	0.613	-0.036	0.182	0.33	0.32	0.17	0.59	0.10
	18(*f*)											
Pd8	9(*b*)	0.43	0.079	0.822	0.387	0.036	0.818	0.33	0.33	0.17	0.60	0.10
Sb3	3(*a*)	0	0	0.261	0	0	0.262	0	0	-0.04	0.04	0.10
	6(*c*)											
Sb6	3(*a*)	0	0	0.763	0	0	0.762	0	0	0.04	0.04	0.10
Sb4	3(*a*)	0	0	0.441	0	0	0.445	0	0	-0.17	0.17	0.10
	6(*c*)											
Sb7	3(*a*)	0	0	0.949	0.	0.	0.945	0	0	0.17	0.17	0.10
Sb5	3(*a*)	0	0	0.607	0	0	0.606	0	0	0.04	0.04	0.10
	6(*c*)											
Sb8	3(*a*)	0	0	0.105	0.	0.	0.106	0	0	-0.04	0.04	0.10

† The value B = 0.75 Å^2 was used throughout.

Table S11(*b*)

Atomic positions for Pd_8Sb_3 at room temperature (Man & Imamov, 1979), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 7. 59 (5), c = 43.2 (1) Å; $z^* = z + 0.180$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3c$, $R\bar{3}c$											
Pd1	18(*b*)	0.262	0.009	0.217	0.287	0.005	0.215	-0.09	0.01	0.04	0.09	0.10
	36(*f*)											
Pd5	18(*b*)	0.306	-0.001	0.287	0.281	-0.005	0.285	0	0.01	-0.09	0.09	0.10
Pd3	18(*b*),18(*e*)	0.646	0	0.251	0.646	0	0.25	0.04	0	0.02	0.04	0.10
Pd9	6(*b*)	0.	0.	0.324	0.	0.	0.327	0	0	-0.09	0.09	0.10
	12(*c*)											
Pd12	6(*b*)	0.	0.	0.669	0.	0.	0.672	0	0	0.02	0.02	0.10
Pd10	6(*b*)	0.	0.	0.385	0.	0.	0.389	0	0	-0.09	0.09	0.10
	12(*c*)											
Sb5	6(*b*)	0	0	0.606	0	0	0.611	0	0	0.04	0.04	0.10
Pd11	6(*b*)	0.	0.	0.543	0.	0.	0.549	0	0	0.09	0.09	0.10
	12(*c*)											
Sb4	6(*b*)	0	0	0.445	0	0	0.451	0	0	-0.17	0.17	0.10
Sb1	18(*b*)	0.613	-0.036	0.182	0.615	-0.024	0.182	-0.02	-0.09	0.0	0.09	0.10
	36(*f*)											
Sb2	18(*b*)	0.36	0.013	0.682	0.362	0.024	0.682	-0.02	-0.09	0.0	0.09	0.10
Sb3	6(*b*),6(*a*)	0	0	0.262	0	0	0.25	0	0	-0.04	0.04	0.10

Table S11(*c*)

Atomic positions for Pd_8Sb_3 at room temperature (Wopersnow & Schubert, 1976), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 7. 6152(7), c = 43.032(7) Å; $z^* = z$ - 0.0338; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position $R3c$, $R\bar{3}\,c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Pd1	18(*b*),18(*d*)	0.588(2)	0.914(2)	-0.0338	0.5	0	0.	0.67	-0.65	-1.45	1.59	0.14
Pd2	6(*a*)	0	0	-0.0234(6)	0	0	0	0	0	-1.01	1.01	0.12
Pd3	6(*a*) 12(*c*)	0	0	0.6342(8)	0	0	0.6408	0	0	-0.28	0.28	0.12
Pd6	6(*b*)	0	0.	0.3526(8)	0.	0.	0.3592	0	0			0.14
Pd4	18(*b*) 36(*f*)	0.350(2)	0.010(2)	-0.0023(5)	0.336	0.016	-0.0504	0.10	-0.05	2.07	2.07	0.12
Sb4†	18(*b*)	0.677(2)	0.978(2)	0.0985(1)	0.663	0.984	0.0504	0.10	-0.05	2.07	2.07	0.12
Pd5	18(*b*) 36(*f*)	0.732(2)	0.003(2)	-0.0311(3)	0.684	0.0005	-0.0475	0.37	0.02	0.71	0.81	0.14
Pd8	18(*b*)	0.364(2)	0.002(2)	0.0638(4)	0.316	-0.0005	0.0475	0.37	0.02	0.71	0.81	0.12
Pd7	6(*b*) 12(*c*)	0	0	0.6963(8)	0	0	0.7190	0	0	-0.98	0.98	0.14
Sb3	6(*b*)	0	0	0.7583(6)	0	0	0.7810	0	-0.02	-0.98	0.98	0.11
Sb2	6(*b*) 12(*c*)	0	0	0.4149(7)	0	0	0.4214	0	0	-0.28	0.28	0.12
Sb1	6(*b*)	0	0	0.0722(6)	0	0	0.0786	0	0	-0.28	0.28	0.12

† Labelled Pd in original report.

Table S12(*a*)

Atomic positions for β-BaB_2O_4 at room temperature (Lu *et al.* 1982),[†] with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 12.532, c = 12.717 Å. $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^{*} - z')\,c$.

	Wyckoff Position *R*3, *R*3*c*	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso} [‡]
Ba1	9(*b*)	0.33004	0.02486	0.00006	0.33009	0.02541	0.00007	-0.001	-0.007	-0.000	0.007	0.13
	18(*f*)											
Ba2	9(*b*)	0.33014	0.30632	0.50008	0.33009	0.30687	0.50007	0.001	-0.007	0.000	0.007	0.13
B1	9(*b*)	0.76709	0.45495	0.03344	0.76586	0.45408	0.03110	0.015	0.011	0.030	0.032	0.15
	18(*f*)											
B2	9(*b*)	0.54679	0.23537	0.52875	0.54592	0.23414	0.53110	0.011	0.015	0.030	0.034	0.15
B3	9(*b*)	0.37631	0.79704	0.12229	0.37599	0.79619	0.12408	0.004	0.011	-0.023	0.026	0.15
	18(*f*)											
B4	9(*b*)	0.20466	0.62433	0.62586	0.20381	0.62401	0.62408	0.011	0.003	0.023	0.023	0.15
O1	9(*b*)	0.64450	0.4282	0.03200	0.6447	0.4281	0.0316	0.003	0.001	0.005	0.005	0.16
	18(*f*)											
O2	9(*b*)	0.57200	0.35501	0.53125	0.5719	0.3553	0.5316	0.001	-0.004	-0.004	0.006	0.16
O3	9(*b*)	0.41953	0.91340	0.12979	0.41951	0.9138	0.13059	0.000	-0.005	-0.010	0.011	0.16
	18(*f*)											
O4	9(*b*)	0.08577	0.58052	0.63140	0.0862	0.58049	0.63059	-0.005	0.000	0.010	0.010	0.16
O5	9(*b*)	0.85833	0.57103	0.02440	0.85926	0.57025	0.0235	-0.012	0.010	0.011	0.015	0.16
	18(*f*)											
O6	9(*b*)	0.86018	0.28979	0.52259	0.85926	0.29057	0.52350		-0.010	-0.012	0.016	0.16
O7	9(*b*)	0.25216	0.70754	0.12073	0.25135	0.70795	0.12178	0.010	-0.005	-0.013	0.014	0.16
	18(*f*)											
O8	9(*b*)	0.29165	0.74946	0.62284	0.29205	0.74865	0.62178	-0.005	0.010	0.013	0.016	0.16

[†] As reported by Xue & Zhang (1998).

[‡] Taken from Fröhlich's (1984) u_{iso} values for equivalent atoms. Atomic coordinate uncertainties not reported.

Table S12(*b*)

Atomic positions for β-BaB_2O_4 at room temperature (Fröhlich, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å, in the hexagonal setting

a = 12.519(6), c = 12.723(6) Å; $z^* = z$ - 0.2030. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3c$, $R\bar{3}c$											
Ba1	18(*f*),18(*e*)	0.3042	0.2442	0.230	0.2742	0.2742	0.2500	0.38	-0.38	-0.56	0.68	0.13
B1	18(*f*)	0.041(2)	-0.087(2)	0.299(2)	-0.029	-0.032	0.380	0.88	-0.69	-1.03	1.31	0.15
	36(*f*)											
B2	18(*f*)	0.023(2)	-0.099(2)	0.038(2)	-0.032	-0.029	0.120	0.69	0.88	-1.04	1.71	0.15
O1	9(*b*)	0.163(1)	0.249(1)	0.305(1)	0.102	0.218	0.255	0.76	0.39	0.64	1.20	0.16
	18(*f*)											
O2	9(*b*)	-0.041(1)	0.085(1)	0.296(1)	-0.102	0.116	0.245	0.76	-0.39	0.64	0.92	0.16
O3	9(*b*)	0.118(1)	0.021(1)	0.038(1)	0.178	0.033	-0.001	-0.75	-0.15	0.51	0.98	0.16
	18(*f*)											
O4	9(*b*)	0.045(1)	0.238(1)	0.540(1)	0.033	0.178	0.499	0.15	0.75	0.51	0.98	0.16

Table S12(*c*)

Modified Lu *et al.*'s (1982) $R3c$ $x'y'z'$ atomic coordinates for β-BaB_2O_4 from Table S12(*a*) with hypothetical $x''y''z''$ coordinates and Δx, Δy, Δz displacements in Å.

a = 12.532, c = 12.717 Å; $z^* = z + 0.1839$ $\Delta x = (x' - x'')a$, $\Delta y = (y' - y'')a$, $\Delta z = (z^{*\prime} - z'')c$.

	Wyckoff Position	x'	y'	$z^{*\prime}$	x''	y''	z''	Δx	Δy	Δz	$\Delta\xi$	u_{iso} †
	$R3c$, $R\bar{3}c$											
Ba1	18(*f*),18(*e*)	0.3301	0.0254	0.1839	0.3301	0.	0.2500	0.0	0.32	-0.84	0.90	0.13
B1	18(*f*)	0.7659	0.4541	0.2150	0.6949	0.4726	0.2035	0.89	-0.23	0.15	0.81	0.15
	36(*f*)											
B4	18(*f*)	0.2038	0.6240	0.8080	0.2223	0.6949	0.7965	-0.23	-0.89	0.15	1.04	0.15
O1	9(*b*)	0.6447	0.4281	0.2155	0.6126	0.4773	0.2005	0.40	-0.62	0.19	0.58	0.16
	18(*f*)											
O4	9(*b*)	0.0862	0.5805	0.8145	0.1354	0.6126	0.7995	-0.62	-0.40	0.19	0.91	0.16
O5	9(*b*)	0.8593	0.5703	0.2074	0.8040	0.5411	0.2009	0.69	0.37	0.08	0.94	0.16
	18(*f*)											
O8	9(*b*)	0.2921	0.7487	0.8057	0.2629	0.8040	0.7991	0.37	-0.69	0.08	0.60	0.16

† From Fröhlich's (1984) u_{iso} values for the equivalent atoms.

Table S13(*a*)

Rhombohedral system atomic coordinates† for $CsCd(NO_2)_3$ (Himmelreich., 1998).

a_R = 5.4579(1) Å; α = 90.220(3)° at 292 K in $R3$; a_R = 5.5087(2) Å, 90° at 475 K in $Pm\bar{3}$.

$\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position $R3$, $Pm\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Cs	1(*a*),1(*a*)	0	0	0	0	0	0	0	0	0	0	0.14
Cd	1(*a*),8(*g*)‡	0.53650(1)	0.53650(1)	0.53650(1)	0.5306	0.5306	0.5306	0.03	0.03	0.03	0.06	0.12
N	3(*b*),6(*f*)	0.0792(2)	0.4857(2)	0.5148(2)	0.075	0.5	0.5	0.02	-0.19	0.08	0.20	0.15
O1	3(*b*) 24(*l*)	-0.0511(2)	0.4904(2)	0.7038(2)	-0.044	0.5	0.6926	-0.04	-0.05	0.06	0.08	0.16
O2	3(*b*)	-0.0349(2)	0.4876(2)	0.3188(2)	-0.044	0.5	0.3074	0.05	-0.07	0.06	0.09	0.16

† Himmelreich's (1998) rhombohedral system coordinates at 292 K. The x'(Cd) and x'(N) coordinates from the structure at 475 K under $Pm\bar{3}$ symmetry are also from the (1998) dissertation.

Table S13(*b*)

Hexagonal system atomic coordinates for $CsCa(NO_2)_3$ (Himmelreich., 1998), see Table S14(*d*) for rhombohedral system coordinates.

a_H = 7.836(2) Å; c_H = 9.660(3) Å. $z^* = z - 0.0045$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3$, $R\bar{3}$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{aniso}
Cs†	3(*a*),3(*a*)	0	0	-0.0045	0.	0.	0.0	0.	0.	-0.04	0.04	0.14
Ca	3(*a*),3(*b*)	0	0	0.5284	0	0	0.5	0.	0.	0.27	0.27	0.12
N	9(*b*),9(*e*)	0.0481(4)	0.5107(4)	0.0160(4)	0.	0.5	0	0.38	0.08	0.15	0.45	0.15
O1	9(*b*) 18(*f*)	0.2352(5)	0.0119(5)	0.7105(5)	0.2698	0.0426	0.7327	-0.27	-0.24	-0.21	0.49	0.17
O2	9(*b*)	-0.3045(5)	-0.0733(5)	0.2451(5)	-0.2698	-0.0426	0.2673	-0.27	-0.24	-0.21	0.49	0.17

† The variable x', y' and z' coordinates at 548 K are from Himmelreich (1998).

Table S13(*c*)

Hexagonal system atomic positions for $CsCd(NO_2)_3$ at room temperature (Avdeev *et al.*, 2002),[†] with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å
$a_H = 7.7305(1)$ Å; $c_H = 9.4170(3)$ Å. $z^* = z - 0.0267$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3,\ R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cs	3(*a*),3(*a*)	0	0	-0.0073	0.	0.	0.0	0.	0.	-0.07	0.04	0.14
Cd	3(*a*),3(*b*)	0	0	0.5286	0	0	0.5	0.	0.	0.27	0.27	0.12
N	9(*b*),9(*e*)	0.0530(4)	0.5014(4)	0.0099(4)	0.	0.5	0	0.41	0.01	0.15	0.45	0.15
O1	9(*b*) 18(*f*)	0.2183(5)	0.0421(5)	0.2486(5)	0.2452	0.0459	0.2642	-0.21	-0.03	-0.15	0.49	0.17
O2	9(*b*)	-0.2721(5)	-0.0497(5)	0.7202(5)	-0.2452	-0.0459	0.7358	-0.21	-0.03	-0.15	0.49	0.17

[†] Following interchange of reported a_1 and a_2 axes, reversal of c axis and $\Sigma\Delta z$ minimization by an origin shift of -0.0267.

Table S14

Atomic positions for $Sc_7Br_{12}C$ at room temperature (Dudis *et al.*, 1986), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 13.628(1)$, $c = 9.203(2)$ Å. ; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position $R3$, $R32$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Br1	9(*b*)	0.0772(3)	0.3088(3)	0.	0.1524	0.3094	-0.0031	-1.02	-0.01	0.03	1.03	0.17
	18(*f*)											
Br3	9(*b*)	0.3100(3)	0.2276(2)	0.0062(3)	0.3094	0.1524	0.0031	0.01	1.02	0.03	1.03	0.12
Br2	9(*b*)	0.1764(2)	0.0495(2)	0.6668(5)	0.1823	0.0924	0.6667	-0.08	-0.58	0.01	0.62	0.15
	18(*f*)											
Br4	3(*a*)	0.1336(2)	0.1882(1)	0.3334(5)	0.0924	0.1823	0.3333	0.56	0.08	0.01	0.60	0.14
Sc1	3(*a*),3(*b*)	0.	0.	0.477 (1)	0.	0.	0.5	0.	0.	-0.21	0.21	0.15
Sc2	9(*b*)	0.1124(3)	0.1566(3)	0.865(3)	0.0775	0.1542	0.858	0.48	0.03	0.06	0.50	0.14
	18(*f*)											
Sc3	9(*b*)	0.1518(3)	0.0425(3)	0.149(1)	0.1542	0.0775	0.142	-0.03	-0.48	0.06	0.50	0.12
C	3(*a*),3(*a*)	0.	0.	0.003	0.	0.	0.0	0.	0.	0.03	0.03	0.12

Table S15(*a*)
Atomic positions for $CsGeCl_3$ at room temperature (Christensen & Rasmussen, 1965), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å
$a_H = 7.674$, $c_H = 9.490$; $z^* = z + 0.0063$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*3*m*	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
Cs	3(*a*),3(*a*)	0	0	0.006	0	0	0	0	0	0.06	0.06	0.16
Ge	3(*a*),3(*a*)	0	0	0.494(5)	0	0	½	0	0	-0.06	0.06	0.20
Cl	9(*b*),9(*b*)	0.147(4)	0.288(4)	0.351(5)	0.145	0.290	0.351	0.02	-0.02	0.0	0.03	0.27

Table S15(*b*)
Atomic positions for $CsGeCl_3$ at room temperature (Thiele *et al.,* 1987), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å
$a_H = 7.666(3)$, $c_H = 9.458(4)$; $z^* = z + 0.0073$.

	Wyckoff position $R3m$,$R\bar{3}m$	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ
Cs	3(*a*),3(*a*)	0	0	0.0073	0	0	0	0	0	0.07	0.23
Ge	3(*a*),3(*a*)	0	0	0.4927(1)	0	0	0.5	0	0	-0.07	0.17
Cl	9(*b*),18(*h*)	0.1555(3)	0.3111(3)	0.3722(3)	0.1555	0.3111	0.3722	0.	0.	0.	0.24

Table S15(*c*)
Atomic positions for $CsGeCl_3$ at room temperature (Yamada *et al.,* 1994), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å
$a_H = 7.672(2)$, $c_H = 9.511(2)$; $z^* = z + 0.002$.

	Wyckoff position $R3m$,$R\bar{3}m$	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	u_{iso}
Cs	3(*a*),3(*a*)	0	0	0.002	0	0	0	0	0	0.02	0.26
Ge	3(*a*),3(*a*)	0	0	0.497(5)	0	0	0.5	0	0	-0.03	0.10
Cl	9(*b*),18(*h*)	0.156(6)	0.311(6)	0.365(7)	0.1557	0.3113	0.365	0.0	0.0	0.0	0.31

Table S16

Atomic positions for $Sn_3PO_4F_3$ at room temperature (Berndt, 1972), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 11.87$, $c = 4.69$ Å; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z - z')\,c$.

	Wyckoff Position *R*3, *R*3*m*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Sn	9(*b*),9(*b*)	0.1213(2)	0.2388(2)	0.512(8)	0.1200	0.2400	0.512	0.02	-0.02	0.	0.02	0.14
P	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	0.13
O1	3(*a*),3(*a*)	0	0	0.648(20)	0.	0.	0.648	0.	0.	0.	0	0.14
O2	9(*b*),9(*b*)	0.069(4)	0.136(4)	0.114(17)	0.068	0.137	0.114	0.01	-0.01	0.	0.01	0.21
F	9(*b*),9(*b*)	0.138(3)	0.401(3)	0.225(12)	0.179	0.359	0.225	-0.49	0.50	0.	0.50	0.19

Table S17

Atomic positions for Ag_8GeTe_6 at room temperature (von Ünterrichter & Range, 1978), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a_H = 8.176(2), c_H = 20.027(5) Å; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position *R*3, *R*3*m*	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	occ.	u_{33}
Te1	3(*a*),3(*a*)	0	0	0.0000(5)	0.0	0.0	0.0	0.0	0.0	0.0	0.	1.0	0.21
Te2	3(*a*),3(*a*)	0	0	0.2550(7)	0.0	0.0	0.255	0.0	0.0	0.0	0.	1.0	0.21
Te3	3(*a*),3(*a*)	0	0	0.6183(5)	0.0	0.0	0.6183	0.0	0.0	0.0	0.	1.0	0.13
Te4	9(*b*),9(*b*)	0.1666(6)	0.3360(5)	0.4510(9)	0.1675	0.3351	0.451	0.0	0.0	-0.01	0.01	1.0	0.08
Ge	3(*a*),3(*a*)	0	0	0.4916(7)	0.	0.	0.4916	-0.01	0.03	-0.02	0.03	1.0	0.05
Ag1	9(*b*) 18(*c*)	-0.326(2)	0.017(4)	0.655(9)	-0.3275	0.0145	0.656	0.02	0.02	-0.03	0.05	0.35†	0.36
Ag3	9(*b*)	-0.012(4)	0.329(4)	0.657(7)	-0.0145	0.3275	0.656	0.02	0.02	0.03	0.05	0.35	0.24
Ag2	9(*b*),9(*b*)	0.557(3)	1.102(3)	0.447(8)	0.553	1.106*	0.447	0.03	0.03	0.	0.05	0.35	0.23
Ag4	9(*b*),9(*b*)	0.101(4)	0.204(4)	0.871(9)	0.102	0.203	0.871	-0.01	0.01	0.	0.01	0.34	0.47
Ag5	9(*b*),9(*b*)	0.141(2)	0.283(2)	0.30(4)	0.141	0.283	0.30	0.	0.	0.	0.	0.06	0.43
Ag6	9(*b*),9(*b*)	-0.149(3)	0.141(3)	0.174(7)	-0.145	0.145	0.174	-0.03	-0.03	0.	0.05	0.13	0.17
Ag7	9(*b*),9(*b*)	0.194(5)	0.363(5)	0.583(9)	0.186	0.371	0.583	0.07	-0.07	0.	0.07	0.19	0.17
Ag8	9(*b*),9(*b*) 18(*c*)	0.394(7)	0.194(4)	0.408(12)	0.420	0.208*	0.426	-0.21	-0.11	-0.37	0.47	0.21	0.69
Ag12	9(*b*),9(*b*)	-0.239(4)	0.223(8)	0.445(12)	-0.212	0.208*	0.426	0.22	0.12	0.37	0.47	0.13	0.26
Ag9	9(*b*),9(*b*)	0.289(6)	0.145(4)	0.363(10)	0.289	0.145	0.363	0.	0.0	0.	0.	0.13	0.37
Ag10	9(*b*) 18(*c*)	0.058(4)	0.364(3)	0.585(14)	0.054	0.365	0.587	0.03	-0.01	-0.01	0.03	0.10	0.24
Ag11	9(*b*),9(*b*)	0.315(3)	0.367(4)	0.59(2)	0.311	0.366	0.59	0.03	0.01	0.	0.04	0.19	0.38
Ag12	9(*b*),9(*b*)	-0.239(4)	0.223(8)	0.445(12)	-0.231	0.231	0.445	-0.06	-0.06	0.	0.10	0.13	0.26
Ag13	9(*b*),9(*b*)	-0.172(5)	0.179(6)	0.521(12)	-0.175	0.176	0.521	0.02	0.02	0.	0.03	0.15	0.18

† Uncertainties for all Ag atom occupancies reported as ~0.02.

Table S18

Atomic positions for lovozerite $[Na_2CaZr(Si_6O_{12}(OH, O)_6]\cdot H_2O$ at room temperature (Yamnova *et al.*, 2001), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 10.18(1)$, $c = 13.13\ (2)$ Å; $z^* = z - 0.160$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*3*m*	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	u_{iso}
Na,K[†]	9(*b*),9(*b*)	0.341(3)	0.172(2)	0.006(2)	0.342	0.171	0.006	-0.01	0.01	0.	0.01	0.23
Ca,Na,Mn	3(*a*),3(*a*)	0	0	0.582	0	0	0.582	0.	0.	0.	0.	0.28
Zr,Fe,Ti,Hf	3(*a*),3(*a*)	0	0	-0.160	0	0	-0.160	0.	0.	0.	0.	0.19
Si1	9(*b*),9(*b*)	0.4829(8)	0.5172(8)	0.0608(6)	0.4829	0.5271	0.0608	0.	0.	0.	0.	0.20
Si2	9(*b*),9(*b*)	0.1835(5)	0.3696(6)	-0.0648(5)	0.1844	0.3687	-0.0648	-0.01	0.01	0.	0.01	0.17
O1	9(*b*),9(*b*)	1.002(8)	0.462(6)	-0.154(4)	0.976	0.488	-0.154	0.26	-0.26	0.	0.26	0.24
O2	9(*b*),9(*b*)	0.447(3)	0.224(3)	-0.163(2)	0.447	0.224	-0.163	0.	0.	0.	0.	0.30
O3	9(*b*),9(*b*)	0.555(3)	0.424(3)	0.088(2)	0.566	0.434	0.088	-0.11	-0.10	0.	0.11	0.29
O4	9(*b*),9(*b*)	0.208(2)	0.104(2)	0.165(1)	0.208	0.104	0.165	0.	0.	0.	0.	0.20
O5	9(*b*) 18(*f*)	0.336(3)	0.433(4)	-0.001(2)	0.335	0.416	-0.001	0.01	0.17	0.	0.17	0.33
O7	9(*b*)	0.601(2)	0.667(2)	0.001(1)	0.584	0.665	0.001	0.17	0.01	0.	0.17	0.25
O6	9(*b*),9(*b*)	0.101(2)	0.184(2)	-0.069(1)	0.095	0.190	-0.069	0.06	-0.06	0.	0.06	0.20

[‡] Occupancies: Na,K 0.73, 0.03; Ca,Na,Mn 0.35, 0.20, 0.08; Zr,Fe,Ti,Hf 0.80, 0.14, 0.03, 0.03.

Table S19(*a*)

Atomic positions for $BiCa_9(VO_4)_7$ at 120 K (Evans *et al.*, 2001) with hypothetical $x'y'z'$ coordinates, and the Δx, Δy, Δz displacements in Å.

$a = 10.8511(2)$, $c = 38.0505(9)$ Å; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position *R*3, *R*3*c*	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
V1	3(*a*)	0.	0.0	0.00367(6)	0.	0.	0.00367	0.	0.0	0.0	0.0	0.08
	6(*a*)											
V2	3(*a*)	0.	0.0	0.50367(7)	0.	0.	0.50367	0.	0.0	0.0	0.0	0.08
V3	9(*b*)	-0.1744(1)	-0.3137(1)	0.13661(5)	-0.1744	-0.3138	0.13663	0.	0.01	0.01	0.01	0.08
	18(*b*)											
V4	9(*b*)	0.3139(1)	0.1745(1)	0.63664(5)	0.3138	0.1744	0.63663	0.	0.01	0.01	0.01	0.09
V5	9(*b*)	-0.3139(1)	-0.1823(1)	-0.09452(5)	-0.3164	-0.1823	-0.09497	0.03	0.0	0.02	0.04	0.07
	18(*b*)											
V6	9(*b*)	0.1823(1)	0.3189(1)	0.40459(5)	0.1823	0.3164	0.40503	0.0	0.03	0.02	0.04	0.07
Ca,Bi1	9(*b*)	-0.1228(3)	-0.2760(3)	-0.0552(1)	-0.1227	-0.2761	-0.0552	0.01	0.01	0.0	0.01	0.15
	18(*b*)†											
Ca,Bi2	9(*b*)	0.2762(4)	0.1226(3)	0.4447(1)	0.2761	0.1227	0.4448	0.01	0.01	0.0	0.01	0.15
Ca,Bi3	9(*b*)	-0.1316(4)	-0.2607(6)	-0.0472(2)	-0.1314	-0.2608	-0.0473	0.01	0.01	0.01	0.02	0.12
	18(*b*)											
Ca,Bi4	9(*b*)	0.2609(6)	0.1312(4)	0.4526(2)	0.2608	0.1314	0.4527	0.01	0.01	0.01	0.02	0.12
Ca,Bi5	9(*b*)	-0.1381(1)	0.1377(1)	-0.15974(5)	-0.1381	0.1377	-0.15976	0.0	0.0	0.01	0.01	0.12
	18(*b*)											
Ca,Bi6	9(*b*)	-0.1377(1)	0.1381(1)	0.34021(5)	-0.1377	0.1381	0.34024	0.0	0.0	0.01	0.01	0.12
Ca,Bi7	9(*b*)	-0.2104(1)	-0.3851(1)	0.03694(5)	-0.2104	-0.3851	0.03695	0.0	0.0	0.0	0.0	0.15
	18(*b*)											
Ca,Bi8	9(*b*)	0.3851(1)	0.2103(1)	0.53691(5)	0.3851	0.2104	0.53695	0.0	-0.01	0.0	0.0	0.15
Ca,Bi9	3(*a*)	0.	0.	0.27075(8)	0.	0.	0.27070	0.0	0.0	0.0	0.0	0.13
	6(*c*)											
Ca,Bi10	3(*a*)	0.	0.	-0.22936(8)	0.	0.	-0.22930	0.0	0.0	0.0	0.0	0.13
O1	9(*b*)	-0.1469(5)	--0.1569(5)	0.0158(2)	-0.1469	-0.1569	0.0158	0.0	0.0	0.0	0.0	0.13
	18(*f*)											
O2	9(*b*)	0.1568(5)	0.1470(5)	0.5159(2)	0.1569	0.1469	0.5158	0.0	0.0	0.0	0.0	0.13
O3	3(*a*)	0.0	0.0	-0.0414(3)	0.0	0.0	-0.0414	0.0	0.0	0.0	0.0	0.17
	6(*a*)											
O4	3(*a*)	0.0	0.0	0.4586(3)	0.0	0.0	0.4586	0.0	0.0	0.0	0.0	0.14
O5	9(*b*)	-0.2427(6)	-0.4917(6)	0.1450(2)	-0.2427	-0.4915	0.1449	0.0	0.0	0.0	0.0	0.16
	18(*b*)											
O6	9(*b*)	0.4914(6)	0.2428(6)	0.6448(2)	0.4915	0.2427	0.6449	0.0	0.0	0.0	0.0	0.15
O7	9(*b*)	-0.2913(5)	-0.2778(5)	0.1597(1)	-0.2915	-0.2779	0.1597	0.0	0.0	0.0	0.0	0.08
	18(*b*)											
O8	9(*b*)	0.2780(5)	0.2918(5)	0.6597(1)	0.2779	0.2915	0.6597	0.0	0.0	0.0	0.0	0.09
O9	9(*b*)	0.0010(6)	-0.2291(7)	0.1491(2)	0.0007	-0.2290	0.1491	0.0	0.0	0.0	0.0	0.14
	18(*b*											
O10	9(*b*)	0.2288(7)	-0.0005(5)	0.6491(2)	0.2290	0.0007	0.6491	0.0	0.0	0.0	0.0	0.14
O11	9(*b*)	-0.1974(7)	-0.2833(9)	0.0945(2)	-0.1971	-0.2833	0.0945	0.0	0.0	0.0	0.0	0.19
	18(*b*)											
O12	9(*b*)	0.2834(9)	0.1968(7)	0.5945(2)	0.2833	0.1971	0.5945	0.0	0.0	0.0	0.0	0.19

O13	9(*b*)	-0.2386(7)	-0.0202(6)	-0.1145(2)	-0.2383	-0.0202	-0.1145	0.0	0.0	0.0	0.0	0.16
	18(*b*)											
O14	9(*b*)	0.0203(6)	0.2380(7)	0.3856(2)	0.0202	0.2383	0.3855	0.0	0.0	0.0	0.0	0.16
O15	9(*b*)	-0.2615(6)	-0.2965(6)	-0.1057(1)	-0.2614	-0.2962	-0.1057	0.0	0.0	0.0	0.0	0.12
	18(*b*)											
O16	9(*b*)	0.2959(6)	0.2613(6)	0.3943(1)	0.2962	0.2614	0.1057	0.0	0.0	0.0	0.0	0.12
O17	9(*b*)	-0.4942(6)	-0.2599(6)	-0.1059(2)	-0.4947	-0.2602	-0.1058	0.01	0.0	0.0	0.01	0.12
	18(*b*)											
O18	9(*b*)	0.2605(5)	0.4952(5)	0.3944(2)	0.2602	0.4947	0.3942	0.0	0.01	0.01	0.01	0.12
O19	9(*b*)	-0.2899(6)	-0.1520(6)	-0.0507(2)	-0.2900	-0.1522	-0.0507	0.0	0.0	0.0	0.0	0.13
	18(*b*)											
O20	9(*b*)	0.1524(6)	0.2901(6)	0.4494(2)	0.1522	0.2900	0.4493	0.0	0.0	0.0	0.0	0.13

† The Ca/Bi1 site occupancy was reported as 0.54(2), that of Ca/Bi3 as 0.35(2) %.

Table S19(*b*)

Comparison of Evans *et al.*'s (2001) *R*3*c*-averaged atomic coordinates for $BiCa_9(VO_4)_7$ with Kim *et al.*'s (2002).

a_{Kim} = 10.857(1), c_{Kim} = 38.063(6) Å. $z^*_{Kim} = z + 0.3062$. $\Delta x = (x_E - x_K)a$, $\Delta y = (y_E - y_K)a$, $\Delta z = (z_E - z_K)c$.

$Atoms_{Evans}$	x_{Evans}	y_{Evans}	z_{Evans}	Equi-valent position†	x_{Kim}	y_{Kim}	z^*_{Kim}	Δx	Δy	Δz	$\Delta\xi$
V1	0.	0.0	0.00367	$V3^1$	0	0	0.0032	0.0	0.0	0.02	0.02
V3	-0.1744	-0.3138	0.13663	$V2^7$	0.8259	0.6857	0.1366	-0.01	0.01	0.00	0.01
V5	-0.3164	-0.1823	-0.09497	$V1^2$	0.6806	0.8188	0.9053	-0.03	-0.01	-0.01	0.04
Ca,Bi1‡	-0.1227	-0.2761	-0.0552	$Ca3^5$	0.8735	0.7291	-0.0528	0.04	-0.06	-0.09	0.10
Ca,Bi3	-0.1314	-0.2608	-0.0473	$Ca3^5$	0.8735	0.7291	-0.0528	0.05	0.11	0.21	0.25
Ca,Bi5	-0.1381	0.1377	-0.15976	$Ca2^3$	0.8613	0.1387	-0.1597	0.01	-0.01	-0.01	0.01
Ca,Bi7	-0.2104	-0.3851	0.03695	$Ca1^5$	0.7906	0.6144	0.0365	-0.01	0.01	0.02	0.02
Ca,Bi9	0.	0.	0.27070	$Ca4^6$	0.	0.	0.2706	0	0.	0.01	0.01
O1	-0.1469	-0.1569	0.0158	$O9^3$	-0.1462	-0.1559	0.0156	-0.01	-0.01	0.01	0.02
O3	0.0	0.0	-0.0414	$O10^4$	0.0	0.0	-0.0409	0	0.0	-0.02	0.02
O5	-0.2427	-0.4915	0.1449	$O6^7$	0.7561	0.5082	0.1458	0.01	0.01	-0.03	0.03
O7	-0.2915	-0.2779	0.1597	$O7^7$	0.7108	0.7240	0.1591	-0.02	-0.02	0.02	0.04
O9	0.0007	-0.2290	0.1491	$O8^7$	0.9988	0.7686	0.1497	0.02	0.03	-0.02	0.05
O11	-0.1971	-0.2833	0.0945	$O5^7$	0.8030	0.7125	0.0938	-0.00	0.05	0.03	0.06
O13	-0.2383	-0.0202	-0.1145	$O2^2$	0.7608	-0.0196	-0.1143	0.01	-0.01	-0.01	0.01
O15	-0.2614	-0.2962	-0.1057	$O4^2$	0.7404	0.7076	-0.1066	-0.02	-0.04	0.03	0.06
O17	-0.4947	-0.2602	-0.1058	$O3^2$	0.5045	0.7401	-0.1066	0.01	-0.01	0.03	0.03
O19	-0.2900	-0.1522	-0.0507	$O1^2$	0.7064	0.8466	-0.0512	0.04	0.01	0.02	0.05

† Equivalent position in *R*3*c*: 1. x, y, z; 2. $\bar{x} + y, y, \frac{1}{2} + z$; 3. $x, x - y, \frac{1}{2} + z$; 4. $\frac{1}{3} + x, \frac{2}{3} + y, \frac{2}{3} + z$; 5. $\frac{1}{3} - x + y, \frac{2}{3} - x, \frac{2}{3} + z$; 6. $\frac{2}{3} - y, \frac{1}{3} - x, \frac{5}{6} + z$; 7. $\frac{2}{3} + x, \frac{1}{3} + x - y, \frac{5}{6} + z$.

‡ Average of the split Ca,Bi1 sites.

Table 19(*c*)
Evans *et al.*'s (2001) atomic positions for $BiCa_9(VO_4)_7$ in a further hypothetical transition to supergroup $R\bar{3}m$, with proposed $x'y'z'$ coordinates and Δx, Δy, Δz displacements in Å, see also Table 19(*a*). $a_{Evans} = 10.8511(2)$, $c_{Evans} = 38.0505(9)$ Å; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$;.

	Wyckoff Position	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3c$, $R\bar{3}m$											
V1	6(*a*),6(*c*)	0.	0.0	0.00367	0.	0.	0.00367	0.0	0.0	0.0	0.0	0.08
V3	18(*b*)	-0.1744	-0.3138	0.13663	-0.1784	-0.3151	0.11580	0.04	0.01	0.79	0.79	0.08
	36(*i*)											
V5	18(*b*)	-0.3164	-0.1823	-0.09497	-0.3151	-0.1784	-0.11580	-0.01	-0.04	0.79	0.79	0.07
Ca,Bi1	18(*b*))	-0.1227	-0.2761	-0.0552	-0.1304	-0.2802	-0.1075	0.08	0.04	1.99	1.99	0.15
	36(*i*)											
Ca,Bi5	18(*b*)	-0.1381	0.1377	-0.15976	-0.1304	0.1417	-0.1075	-0.08	-0.04	-1.99	1.99	0.12
Ca,Bi3	18(*b*)	-0.1314	-0.2608	-0.0473	-0.1709	-0.3229	-0.0421	0.43	0.67	-0.20	0.98	0.12
	36(*i*)											
Ca,Bi7	18(*b*)	-0.2104	-0.3851	0.03695	-0.1709	-0.3229	0.0421	-0.43	-0.67	-0.20	0.98	0.15
O1	18(*b*),18(*f*)	-0.1469	-0.1569	0.0158	-0.1519	-0.1519	0.	0.05	-0.05	0.60	0.60	0.13
O3	6(*a*),6(*c*)	0.0	0.0	-0.0414	0.0	0.0	-0.0414	0.0	0.0	0.0	0.0	0.17
O5	18(*b*)	-0.2427	-0.4915	0.1449	-0.2525	-0.4931	0.1254	0.10	0.02	0.74	0.75	0.16
	36(*i*)											
O17	18(*b*)	-0.4947	-0.2602	-0.1058	-0.4931	-0.2525	-0.1254	-0.02	-0.08	0.74	0.75	0.12
O7	18(*b*)	-0.2915	-0.2779	0.1597	-0.2939	-0.2696	0.1327	0.03	-0.09	1.03	1.03	0.08
	36(*i*)											
O15	18(*b*)	-0.2614	-0.2962	-0.1057	-0.2696	-0.2939	-0.1327	0.09	-0.02	1.03	1.03	0.12
O9	18(*b*)	0.0007	-0.2290	0.1491	-0.0098	-0.2336	0.1318	0.14	0.05	0.66	0.68	0.14
	36(*i*)											
O13	18(*b*)	-0.2383	-0.0202	-0.1145	-0.2336	-0.0098	-0.1318	-0.05	-0.12	0.66	0.68	0.16
O11	18(*b*)	-0.1971	-0.2833	0.0945	-0.1746	-0.2866	0.0726	0.24	0.04	0.83	0.87	0.19
	36(*i*)											
O19	18(*b*)	-0.2900	-0.1522	-0.0507	-0.2866	-0.1746	-0.0726	-0.04	0.24	0.83	0.86	0.13

Table 19(*d*)
Kim *et al.*'s (2002) atomic positions for $BiCa_9(VO_4)_7$ in a hypothetical transition to supergroup $R\bar{3}m$ with proposed $x'y'z'$ coordinates and Δx, Δy, Δz displacements in Å.
a_{Kim} = 10.857(1), c_{Kim} = 38.063(6) Å. $z^* = z + 0.3062$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3c$, $R\bar{3}m$											
V1†	6(*a*),6(*c*)	0.	0.0	0.0032	0.	0.	0.0032	0.0	0.0	0.0	0.0	0.08
V2	18(*b*)	-0.1741	-0.3143	0.1366	-0.1776	-0.3169	0.11565	0.04	0.03	0.79	0.79	0.08
	36(*i*)											
V1	18(*b*)	-0.3194	-0.1812	-0.0947	-0.3169	-0.1776	-0.11565	-0.03	-0.04	0.79	0.79	0.07
Ca5	18(*b*)	-0.1387	0.1387	-0.1597	-0.1385	0.1326	-0.1062	-0.0	0.07	-2.04	2.04	0.12
	36(*i*)											
Ca1,3	18(*b*))	-0.1265	-0.2709	-0.0528	-0.1326	-0.2711	-0.1062	0.07	0.0	2.03	2.03	0.15
Ca7	18(*b*),18(*h*)	-0.2094	-0.3856	0.0365	-0.1983	-0.3967	0.0365	-0.12	0.12	0.0	0.12	0.12
Ca9	6(*a*),6(*c*)	0.	0.	0.2706	0.	0.	0.2706	0.0	0.0	0.0	0	
O1	18(*b*),18(*f*)	-0.1462	-0.1559	0.0156	-0.1511	-0.1511	0.	0.05	-0.05	0.60	0.60	0.13
O3	6(*a*),6(*c*)	0.0	0.0	-0.0409	0.0	0.0	-0.0409	0.0	0.0	0.0	0	0.17
O5	18(*b*)	-0.2439	-0.4918	0.1458	-0.2515	-0.4936	0.1262	0.08	0.02	0.75	0.76	0.16
	36(*i*)											
O17	18(*b*)	-0.4955	-0.2599	-0.1066	-0.4936	-0.2515	-0.1262	-0.02	-0.09	0.72	0.73	0.12
O7	18(*b*)	-0.2892	-0.2760	0.1591	-0.2908	-0.2678	0.1329	-0.02	-0.09	1.00	1.01	0.08
	36(*i*)											
O15	18(*b*)	-0.2596	-0.2924	-0.1066	-0.2678	-0.2908	-0.1329	0.09	-0.02	1.00	1.00	0.12
O9	18(*b*)	0.0012	-0.2314	0.1497	-0.0092	-0.2353	0.1320	0.11	0.04	0.67	0.68	0.14
	36(*i*)											
O13	18(*b*)	-0.2392	-0.0196	-0.1143	-0.2353	-0.0092	-0.1320	-0.04	-0.11	0.67	0.68	0.16
O11	18(*b*)	-0.1970	-0.2875	0.0938	-0.1752	-0.2905	0.0726	-0.24	0.03	0.81	0.84	0.19
	36(*i*)											
O19	18(*b*)	-0.2936	-0.1534	-0.0512	-0.2905	-0.1752	-0.0726	-0.03	0.24	0.81	0.84	0.13

† Evans *et al.*'s (2001) atom numbering.

Table S20

Atomic positions† for $CoGe_{1.5}S_{1.5}$ and $CoGe_{1.5}Se_{1.5}$ at room temperature (Partik *et al.*, 1996)† with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 11.3363(10)$, $c = 13.9176(9)$ Å. $z^* = z - 0.2572$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3,R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Co1	3(*a*)	0	0	0.7428	0	0	0.7451	0	0	-0.03	0.03	0.05
	6(*c*)											
Co2	3(*a*)	0	0	0.2526(2)	0	0	0.2549	0	0	-0.03	0.03	0.05
Co3	9(*b*)	0.3324(2)	0.1651(3)	0.4091(3)	0.3328	0.1642	0.4104	-0.01	0.01	-0.02	0.03	0.05
	18(*f*)											
Co4	9(*b*)	0.6667(2)	0.8367(2)	0.5883(3)	0.6672	0.8358	0.5896	-0.01	0.01	-0.02	0.03	0.06
S1	9(*b*)	0.2810(4)	0.0675(4)	0.0661(4)	0.2806	0.0670	0.0675	0.01	0.01	-0.02	0.03	0.07
	18(*f*)											
S4	9(*b*)	0.2142(4)	0.2801(4)	0.9312(4)	0.2137	0.2806	0.9325	0.01	-0.01	-0.02	0.03	0.06
S3	9(*b*)	0.1624(4)	0.9799(4)	0.3336(4)	0.1621	0.9803	0.3340	0.01	-0.01	0.04	0.05	0.05
	18(*f*)											
S2	9(*b*)	0.8382(4)	0.0193(4)	0.6655(4)	0.8379	0.0197	0.6659	0.02	-0.01	-0.07	0.07	0.06
Ge1	9(*b*)	0.8310(2)	0.3227(2)	0.1729(3)	0.8292	0.3212	0.1731	0.02	0.02	0.01	0.04	0.07
	18(*f*)											
Ge2	9(*b*)	0.1726(2)	0.6803(2)	0.8267(3)	0.1708	0.6788	0.8269	0.02	0.02	0.01	0.04	0.06
Ge3	9(*b*)	0.0635(2)	0.7902(2)	0.4376(3)	0.0632	0.7895	0.4385	0 .01	0.01	-0.01	0.02	0.07
	18(*f*)											
Ge4	9(*b*)	-0.0628(2)	0.2112(2)	0.5606(3)	-0.0631	0.2105	0.5615	0.01	0.01	-0.01	0.02	0.07

† With several S and Ge atoms in rhombohedral equivalents of reported locations.

Table S21(*a*)

Atomic positions for $K_2Sn_2O_3$ at room temperature (Braun & Hoppe, 1978) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

$a = 6.001$, $c = 14.33$ Å.[†] $z^* = z + 0.0093$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff position $R3$, $R\bar{3}m$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
K1	3(a) 6(c)	0	0	0.7538(20)	0	0	0.7533	0	0	0.01	0.01	0.13
K2	3(a)	0	0	0.2473(2)	0	0	0.2467	0	0	0.01	0.01	0.11
Sn1	3(a),3(a)	0	0	0.0093	0	0	0	0	0	0.13	0.13	0.12
Sn2	3(a),3(b)	0	0	0.4895(1)	0	0	0.5000	0	0	-0.15	0.15	0.09
O1	9(b),18(h)	0.1685(20)	0.338(2)	0.0711(10)	0.169	0.338	0.0711	0.0	0.0	0.0	0.0	~0.2

[†] Uncertainties in lattice constants and u_{33} not stated.

Table S21(*b*)

Revised atomic positions for $K_2Sn_2O_3$ at room temperature (Braun & Hoppe, 1981)

$a = 6.001(1)$, $c = 14.327(1)$ Å.

	Wyckoff position $R\bar{3}m$	x	y	z[†]	u_{33}
K1	3(*b*)	0	0	0.5	0.15
K2	3(*a*)	0	0	0.	0.13
Sn	6(*c*)	0	0	0.24013(3)	0.11
O	9(*d*)	0.1667	0.3333	0.8333	0.21

[†] An origin shift of ¼ in the *z*-coordinates of Table S21(*a*) reveals the near identity of the derived $x'y'z'$ coordinates and the experimental values in Table S21(*b*); Sn1 and Sn2 can occupy either the 3(*a*) and 3(*b*) sites as in Table S21(*a*) or the 6(*c*) site as in Table S21(*b*).

Table S22

Atomic positions for $[Cr(H_2O)_6]F_3 \cdot (H_2O)_3$ at room temperature (Epple & Massa, 1978) with hypothetical $x'y'z'$ coordinates, the Δx, Δy, Δz and u_{33}/u_{iso} displacements in Å

$a = 10.837(9)$, $c = 8.157(3)$ Å. $z^* = z - 0.0014$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33} †
Cr	3(*a*)	0	0	-0.0014	0.	0	0.	0	0	-0.01	0.01	0.13
O1	9(*b*)	0.6503(9)	0.4747(10)	0.1914(9)	0.6562	0.4764	0.1970	-0.06	-0.02	-0.05	0.09	0.16
O2	18(*f*) 9(*b*)	0.3379(9)	0.5220(9)	0.7974(9)	0.3437	0.5236	0.8030	-0.06	-0.02	-0.05	0.09	0.17
O3	9(*b*)	0.0884(10)	0.5170(10)	0.2395(10)	0.0885	0.5176	0.2438	-0.01	-0.01	-0.04	0.04	0.17
F1	18(*f*) 9(*b*)	0.9115(9)	0.4817(9)	0.7515(9)	0.9115	0.4824	0.7562	-0.01	-0.02	-0.04	0.05	0.21
H1	9(*b*)	0.447(2)	0.258(2)	0.869 (2)	0.469	0.309	0.841	-0.24	-0.55	0.23	0.74	0.3
H2	18(*f*) ‡ 9(*b*)	0.510(2)	0.639(2)	0.186(2)	0.531	0.691	0.159	-0.23	-0.56	0.22	0.74	0.3
H3	9(*b*)	0.524(2)	0.365(2)	0.550(2)	0.525	0.362	0.556	-0.01	0.03	-0.05	0.06	0.3
H6	18(*f*) 9(*b*)	0.475(1)	0.642(2)	0.438(2)	0.475	0.638	0.444	0.00	0.04	-0.05	0.06	0.3
H4	9(*b*)	0.439(2)	0.265(2)	0.447(3)	0.430	0.261	0.456	0.09	0.04	-0.07	0.13	0.3
H5	18(*f*) 9(*b*)	0.579(2)	0.744(2)	0.534(3)	0.570	0.739	0.544	0.09	0.05	-0.08	0.15	0.3

† Values of u_{33} determined for Cr, O and F; that of u_{iso}(H) is assumed.

‡ H1, H2 and O3 form the H_2O molecule.

Table S23(*a*)

Atomic positions for $Cs[SbF_5OH]$ at room temperature (Nolte & de Beer, 1979) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

a = 7.94(1), c = 8.28(1) Å. $z^* = z - 0.0082$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Cs	3(*a*),3(*b*)	0	0	0.4917(8)	0	0	½	0	0	-0.07	0.07	0.19(4)
Sb	3(*a*),3(*a*)	0	0	-0.0082	0	0.	0	0	0	-0.07	0.07	0.21(4)
F1,O[†]	9(*b*)	0.0795(38)	0.2099(45)	0.1433(31)	0.0655	0.2131	0.1351	0.11	-0.03	0.07	0.12	0.19(9)
F2	18(*f*) 9(*b*)	0.2162(36)	0.1616(33)	-0.1269(35)	0.2131	0.1476	-0.1351	0.03	0.11	0.07	0.15	0.26(12)

[†] Occupancy of F1 and O sites given as $^5/_6$ F, $^1/_6$ O. The equivalence of F1,O and F2 in $R\bar{3}$ strongly suggests equal occupancy of both sites.

Table S23(*b*)

Atomic positions for $CsSbF_6$ at room temperature (de Steyn *et al.,* 1984) for comparison with derived values in Table 24(*a*).

a = 7.904(1), c = 8.261(1) Å.

	Wyckoff position $R\bar{3}$, $R\bar{3}m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Cs	3(*b*),3(*b*)	0	0	½	0	0	½	0	0	0	0	0.19(3)
Sb	3(*a*),3(*a*)	0	0	0	0	0.	0	0	0	0	0	0.18(3)
F	18(*f*),18(*h*)	0.0656(16)	0.2158(15)	0.1337(14)	0.0938	0.1876	0.1337	-0.22	0.22	0	0.22	0.26(8)

Table S24

Atomic positions for $(BN)_3Cl_6$ at room temperature (Gopinathan *et al.*, 1974), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å

$a = 8.847(4)$, $c = 10.321(5)$ Å. $z^* = z + 0.0026$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c = 0$.

	Wyckoff position $R3, R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Cl1	9(*b*)	-0.4062(1)	-0.2654(3)	0.0026	-0.4066	-0.2656	0.0026	0.00	0.00	0.00	0.00	0.27(3)
	18(*f*)	.										
Cl2	9(*b*)	0.4069(2)	0.2657(2)	-0.0026(1)	0.4066	0.2657	-0.0026	0.00	0.00	0.00	0.00	0.29(3)
N	9(*b*)	-0.1808 (5)	-0.1176(3)	0.0005(6)	-0.1831	-0.1191	0.0005	0.02	0.01	0.00	0.02	0.22(5)
	18(*f*)											
B	9(*b*)	0.1854(5)	0.1205(3)	-0.0005(6)	0.1831	0.1191	-0.0005	0.02	0.01	0.00	0.02	0.22(5)

Table S25

Atomic positions for Li_7SbO_6 at room temperature (Hauck, 1969) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

$a = 5.393(3)$, $c = 15.084(8)$ Å. $z^* = z$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq} †
Sb	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	0.13
O1	9(*b*)	0.32	0.03	0.082	0.175	0.175	0.082	0.78	-0.78	0	0.78	0.14
O2	18(*c*) 9(*b*)	-0.03	-0.32	-0.082	-0.175	-0.175	-0.082	0.78	-0.78	0	0.78	0.14
Li1	9(*b*)	-0.36	-0.33	-0.11	-0.345	-0.345	-0.11	-0.08	0.08	0	0.08	0.16
Li2	18(*c*) 9(*b*)	0.33	0.36	0.11	0.345	0.345	0.11	-0.08	0.08	0	0.08	0.16
Li3	3(*a*),6(*c*)‡	0	0	0.67	0	0	0.67	0	0.0	0	0.0	0.16

† Values from centrosymmetric Li_7SbO_6 in $P\bar{1}$ by Mühle *et al*. (2004); the dimensionless 'U_{eq}' values reported therein, ranging from 1.53 to 4.19, were taken as B_{eq}(Å^2), not $B/8\pi^2$.

‡ The use of position 6(*c*) by Li3 implies disorder with 50 % occupancy; if Li3 remains in 3(*a*), then $\Delta z = 2.56$ Å.

Table S26(*a*)
Atomic positions for $Fe_2P_2Se_6$ at room temperature (Klingen *et al.*, 1973) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å
$a = 6.265(6)$, $c = 19.80(2)$ Å. $z^* = z + 0.0013$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position $R3,R\bar{3}$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u†
Fe1	3(*a*) 6(*c*)	0	0	0.1671(15)	0	0	0.1672	0	0	-0.01	0.01	n/r
Fe2	3(*a*)	0	0	-0.1674(21)			-0.1672	0	0	-0.01	0.01	n/r
P1	3(*a*) 6(*c*)	0	0	0.4450(22)	0	0	0.4434	0	0	0.01	0.01	n/r
P2	3(*a*)	0	0	-0.4418(24)	0	0	-0.4434	0	0	0.01	0.01	n/r
Se1	9(*b*) 18(*f*)	0.3315(7)	-0.0030(17)	0.0813(11)	0.3382	0.0121	0.0827	-0.04	-0.09	-0.03	0.12	n/r
Se2	9(*b*)	-0.3449(28)	-0.0272(31)	-0.0841(12)	-0.3382	-0.0121	-0.0827	-0.04	-0.09	-0.03	0.12	n/r

† Thermal/static displacement factors not reported.

Table S26(*b*)
Atomic positions for $Fe_2P_2Se_6$ at room temperature (Wiedenmann *et al.*, 1981) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å
$a = 6.262(3)$, $c = 19.805(5)$ Å.

	Wyckoff position $R\bar{3}$	x	y	z†
Fe1	6(*c*)	0	0	0.1671
P1	6(*c*)	0	0	0.4455
Se1	9(*b*)	0.3314	0.0059	0.0828

† Coordinate uncertainties not reported.

Table S27

Atomic positions for Ni_3TeO_6 at room temperature (Newnham & Meagher, 1967), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 5.103(2)$, $c = 13.755(10)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u‡
	$R3$, $R\bar{3}$											
Ni1†	3(*a*)	0	0	0.352	0	0	0.352	0	0	0	0	0.1
	6(*c*)											
Ni2	3(*a*)	0	0	0.648	0	0	0.648	0	0	0	0	0.1
Ni3†	3(*a*)	0	0	0.852	0	0	0.852	0	0	0	0	0.1
	6(*c*)											
Te1	3(*a*)	0	0	0.148	0	0	0.148	0	0	0	0	0.1
O1	9(*b*)	0.306	0	0.25	0.306	0	0.25	0	0	0	0	0.1
	18(*f*)											
O2	9(*b*)	0.694	0	0.75	0.694	0	0.75	0	0	0	0	0.1

† Ni3 and Te1 sites each with 0.5 Ni and 0.5 Te occupancy.

‡ Values of u (Å) assumed, not reported.

Table S28

Atomic positions for $2CeFCO_3 \cdot CaCO_3$ (parisite) at room temperature (Donnay & Donnay, 1953), with hypothetical $x'y'z'$ coordinates, the Δx, Δy, Δz displacements in Å, and u assumed as 0.1 Å.

$a = 7.124$, $c = 84.11$ Å. $z^* = z - 0.138$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	*u*
Ce1	9(*b*)	0.333	0.0	-0.138	0.333	0.	-0.138	0.	0.	0.08	0.08	0.1
	18(*f*)											
Ce4	9(*b*)	0.333	0	0.137	0.333	0	0.138	0.	0.	-0.08	0.08	0.1
Ce2	9(*b*)	0.333	0.	-0.030	0.333	0.	-0.030	0.	0.	-0.08	0.08	0.1
	18(*f*)											
Ce3	9(*b*)	0.333	0	0.029	0.333	0.	0.030	0.	0.	0.08	0.08	0.1
Ca1	9(*b*)	0.333	0.	-0.084	0.333	0.	-0.083	0.	0.	0.0	0.0	0.1
	18(*f*)											
Ca2	9(*b*)	0.333	0.	0.083	0.333	0.	0.083	0.	0.	0.0	0.0	0.1
F1	3(*a*)	0.	0.	-0.138	0.	0.	-0.138	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F10	3(*a*)	0.	0.	0.137	0.	0.	0.138	0.	0.	0.08	0.08	0.1
F2	3(*a*)	0.	0.	0.195	0.	0.	0.196	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F12	3(*a*)	0.	0.	0.804	0.	0.	0.805	0.	0.	0.08	0.08	0.1
F3	3(*a*)	0.	0.	0.529	0.	0.	0.530	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F11	3(*a*)	0.	0.	0.470	0.	0.	0.471	0.	0.	0.08	0.08	0.1
F4	3(*a*)	0.	0.	-0.030	0.	0.	-0.030	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F7	3(*a*)	0.	0.	0.029	0.	0.	0.030	0.	0.	-0.08	0.08	0.1
F5	3(*a*)	0.	0.	0.303	0.	0.	0.304	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F9	3(*a*)	0.	0.	0.697	0.	0.	0.697	0.	0.	-0.08	0.08	0.1
F6	3(*a*)	0.	0.	0.637	0.	0.	0.638	0.	0.	-0.08	0.08	0.1
	18(*f*)											
F8	3(*a*)	0.	0.	0.362	0.	0.	0.362	0.	0.	-0.08	0.08	0.1
C1[†]	9(*b*)	0.245	0.333	-0.083	0.245	0.333	-0.085	0.	0.	0.17	0.17	0.1
	18(*f*)											
C2	9(*b*)	0.245	0.333	0.083	0.245	0.333	0.085	0.	0.	-0.17	0.17	0.1
O1	9(*b*)	0.067	0.333	-0.083	0.067	0.333	-0.083	0.	0.	0.	0.	0.1
	18(*f*)											
O2	9(*b*)	0.333	0.067	0.083	0.333	0.067	0.083	0.	0.	0.	0.	0.1
	18(*f*)											
O3	9(*b*)	0.333	0.333	-0.097	0.333	0.333	-0.097	0.	0.	-0.08	0.08	0.1
	18(*f*)											
O6	9(*b*)	0.333	0.333	0.096	0.333	0.333	0.096	0.	0.	-0.08	0.08	0.1
O4	9(*b*)	0.333	0.333	-0.070	0.333	0.333	-0.070	0.	0.	0.	0.	0.1
	18(*f*)											
O5	9(*b*)	0.333	0.333	0.070	0.333	0.333	0.070	0.	0.	0.	0.	0.1

[†] A displacement of ~c/12 by the CO_3 group in addition to the origin displacement along the c axis, together with an exchange of O2(*yxz*) for O2(*xyz*), results in a close approach to space group *R*32.

Table S29

Atomic positions for $3CeFCO_3 \cdot 2CaCO_3$ (röntgenite) at room temperature (Donnay & Donnay, 1953), with hypothetical $x'y'z'$ coordinates, the Δx, Δy, Δz displacements in Å and u assumed as 0.1 Å.

$a = 7.131$, $c = 69.41$ Å. $z^* = z - 0.1314$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u
Ce1	9(*b*)	0.333	0.0	-0.131	0.333	0.0	-0.131	0.	0.	0.	0.	0.1
	18(*f*)											
Ce3	9(*b*)	0.333	0	0.131	0.333	0	0.131	0	0	0	0	0.1
Ce2	9(*b*),9(*d*)	0.333	0.	0.0	0.333	0.	0.0	0.	0.	0.	0.	0.
Ca1	9(*b*)	0.333	0.	-0.065	0.333	0.	-0.065	0.	0.	0.	0.	0.1
	18(*f*)											
Ca2	9(*b*)	0.333	0.	0.066	0.333	0.	0.066	0.	0.	0.	0.	0.1
F1	3(*a*)	0.	0.	-0.131	0.	0.	-0.131	0	0	0	0	0.1
	18(*f*)											
F7	3(*a*)	0.	0.	0.132	0.	0.	0.132	0.	0.	0.	0.	0.1
F2	3(*a*)	0.	0.	0.202	0.	0.	0.202	0.	0.	0.	0.	0.1
	18(*f*)											
F9	3(*a*)	0.	0.	0.798	0.	0.	0.798	0.	0.	0.	0.	0.1
F3	3(*a*)	0.	0.	0.536	0.	0.	0.536	0.	0.	0.	0.	0.1
	18(*f*)											
F8	3(*a*)	0.	0.	0.464	0.	0.	0.464	0.	0.	0.	0.	0.1
F4	3(*a*),3(*a*)	0.	0.	0.0	0.	0.	0.0	0.	0.	0.	0.	0.1
F5	3(*a*)	0.	0.	0.333	0.	0.	0.333	0.	0.	0.	0.	0.1
	18(*f*)											
F6	3(*a*)	0.	0.	0.667	0.	0.	0.667	0.	0.	0.	0.	0.1
C†	9(*b*),9(*d*)	0.245	0.333	0.0	0.289	0.289	0.0	-0.31	0.31	0	0.31	0.1
O1	9(*b*),9(*d*)	0.067	0.333	0.0	0.	0.333	0.	0.48	0.	0.	0.48	0.1
O2	9(*b*)	0.333	0.333	-0.016	0.333	0.333	-0.016	0.	0.	0.	0.	0.1
	18(*f*)											
O3	9(*b*)	0.333	0.333	0.016	0.333	0.333	0.016	0.	0.	0.	0.	0.1

† With an additional displacement of $^1/_6$ along the c axis by the CO_3 group.

Table S30

Atomic positions for $NiTiO_3$ at room temperature (Sullivan & Pavlovic, 1962), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

a = 5.443 Å, α = 55.05º; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Ni	2(a)	±(0.352	0.352	0.352)	±(0.352	0.352	0.352)	0	0	0.	0	0.12
Ti	2(a)	±(0.142	0.142	0.142)	±(0.142	0.142	0.142)	0	0	0	0	0.12
O1	6(b)	±(0.307	0.008	0.223)	±(0.53	-0.075	0.215)	0.	0.	0.	0	0.14

Table S31

Atomic positions for $Er_{13}Ge_6O_{31}(OH)$ at room temperature (Genkina *et al.*, 1990), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 15.617\ (7)$, $c = 9.398\ (5)$ Å; $z^* = z + 0.0312$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{aniso}
	$R3,\ R\bar{3}$											
Er1	3(*a*),3(*a*)	0	0	0.0312	0	0	0	0	0	0.29	0.29	0.07
Er2	9(*b*) 18(*f*)	0.7470(1)	0.1608(1)	0.3129(2)	0.7472	0.1607	0.3123	-0.01	0.01	0.01	0.01	0.08
Er3	9(*b*)	0.2525(1)	0.8395(1)	0.6884(2)	0.2529	0.8394	0.6877	-0.01	0.01	0.01	0.01	0.05
Er4	9(*b*) 18(*f*)	0.8542(1)	0.0016(1)	0.3263(3)	0.8539	0.0009	0.3250	0.01	0.01	0.01	0.02	0.09
Er5	9(*b*)	0.1464(1)	0.9997(1)	0.6762(3)	0.1461	0.9991	0.6750	0.01	0.01	0.01	0.02	0.07
Ge1	9(*b*) 18(*f*)	0.3127(4)	0.4103(4)	0.3440(6)	0.3127	0.4116	0.3432	0.00	-0.02	0.01	0.02	0.07
Ge2	9(*b*)	0.6873(4)	0.5871(4)	0.6590(6)	0.6873	0.5884	0.6567	0.00	-0.02	0.01	0.02	0.06
O1	9(*b*) 18(*f*)	0.005(2)	0.708(2)	0.309(3)	0.005	0.711	0.300	-0.01	-0.05	0.08	0.10	0.08
O2	9(*b*)	0.994(2)	0.286(2)	0.709(3)	0.995	0.289	0.700	-0.01	-0.05	0.08	0.10	0.10
O3	9(*b*) 18(*f*)	0.941(2)	0.801(2)	0.549(3)	0.944	0.802	0.549	-0.05	-0.02	0.00	0.06	0.07
O4	9(*b*)	0.052(2)	0.196(2)	0.452(3)	0.055	0.198	0.451	-0.05	-0.02	0.01	0.06	0.07
O5	9(*b*) 18(*f*)	0.769(2)	0.157(2)	0.057(3)	0.769	0.159	0.058	0.00	-0.04	-0.01	0.04	0.13
O6	9(*b*)	0.231(2)	0.838(2)	0.940(2)	0.231	0.841	0.942	0.00	-0.04	-0.02	0.04	0.04
O7	9(*b*) 18(*f*)	0.581(2)	0.830(2)	0.496(2)	0.583	0.832	0.498	-0.05	-0.03	-0.02	0.07	0.06
O8	9(*b*)	0.424(2)	0.166(2)	0.500(4)	0.427	0.168	0.502	-0.05	-0.03	-0.02	0.07	0.12
O9	9(*b*) 18(*f*)	0.879(2)	0.028(2)	0.098(3)	0.881	0.027	0.100	-0.03	0.02	-0.02	0.03	0.05
O10	9(*b*)	0.116(2)	0.974(2)	0.898(4)	0.118	0.973	0.900	-0.03	0.02	-0.02	0.03	0.15
O11	3(*a*) 6(*c*)	0	0	0.306(4)	0	0	0.328	0	0	-0.21	0.21	0.16
O12	3(*a*)	0	0	0.649(6)	0	0	0.672	0	0	-0.22	0.22	0.08

Table S32(*a*)

Atomic positions for II-$In_4(P_2Se_6)_3$ (Voroshilov *et al.*, 1991), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 6.362$, $c = 7.590$ Å; $z^* = z + 0.0012$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	occ.	u_{iso}
	$R3$, $R\bar{3}$												
In1	3(*a*)	0	0	0.1683	0	0	0.1683	0	0	0	0	0.666	0.07
	6(*c*)												
In2	9(*b*)	0	0	0.8317	0	0	0.8317	0	0	0	0	0.666	0.08
P1	9(*b*)	0	0	0.4195	0	0	0.4172	0	0	0.02	0.02	1	0.05
	6(*c*)												
P2	9(*b*)	0	0	0.5852	0	0	0.5828	0	0	0.02	0.02	1	0.09
Se1	9(*b*)	0.3507	0.0367	0.0808	0.3520	0.0361	0.0796	-0.01	0.01	0.01	0.01	1	0.07
	18(*f*)												
Se2	9(*b*)	0.6468	0.9646	0.9216	0.6480	0.9639	0.9204	-0.01	0.01	0.01	0.01	1	0.06

Table S32(*b*)

Revised atomic positions for II-$In_4(P_2Se_6)_3$ (Voroshilov *et al.*, 1991) in ICSD #56891.

$a = 6.362$, $c = 7.590$ Å.

	Wyckoff Position	x	y	z^*	occ.	u_{iso}
	$R\bar{3}$					
In	6(*c*)	0	0	0.1683	0.666	0.06
P	6(*c*)	0	0	0.4172	1	0.06
Se	18(*f*)	0.3519	0.0361	0.0796	1	0.061

Table S33(*a*)
Atomic positions for $NaNiAsO_4$ at room temperature (Range & Meister, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å
$a = 4.955(3)$ (5), $c = 26.47$ (3) Å; $z^* = z - 0.2881$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ni1	3(*a*)	0.0	0.0	-0.1641(3)	0.0	0.0	-0.1644	0.0	0.0	0.01	0.01	0.09
	6(*c*)											
Ni2	3(*a*)	0.0	0.0	0.1647(3)	0.0	0.0	0.1644	0.0	0.0	0.01	0.01	0.07
As1	3(*a*)	0.0	0.0	0.4333(3)	0.0	0.0	0.4340	0.0	0.0	-0.01	-0.01	0.09
	6(*c*)											
As2	3(*a*)	0.0	0.0	0.5653(4)	0.0	0.0	0.5660	0.0	0.0	-0.01	-0.01	0.07
O1	9(*b*)	0.0015(12)	0.3506(12)	0.1202(3)	0.0029	0.3442	0.1211	-0.01	0.03	-0.02	0.04	0.09
	18(*f*)											
O2	9(*b*)†	-0.0042(13)	-0.3377(12)	-0.1220(3)	-0.0029	-0.3442	-0.1211	-0.01	0.03	-0.02	0.04	0.09
O3	3(*a*)	0.0	0.0	0.3716(4)	0.0	0.0	0.3717	0.0	0.0	-0.01	-0.01	0.18
	6(*c*)											
O4	3(*a*)	0.0	0.0	0.6282(4)	0.0	0.0	0.6283	0.0	0.0	-0.01	-0.01	0.11
Na1	3(*a*)	0.0	0.0	-0.2881	0.0	0.0	-0.2887	0.0	0.0	0.02	0.02	0.16
	6(*c*)											
Na2	3(*a*)	0.0	0.0	0.2893(4)	0.0	0.0	0.2887	0.0	0.0	0.02	0.02	0.18

Table S33(*b*)
Revised atomic positions for $NaNiAsO_4$ at room temperature (Jones *et al.,* 1987)
$a = 4.955(3)$ (5), $c = 26.47$ (3) Å

	Wyckoff Position	x	y	z^*	u_{iso}
	$R\bar{3}$				
Ni	6(*c*)	0.0	0.0	0.16443(2)	0.09
As	6(*c*)	0.0	0.0	0.56604(1)	0.08
O1	18(*f*)	0.0024(3)	0.3449(3)	0.1212(1)	0.10
O2	6(*c*)	0.0	0.0	0.6285(4)	0.17
Na	6(*c*)	0.0	0.0	0.2835(8)	0.18

Table S34

Atomic positions for Mg_3In at room temperature (Schubert *et al.*, 1963)
a = 6.323, c = 31.06 Å. $z^* = z_{Schubert} - 0.125$.

	Wyckoff position	x	y	z^*
	$R3, R\bar{3}$ †			
In1	3(*a*)	0	0	-0.125
	6(*c*)			
In2	3(*a*)	0	0	0.125
In3	3(*a*)	0.	0.	0.292
	6(*c*)			
In4	3(*a*)	0.	0.	-0.292
Mg1	9(*b*)	0.5	0.5	-0.125
	18(*f*)			
Mg4	9(*b*)	0.5	0.5	0.125
Mg2	9(*b*)	0.167	0.833	-0.042
	18(*f*)			
Mg3	9(*b*)	0.833	0.167	0.042

† $R3$ proposed by authors, $R\bar{3}$ symmetry demonstrated by the x, y, z: $\bar{x}, \bar{y}, \bar{z}$ relationship between related pairs of atomic coordinates.

Table S35

Atomic positions for $AsTe_2I{\cdot}0.5H_2O$ at room temperature (Stergiou, 1994), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 7.221(1)$, $c = 21.478(7)$ Å; $z^* = z + 0.0016$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
	$R3,\ R\bar{3}$											
As1	3(*a*)	0.0	0.0	0.6995	0.0	0.0	0.6960	0.0	0.0	0.08	0.08	0.23
	6(*c*)											
As2	3(*a*)	0.0	0.0	0.3075(2)	0.0	0.0	0.3040	0.0	0.0	0.08	0.08	0.23
Te1/I1	9(*b*)	0.3228(2)	-0.0016(3)	0.7463(2)	0.3216	-0.0001	0.7499	-0.01	-0.01	-0.08	0.08	0.22
	18(*f*)†											
Te2/I2	9(*b*)	0.6796(2)	-0.0015(2)	0.2466(3)	0.6784	0.0001	0.2501	0.01	-0.01	-0.08	0.08	0.23
O1	3(*a*)	0.0	0.0	0.1896(4)	0.0	0.0	0.1896	0.0	0.0	0.0	0.0	0.15
	6(*c*)‡											
O2	3(*a*)	0.0	0.0	-0.1896(4)	0.0	0.0	-0.1896	0.0	0.0	0.0	0.0	0.15

† 67 % occupancy by Te, 33 % by I.

‡ The original O1 site occupancy, reported by Stergiou (1994) as 50 %, is assumed here to be 25 % at both the O1 and *O2* sites, with u_{iso}(*O2*) identical to u_{iso}(O1). The *O2* atom was not previously reported.[4]

Table S36(*a*)
Atomic positions for Au_5Sn at room temperature (Osada *et al.*, 1974), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å
$a = 5.092$, $c = 14.333$ Å. $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^{*} - z')\,c$.

	Wyckoff Position $R3$, $R32$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u[†]
Au1	3(*a*) 6(*c*)	0	0	0.3307	0.	0.	0.3307	0	0	0	0	n/r
Au2	3(*a*)	0	0	0.6693	0	0	0.6693	0	0	0	0	n/r
Au3[‡]	9(*b*),9(*e*)	0	0.6736	0.5	0	0.6736	0.5	0	0	0	0	n/r
Sn	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	n/r

[†] *u*-values not reported.
[‡] Au3 reported coordinates + ⅔, ⅓, ⅓.

Table S36(*b*)
Atomic positions for Au_5Sn (Osada *et al.*, 1974) in room temperature and hypothetical phase above $T_{PT} \approx 459$ K with Δx, Δy, Δz displacements in Å

	Wyckoff Position $R32$,$R\bar{3}m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u
Au1	6(*c*),6(*c*)	0	0	0.3307	0.	0.	0.3307	0.	0.	0.	0.	n/r
Au3	9(*b*),9(*d*)	0	0.6736	0.5	0	0.5	0.5	0.88	0.	0.	0.88	n/r
Sn	3(*a*),3(*a*)	0	0	0	0.	0	0	0	0.	0.	0.	n/r

Table S37

Atomic positions for $InBrI_2$ at room temperature (Kniep & Blees, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 7.063(2)$, $c = 20.158(5)$ Å. $z^* = z + 0.0444$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3, R\bar{3}$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
In1	3(*a*) 6(*c*)	0	0	0.3325	0.	0.	0.3337	0.	0.	-0.02	-0.02	0.15
In2	3(*a*)	0	0	0.6650	0	0	0.6663	0.	0.	-0.03	-0.03	0.18
I1,Br1	9(*b*),9(*e*)	0.6558(6)	0.0017(6)	0.0833(2)	0.6564	0.0012	0.0821	-0.01	0.01	0.02	0.02	0.16
I2,Br2	9(*b*),9(*a*)	0.3430(6)	0.9993(6)	0.9191(2)	0.3436	0.9988	0.9179	-0.01	0.01	0.02	0.02	0.16

Table S38

Atomic positions for $H_3O^+ \cdot Al_4SiP_3O_{16}^- \cdot nH_2O$ at room temperature (Ito *et al.*, 1985), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a = 13.781(1)$, $c = 14.846(2)$ Å. $z^* = z - 0.0053$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
P1,Si1	9(*b*) 18(*f*)	0.0038(3)	0.2261(3)	0.1029(3)	0.0033.	0.2279	0.1081	0.01	-0.02	-0.08	0.08	0.14
P2,Si2	9(*b*)	0.9973(4)	0.7703(4)	0.8868(3)	0.9967	0.7721	0.8919	0.01	-0.02	-0.08	0.08	0.14
Al1	9(*b*) 18(*f*)	0.2287(4)	0.2266(4)	0.0976(3)	0.2289	0.2261	0.1036	-0.00	0.01	-0.09	0.09	0.13
Al2	3(*a*)	0.7709(4)	0.7745(4)	0.8904(3)	0.7711	0.7739	0.8964	-0.00	0.01	-0.09	0.09	0.14
O1	3(*a*) 18(*f*)	0.0025(10)	0.2638(9)	0.0019(6)	0.0037	0.2582	0.0084	-0.02	0.08	-0.09	0.12	0.16
O5	9(*b*)	0.9950(11)	0.7474(13)	0.9851(8)	0.9963	0.7418	0.9916	-0.02	0.08	-0.10	0.12	0.21
O2	9(*b*) 18(*f*)	0.1139(9)	0.2333(11)	0.1265(8)	0.1162	0.2389	0.1350	-0.03	-0.08	-0.13	0.16	0.19
O6	9(*b*)	0.8814(9)	0.7556(10)	0.8564(8)	0.8838	0.7611	0.8650	-0.03	-0.08	-0.13	0.16	0.18
O3	9(*b*) 18(*f*)	0.2005(10)	0.0908(9)	0.1238(9)	0.1955	0.0898	0.1256	0.07	0.01	-0.03	0.08	0.19
O7	9(*b*)	0.8095(10)	0.9112(9)	0.8726(9)	0.8045	0.9102	0.8744	0.07	0.01	-0.03	0.08	0.19
O4	9(*b*) 18(*f*)	0.3247(9)	0.0147(10)	0.1653(8)	0.3245	0.0144	0.1674	0.01	0.00	-0.03	0.03	0.19
O8	9(*b*)	0.6757(8)	0.9859(9)	0.8305(7)	0.6755	0.9856	0.8326	0.00	0.00	-0.03	0.03	0.17
O9[†]	3(*a*),3(*a*)	0	0	0.98 (40)	0	0	0	0.00	0.00	-0.30	0.30	0.38
O10	9(*b*) 18(*f*)	0.668(10)	0.357(6)	0.045(2)	0.630	0.353	0.025	0.52	0.06	0.30	0.63	0.19
O11	9(*b*)	0.408(10)	0.651(10)	-0.005(8)	0.370	0.647	-0.025	0.52	0.06	0.30	0.63	0.17
O12	9(*b*) 18(*f*)	0.401(9)	0.678(10)	0.347(7)	0.379	0.631	0.331	0.30	0.65	0.23	0.87	0.17
O16	9(*b*)	0.644(11)	0.417(11)	0.684(9)	0.621	0.369	0.669	0.32	0.66	0.23	0.90	0.21
O13	9(*b*) 18(*f*)	0.232(9)	0.428(9)	0.296(7)	0.187	0.494	0.290	0.62	-0.90	0.09	0.80	0.17
O15	9(*b*)	0.559(9)	0.353(9)	0.716(7)	0.494	0.307	0.710	0.90	0.63	0.09	1.33	0.21
O14	9(*b*),9(*e*)	0.635(15)	0.412(14)	-0.001(11)	0.5	0.5	0	1.86	-1.21	-0.01	1.63	0.17

[†] Occupancy factor for the ordered water O9-O16 given as 0.03 for O9, 0.25 for O10 and 0.10 for O11- O16.

Table S39

Atomic positions for $(NH_4)_3Sc(SeO_4)_3$ at room temperature (Valkonen & Niinstö, 1978) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

$a = 15.567(5)$, $c = 9.871(3)$ Å. $z^* = z + 0.0189$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff position $R3$, $R\bar{3}c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Se1	9(*b*)	0.1831(2)	0.5025(2)	0.4067(2)	0.1690	0.5072	0.4155	0.22	-0.07	-0.09	0.21	0.16
	18(*b*)											
Se2	9(*b*)	0.3523(1)	0.5120(1)	0.9244(2)	0.3382	0.5072	0.9155	0.22	0.07	0.09	0.28	0.12
Sc1	3(*a*)	0	0	0.488815)	0	0	0.4875	0	0	0.01	0.01	0.10
	6(*a*)											
Sc2	3(*a*)	0	0	0.9862(17)	0	0	0.9875	0	0	-0.01	0.01	0.09
O1	9(*b*)	0.7268(12)	0.7684 (12)	0.7383(19)	0.7446	0.7474	0.7536	-0.28	0.33	-0.15	0.34	0.22
	18(*b*)											
O7	9(*b*)	0.2736(16)	0.2376 (16)	0.2310(24)	0.2526	0.2554	0.2464	0.32	-0.28	-0.15	0.34	0.25
O2	9(*b*)	0.5479(9)	0.2406 (11)	0.9382(16)	0.4304	0.2321	0.8370	1.83	0.13	1.00	2.15	0.18
	18(*b*)											
O6	9(*b*)	0.2236(17)	0.6871 (21)	0.7642(24)	0.2321	0.5696	0.6630	-0.13	1.83	1.00	2.03	0.22
O3	9(*b*)	0.0902(13)	0.9724 (12)	0.8721(16)	0.0978	0.9193	0.8224	-0.12	0.83	0.49	0.92	0.15
	18(*b*)											
O4	9(*b*)	0.8660(16)	0.1053 (20)	0.7272(25)	0.9193	0.0978	0.6776	-0.83	0.12	0.49	0.92	0.25
O5	9(*b*)	0.7983(16)	0.4376 (16)	0.7085(19)	0.6870	0.4544	0.6534	-1.73	-0.26	0.54	1.95	0.16
	18(*b*)											
O8	9(*b*)	0.4711(11)	0.5757(13)	0.9018(19)	0.4544	0.6870	0.8466	0.26	-1.73	0.54	1.70	0.21
N1	9(*b*)	0.5921(15)	0.5678 (12)	0.7065(21)	0.4576	0.6293	0.7907	2.09	-0.96	-0.83	1.99	0.20
	18(*b*)											
N2	9(*b*)	0.2317(18)	0.3093(19)	0.6251(26)	0.0973	0.3707	0.7093	2.09	-0.96	-0.83	1.99	0.22

Table S40(*a*)

Atomic positions for $Cu_7As_6Se_{13}$ at room temperature (Takeuchi & Horiuchi, 1972) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

$a = 14.025(3)$, $c = 9.61(3)$ Å. $z^* = z - 0.1259$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu1	9(*b*)	0.3697(5)	0.5313(5)	0.6357(1)	0.3828	0.5320	0.5015	-0.18	-0.01	1.29	1.30	0.13
	18(*f*)											
Cu2	9(*b*)	0.5327(5)	0.1362(6)	0.6328(2)	0.5320	0.1492	0.4985	0.01	-0.18	1.29	1.30	0.16
Cu3	3(*a*),3(*b*)	0	0	0.6102(2)	0	0	½	0	0	1.05	1.05	0.21
As1	9(*b*)	0.0755(5)	0.3104(5)	0.6276(1)	0.0767	0.3102	0.5026	-0.02	0.01	1.20	1.20	0.16
	18(*f*)											
As2	9(*b*)	0.3100(6)	0.2341(8)	0.6224(1)	0.3102	0.2335	0.4974	-0.01	0.01	1.20	1.20	0.16
Se1	9(*b*)	0.0711(4)	0.2938(4)	-0.1325(1)	0.0719	0.3045	0.0024	-0.01	-0.15	-1.30	1.31	0.14
	18(*f*)											
Se2	9(*b*)	0.3151(5)	0.2318(5)	-0.1372(13)	0.3045	0.2326	-0.0024	0.15	-0.01	-1.30	1.31	0.15
Se3	9(*b*)	0.3830(5)	0.5488(5)	-0.1112(10)	0.3867	0.5453	0.0056	-0.05	0.05	-1.12	1.12	0.16
	18(*f*)											
Se4	9(*b*)	0.5418(3)	0.1549(3)	-0.1223(12)	0.5453	0.1586	-0.0056	-0.05	-0.05	-1.05	1.05	0.09
Se5	3(*a*),3(*a*)	0	0	-0.1259	0	0	0	0	0	-1.21	1.21	n/r[†]

[†] Not reported.

Table S40(*b*)

Modified Cu atom positions[†] for $Cu_7As_6Se_{13}$ at room temperature with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{33} displacements in Å

$a = 14.025(3)$, $c = 9.61(3)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z[†]	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu1	9(*b*) 18(*f*)	0.3697(5)	0.5313(5)	0.5116(1)	0.3828	0.5320	0.5015	-0.18	-0.01	0.10	0.21	0.13
Cu2	9(*b*) 18(*f*)	0.5327(5)	0.1362(6)	0.5087(2)	0.5320	0.1492	0.4985	0.01	-0.18	0.10	0.21	0.16
Cu3	3(*a*),3(*b*)	0	0	0.4861(2)	0	0	½	0	0	-0.13	0.13	0.21
As1	9(*b*) 18(*f*)	0.0755(5)	0.3104(5)	0.5035(1)	0.0767	0.3102	0.5026	-0.02	0.01	0.01	0.03	0.16
As2	9(*b*) 18(*f*)	0.3100(6)	0.2341(8)	0.4983(1)	0.3102	0.2353	0.4974	-0.01	-0.02	0.01	0.03	0.16
Se1	9(*b*) 18(*f*)	0.0711(4)	0.2938(4)	-0.0661(1)	0.0719	0.3045	0.0024	-0.01	-0.15	-0.09	0.18	0.14
Se2	9(*b*) 18(*f*)	0.3151(5)	0.2318(5)	-0.0113(13)	0.3045	0.2326	-0.0024	0.15	-0.01	-0.09	0.18	0.15
Se3	9(*b*) 18(*f*)	0.3830(5)	0.5488(5)	0.0147(10)	0.3867	0.5453	0.0056	-0.05	0.05	0.09	0.11	0.16
Se4	9(*b*) 18(*f*)	0.5418(3)	0.1549(3)	0.0036(12)	0.5453	0.1586	-0.0056	-0.05	-0.05	0.09	0.12	0.09
Se5	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	n/r[‡]

[†] With general shift in origin from that reported of 0.1259 [= -*z*(Se5)] and replacement of each *z*(Cu1), *z*(Cu2), *z*(Cu3), *z*(As1) and *z*(As2) magnitude by *z* - ¼.

[‡] Not reported.

Table 41(*a*)
Atomic positions (X-ray) for $MgHPO_3 \cdot 6H_2O$ at 108 K (Powell *et al.*, 1994) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å
$a = 8.8281(11)$, $c = 9.104(2)$ Å. $z^* = z + 0.0133$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{eq}
Mg1	3(*a*),3(*a*)	0	0	-0.0062(2)	0	0	0	0	0	-0.06	0.06	0.11
P1	3(*a*),3(*b*)	0	0	0.5133	0	0	½	0	0	0.12	0.12	0.12
H1	3(*a*)	0	0	0.370(6)	0	0	0.357	0	0	0.12	0.13	0.17
	6(*c*)											
H1′ †	*3(a)*	*0*	*0*	*0.657*	*0*	*0*	*0.643*	*0*	*0*	*0.12*	*0.13*	-
O1	9(*b*),9(*d*)	0.1845(2)	0.1320(2)	0.5641(2)	0.1582	0.1582	½	0.23	-0.23	0.58	0.62	0.13
O2	9(*b*)	0.1916(2)	0.1893(2)	0.8553(2)	0.1933	0.0951	0.8687	-0.02	0.83	-0.12	0.85	0.16
	18(*f*)											
O3	9(*b*)	0.0009(3)	0.1951(3)	0.1179(2)	0.0951	0.1933	0.1313	-0.83	0.02	-0.12	0.85	0.14
H2	9(*b*)	0.288(5)	0.232(4)	0.875(4)	0.2865	0.154	0.8605	0.01	0.69	0.13	0.70	0.17
	18(*f*)											
H5	9(*b*)	0.076(5)	0.285(6)	0.154(4)	0.154	0.2865	0.1395	-0.69	-0.01	0.13	0.70	0.17
H3	9(*b*)	0.187(4)	0.166(5)	0.777(4)	0.1855	0.039	0.814	0.01	1.12	-0.34	1.17	0.17
	18(*f*)											
H4	9(*b*)	-0.088(5)	0.184(4)	0.149(3)	0.039	0.1855	0.186	-1.12	-0.01	-0.34	1.17	0.17

† The H1′ site is unoccupied at room temperature. If it is assumed 50 % occupied following a minimum migration of 2.8 Å by half the H1,[4] with all other atoms in their *x*′ *y*′ *z*′ sites, then *R*32 symmetry is achievable.

Table S41(*b*)

Nuclear positions for $MgHPO_3 \cdot 6H_2O$ at 293 K (Powell *et al.*, 1994), see Table S39(*a*).
$a = 8.868(2)$, $c = 9.150(2)$ Å. $z^* = z + 0.0151$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	*x*	*y*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{eq}
Mg1	3(*a*),3(*a*)	0	0	-0.0054(6)	0	0	0	0	0	-0.05	0.05	0.14
P1	3(*a*),3(*b*)	0	0	0.5151	0	0	½	0	0	0.14	0.14	0.15
H1	3(*a*)	0	0	0.3622(9)	0	0	0.3471	0	0	0.14	0.14	0.24
	6(*c*)											
H1′ †	*3(a)*	*0*	*0*	*0.6680*	*0*	*0*	*0.6529*	*0*	*0*	*0.14*	*0.14*	-
O1	9(*b*), 9(*d*)	0.1837(3)	0.1315(3)	0.5658(5)	0.1576	0.1576	½	0.23	-0.23	0.60	0.64	0.16
O2	9(*b*)	0.1929(3)	0.1883(3)	0.8559(5)	0.1945	0.0952	0.8687	-0.01	0.83	-0.12	0.84	0.16
	18(*f*)											
O3	9(*b*)	0.0022(4)	0.1962(3)	0.1195(5)	0.0952	0.1945	0.1313	-0.83	0.02	-0.11	0.84	0.18
H2	9(*b*)	0.3173(6)	0.2507(6)	0.8796(7)	0.3086	0.1754	0.8594	0.08	0.67	0.18	0.74	0.19
	18(*f*)											
H5	9(*b*)	0.1001(6)	0.2998(6)	0.1609(6)	0.1754	0.3086	0.1406	-0.67	-0.08	0.19	0.74	0.20
H3	9(*b*)	0.1888(5)	0.1595(5)	0.7522(6)	0.1888	0.0292	0.7981	0.00	1.16	-0.42	1.23	0.19
	18(*f*)											
H4	9(*b*)	-0.1012(6)	0.1887(5)	0.1560(6)	0.0292	0.1888	0.2019	-1.16	-0.00	-0.42	1.23	0.21

† The H1′ site is unoccupied at room temperature. If assumed 50 % occupied following a minimum migration of 2.8 Å by half the H1 atoms,[4] with all other atoms in their *x*′ *y*′ *z*′ sites, then *R*32 symmetry is achievable.

Table S42

Atomic positions for cronstedtite-6R $Fe_3((FeSi)O_4)(OH)_5$ at room temperature (Steadman & Nuttal, 1963) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.
$a = 5.49(1)$, $c = 42.5(1)$ Å. $z^* = z - 0.132$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u‡
	$R3$, $R\bar{3}$											
Fe1,Si1†	3(*a*)	0	0	0.383	0	0	0.417	0	0	-1.42	1.42	n/d
	6(*c*)											
Fe4,Si4	3(*a*)	0	0	0.550	0	0	0.583	0	0	-1.42	1.42	n/d
Fe2,Si2	3(*a*)	0	0	0.717	0	0	0.750	0	0	-1.40	1.40	n/d
	6(*c*)											
Fe3,Si3	3(*a*)	0	0	0.217	0	0	0.250	0	0	-1.40	1.40	n/d
Fe5	9(*b*)	0.6667	0	-0.049	0.6667	0	-0.083	0	0	1.45	1.45	n/d
	18(*f*)											
Fe6	9(*b*)	0.3333	0	0.117	0.3333	0	0.083	0	0	1.45	1.45	n/d
O1	9(*b*)	0.49	0	-0.132	0.49	0	-0.083	0	0	-2.06	2.06	n/d
	18(*f*)											
O2	9(*b*)	0.51	0	0.035	0.51	0	0.083	0	0	-2.06	2.06	n/d
O3	3(*a*)	0	0	-0.075	0	0	-0.085	0	0	0.28	0.28	n/d
	6(*c*)											
O4	3(*a*)	0	0	0.091	0	0	0.085	0	0	0.28	0.28	n/d
O5	3(*a*)	0	0	0.425	0	0	0.417	0	0	0.34	0.34	n/d
	6(*c*)											
O8	3(*a*)	0	0	0.591	0	0	0.583	0	0	0.34	0.34	n/d
O6	3(*a*)	0	0	0.758	0	0	0.750	0	0	0.34	0.34	n/d
	6(*c*)											
O7	3(*a*)	0	0	0.258	0	0	0.250	0	0	0.34	0.34	n/d
O9	9(*b*)	0.3333	0	-0.024	0.3333	0	-0.083	0	0	2.53	2.53	n/d
	18(*f*)											
O10	9(*b*)	0.6667	0	0.143	0.6667	0	0.083	0	0	2.53	2.53	n/d

† The four Fe, Si sites are reported as occupied equally by both constituents.

‡ Values of u not determined.

Table S43(*a*)

Atomic positions for $Cu_6Hg_3As_4S_{12}$ (aktashite) at room temperature (Kaplunnik *et al.,* 1980), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å

a = 13.730(3), c = 9.329(1) Å. $z^* = z - 0.0405$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu1†	9(*b*), 9(*d*)	0.076(1)	0.2921(5)	-0.0375(2)	0	0.2921	0	1.04	0	-0.35	1.10	0.11
Cu2	9(*b*), 9(*d*)	0.3915(4)	0.552(3)	-0.0225(6)	0.4718	0.4718	0	-1.10	1.10	-0.21	1.12	0.11
Hg	9(*b*), 9(*d*)	0.310(2)	0.2263(4)	-0.0324(5)	0.2682	0.2682	0	0.57	-0.57	-0.30	0.64	0.16
As1	9(*b*), 9(*d*)	0.5610(6)	0.178(2)	-0.0405(4)	0.5610	0	0	0	2.44	-0.38	2.47	0.10
As2	3(*a*),3(*a*)	0	0	-0.0597	0	0	0	0	0	-0.56	0.56	0.05
S1	9(*b*), 9(*d*))	0.3729(8)	0.0899(5)	0.045(2)	0.3729	0	0	0	1.23	0.42	1.30	0.08
S2	9(*b*), 9(*d*)	0.4579(7)	0.428(3)	0.0255(5)	0.4430	0.4430	0	0.21	-0.21	0.24	0.32	0.07
S3	9(*b*), 9(*d*)	0.1186(3)	0.1561(5)	0.0674(4)	0.1374	0.1374	0	-0.26	0.26	0.63	0.68	0.09
S4	9(*b*), 9(*d*)	0.2036(8)	0.475(3)	0.0556(6)	0.3393	0.3393	0	-1.86	1.86	0.52	1.93	0.08

† Occupancies, after Nowacki (1982): all sites 100% filled by the nominal occupant.

Table S43(*b*)

Atomic positions for $Cu_6Zn_3As_4S_{12}$ (nowackiite) at room temperature (Marumo, 1967).

a = 13.440(15), c = 9.17(1) Å. $z^* = z - 0.0360$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu1†	9(*b*), 9(*d*)	0.0741(3)	0.2932(3)	-0.0373(3)	0	0.2932	0.	0.99	0	-0.34	1.05	0.11
Cu2,	9(*b*), 9(*d*)	0.3088(3)	0.2275(3)	-0.0440(3)	0.2682	0.26842	0	0.55	-0.55	-0.40	0.68	0.10
Cu3,	9(*b*), 9(*d*)	0.3895(3)	0.5539(3)	-0.0272(4)	0.4717	0.4717	0	-1.13	1.13	-0.25	1.16	0.14
As1	9(*b*), 9(*d*)	0.5533(2)	0.1680(2)	-0.0289(2)	0.5532	0	0	0	2.25	-0.27	2.27	0.10
As2	3(*a*),3(*a*)	0	0	-0.0552(2)	0	0	0	0	0	-0.51	0.51	0.08
S1	9(*b*), 9(*d*)	0.3695(4)	0.1026(4)	0.0432(5)	0.3695	0	0.	0	1.38	0.40	1.44	0.11
S2	9(*b*), 9(*d*)	0.4380(4)	0.4150(4)	0.0348(5)	0.4265	0.4265	0.	0.15	-0.15	0.32	0.35	0.11
S3	9(*b*), 9(*d*)	0.1251(4)	0.1646(4)	0.0549(6)	0.1449	0.1449	0	-0.27	0.27	0.50	0.57	0.11
S4	9(*b*), 9(*d*)	0.2036(4)	0.4750(4)	0.0601(5)	0.3393	0.3393	0	-1.82	1.82	0.55	1.90	0.10

† Occupancies, after Nowacki (1982): Cu1:Zn1:: 0.9:0.1, Cu2:Zn2:: 0.2:0.8, Cu3:Zn3:: 0.9:0.1.

Table S44

Atomic positions for $Na_{0.55}TiS_2$ at room temperature (Rouxel *et al.,* 1971; Cenzual *et al.,* 1991), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å[†]

$a = 3.433$, $c = 20.94$ Å. $z^* = z - 0.002$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3(m)$,[‡] $R\bar{3}m$	x	y	z*	occ.	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	occ.
Na1	3(*a*)	0	0	0.168	0.55	0.0	0.0	0.170	0.0	0.0	-0.04	0.04	0.275
	6(*c*)[††]												
Na2	*3(a)*	*0*	*0*	*-0.172*	*0.0*	*0.0*	*0.0*	*-0.170*	*0.0*	*0.0*	*-0.04*	*0.04*	*0.275*
Ti	3(*a*), 3(*b*)	0	0	-0.002	1.0	0.0	0.0	0.0	0.0	0.0	-0.04	0.04	1.0
S1	3(*a*)	0	0	0.398	1.0	0.0	0.0	0.395	0.0	0.0	0.06	0.06	1.0
	6(*c*)												
S2	3(*a*)	0	0	0.608	1.0	0.0	0.0	0.605	0.0	0.0	0.06	0.06	1.0

† Retaining the inverse setting used in the $Na_{1-x}VS_2$ structure.

‡ *R*3 used by Rouxel *et al.,* (1971); *R*3*m* proposed by Cenzual *et al.* (1991).

†† Total occupancy of 0.55 at the Na site; a transition to $R\bar{3}m$, assuming the *Na2* site is also occupied,[4] requires an occupancy of 0.275 at both sites.

Table S45

Atomic positions for $H_6As_{6.3}Cu_{0.84}FeMg_{0.1}Mn_{13.9}O_{33}Si_{17}$ (dixenite) at room temperature (Araki & Moore, 1981), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å.
a = 8.233(4), c = 37.499(1) Å. $z^* = z - 0.0095$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*32	*x*	*y*	*z**	*x′*	*y′*	*z′*	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	occ.	u_{iso}
Mn1	3(*a*),3(*a*)	0.	0.	-0.0095	0.	0.	0	0.	0.	-0.36	0.36	1.0	0.10
Mn2,Mgl	3(*a*)	0.	0.	0.3301(1)	0.	0.	0.3349	0.	0.	-0.17	0.17	0.9,0.1	0.13
	6(*c*)												
Cu2	3(*a*)	0.	0.	-0.3398(3)	0.	0.	-0.3349	0.	0.	-0.18	0.18	0.19(1)	0.12
Fe1	3(*a*)	0.	0.	0.2480(1)	0.	0.	0.2605	0.	0.	-0.47	0.47	0.5	0.09
	6(*c*)												
As4	3(*a*)	0.	0.	-0.2729(1)	0.	0.	-0.2605	0.	0.	-0.47	0.47	1.	0.09
Si3,As3	3(*a*)	0.	0.	-0.5626(1)	0.	0.	-0.5685	0.	0.	0.22	0.22	0.24(1), 0.76	0.08
	6(*c*)												0.10
As5	3(*a*)	0.	0.	0.5744(1)	0.	0.	0.5685	0.	0.	0.58	0.58	1.0	0.09
Mn3	9(*b*)	0.3741(1)	-0.0716(1)	-0.2750(1)	0.3016	-0.1935	-0.2634	0.60	0.97	-0.43	1.44	1.0	0.10
	18(*f*)												
Mn6	9(*b*)	0.4226(1)	0.3154(1)	0.2518(1)	0.4951	0.1935	0.2634	-0.60	1.00	-0.43	0.97	1.0	0.11
Mn4	9(*b*)	-0.2509(2)	0.0026(2)	-0.2130(1)	-0.1799	0.1102	-0.1979	-0.58	-0.89	-0.57	1.40	1.0	0.11
	18(*f*)												
Mn5	9(*b*)	0.1089(1)	0.3976(1)	0.1828(1)	0.1799	0.2901	0.1979	-0.58	0.89	-0.57	0.97	1.0	0.11
Sil,Asl	3(*a*)	0.	0.	0.8451(1)	0.	0.	0.8542	0.	0.	-0.34	0.34	0.86(1), 0.14	0.09
	6(*c*)												
Si2,As2		0.	0.	0.1367 (1)	0.	0.	0.1458	0.	0.	-0.34	0.34	0.60(1), 0.40	0.09
Cul[†]	3(*a*)	0.	0.	0.6367(9)	0.	0.	0.6233	0.	0.	0.50	0.50	0.65 (1)	0.10
	6(*c*)												
Cu3	*3(a)*	*0.*	*0.*	*0.39*	*0.*	*0.*	*0.3767*	*0.*	*0.*	*0.50*	*0.50*	*n/d*[‡]	*0.1*
As6	9(*b*),9(*d*)	0.4219(1)	0.0404(1	-0.0269(1)	0.4219	0.	0.	0.	0.33	-1.01	1.06	1.	0.09
01	3(*a*)	0.	0.	0.0924(2)	0.	0.	0.1020	0.	0.	-0.36	0.36	1.	0.12
	6(*c*)												
03	3(*a*)	0.	0.	0.8883(2)	0.	0.	0.8980	0.	0.	-0.36	0.36	1.	0.09
02	3(*a*),3(*b*)	0.	0.	0.4822(3)	0.	0.	0.5	0.	0.	-0.67	0.67	1.	0.12
04	9(*b*)	0.4232(7)	0.1111(7)	-0.3216(2)	0.4189	0.1327	-0.3135	0.04	-0.18	-0.30	0.34	1.	0.12
	18(*f*)												
012	9(*b*)	-0.4527(7)	-0.1542(7)	-0.3053(2)	-0.4484	-0.1327	-0.3135	-0.04	-0.18	0.31	0.41	1.	0.11
05	9(*b*)	-0.1969(7)	-0.1674(7)	-0.2479(1)	-0.1237	-0.1973	-0.2645	-0.60	0.25	0.62	0.81	1.	0.10
	18(*f*)												
010	9(*b*)	0.1468(7)	0.2272(7)	0.2810(1)	0.0736	0.1973	0.2645	0.60	0.25	0.62	0.98	1.	0.11
06	9(*b*)	-0.3830(7)	0.1212(7)	-0.2440(2)	-0.3760	0.1231	-0.2311	-0.06	-0.02	-0.48	0.49	1.	0.11
	18(*f*)												
09	9(*b*)	0.3690(7)	0.5010(7)	0.2182(1)	0.3760	0.4991	0.2311	-0.06	0.02	-0.48	0.48	1.	0.11
07	9(*b*)	-0.5012(7)	-0.1252(6)	-0.1811(1)	-0.5817	-0.1219	-0.2336	0.66	-0.02	1.97	2.07	1.	0.10
	18(*f*)												
011	9(*b*)	0.4608(7)	0.1185(7)	0.2861(1)	0.5413	0.1219	0.2336	-0.66	-0.03	1.97	2.07	1.	0.10
08	9(*b*)	0.5194(7)	0.1277{7)	0.1612(1)	0.4754	0.1756	0.1385	0.36	-0.39	0.85	0.93	1.	0.10
	18(*f*)												
013	9(b)	0.5685(7)	0.7481(7)	0.8843(1)	0.5246	0.7002	0.8615	0.36	0.39	0.85	0.36	1.	0.10

[†] $\Delta z(\text{Cu1}) \gtrsim 5$ Å unless a third *Cu* atom is present at [1 - *z*(Cu1) + δ], as shown in italic, but was not detected; the value of Δ*z*(*Cu3*) in such a case depends on the magnitude of δ.[4] Note the short $d_{\text{Cu1-Cu2}}$ = 0.88 Å.

[‡] Neither occupancy nor u_{iso} for *Cu3* determined; the latter is assumed to be 0.1 Å.

Table S46

Atomic positions for $[C(NH_2)_3]_6As_2Mo_{18}O_{62}\cdot 9H_2O$ at room temperature (Ichida & Sasaki, 1983), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å

$a_H = 20.158(2)$, $c_H = 15.783(1)$ Å. $z^* = z + 0.00069$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.

	Wyckoff Position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
As1	3(*a*)	0	0	0.37103	0	0	0.37202	0	0	-0.02	0.02	0.12
	6(*c*)											
As2	3(*a*)	0	0	0.62699	0	0	0.62798	0	0	-0.02	0.02	0.12
Mo1	9(*b*)	-0.1517	-0.18752	0.36333	-0.14823	-0.19107	0.36289	-0.07	0.07	0.01	0.07	0.14
	18(*f*)											
Mo2	9(*b*)	0.04638	-0.14476	0.63756	0.04249	-0.14823	0.63711	0.08	0.07	0.01	0.13	0.12
Mo3	9(*b*)	0.04753	-0.14787	0.39278	0.04329	-0.15115	0.39281	0.09	0.07	0.01	0.14	0.13
	18(*f*)											
Mo4	9(*b*)	-0.15443	-0.19019	0.60715	-0.15115	-0.19444	0.60718	0.08	0.08	0.01	0.14	0.12
Mo5	9(*b*)	-0.01888	-0.10508	0.18155	0.00766	-0.07738	0.18099	-0.53	-0.56	0.01	0.94	0.14
	18(*f*)											
Mo6	9(*b*)	-0.04968	-0.11158	0.81957	-0.07738	-0.08504	0.81901	0.56	-0.53	0.01	0.55	0.12
O1	9(*b*)	-0.0885	-0.0619	0.4037	-0.0594	-0.0901	0.4033	-0.57	0.57	0.01	0.57	0.13
	18(*f*)											
O2	9(*b*)	0.0588	-0.0302	0.5970	0.0306	-0.0594	0.5967	0.57	0.59	0.01	1.00	0.13
O3	3(*a*)	0	0	0.2629	0	0	0.2625	0	0	0.01	0.01	0.11
	18(*f*)											
O4	3(*a*)	0	0	0.7379	0	0	0.7375	0	0	0.01	0.01	0.13
O5	9(*b*)	-0.2240	-0.1529	0.3664	-0.2029	-0.1499	0.3830	-0.42	-0.06	-0.26	0.52	0.17
	18(*f*)											
O10	9(*b*)	-0.0561	-0.1819	0.6004	-0.0531	-0.2029	0.6170	-0.06	0.42	-0.26	0.47	0.13
O7	9(*b*)	-0.0859	-0.0636	0.1353	-0.0534	-0.0761	0.1340	-0.66	0.25	0.02	0.58	0.15
	18(*f*)											
O8	9(*b*)	-0.0885	-0.0553	0.8673	-0.0761	-0.0228	0.8660	-0.25	-0.66	0.02	0.81	0.14
O6	9(*b*)	-0.2243	-0.1538	0.6365	-0.2047	-0.1495	0.6191	-0.40	-0.09	0.27	0.53	0.15
	18(*f*)											
O9	9(*b*)	-0.0596	-0.1851	0.3984	-0.0553	-0.2047	0.3809	-0.09	0.40	0.28	0.46	0.13
O11	9(*b*)	0.0285	-0.1255	0.2631	0.0324	-0.1208	0.2637	-0.08	-0.09	-0.01	0.15	0.14
	18(*f*)											
O12	9(*b*)	-0.1160	-0.1571	0.7357	-0.1208	-0.1532	0.7363	0.10	-0.09	-0.01	0.10	0.12
O13	9(*b*)	-0.1143	-0.1599	0.2588	-0.1213	-0.1530	0.2581	0.14	-0.14	0.01	0.14	0.12
	18(*f*)											
O14	9(*b*)	0.0248	-0.1283	0.7426	0.0317	-0.1213	0.7419	-0.14	-0.14	0.01	0.24	0.13
O15	9(*b*)	-0.1682	-0.1950	0.4959	-0.1574	-0.2075	0.4965	-0.22	0.25	-0.01	0.24	0.16
	18(*f*)											
O16	9(*b*)	0.0626	-0.1466	0.5030	0.0501	-0.1574	0.5035	0.25	0.22	-0.01	0.41	0.14
O17	9(*b*)	-0.2159	-0.2821	0.3507	-0.2208	-0.2626	0.3520	0.10	-0.39	-0.02	0.35	0.17
	18(*f*)											
O18	9(*b*)	0.0504	-0.2258	0.6468	0.0558	-0.2208	0.6480	-0.10	-0.39	-0.02	0.49	0.17
O19	9(*b*)	0.0516	-0.2257	0.3608	0.0580	-0.2185	0.3625	-0.13	-0.15	-0.03	0.24	0.15
	18(*f*)											
O20	9(*b*)	-0.2112	-0.2829	0.6359	-0.2185	-0.2765	0.6375	0.15	-0.13	-0.03	0.14	0.16

O21	9(*b*)	-0.0380	-0.1744	0.1087	-0.0543	-0.1784	0.1099	0.32	0.08	-0.02	0.37	0.14
O22	(18(*f*)† 9(*b*)	-0.0706	-0.1824	0.8889	-0.0543	-0.1784	0.8901	-0.33	-0.08	-0.02	0.38	0.11
C1‡	9(*b*)	0.3709	0.2596	0.2568	0.3649	0.2544	0.2555	0.12	0.10	0.02	0.19	0.22
C2	18(*f*) 9(*b*)	-0.3588	-0.2492	0.7458	-0.3649	-0.2544	0.7445	0.12	0.10	0.02	0.19	0.15
C3	9(*b*),9(*d*)††	0.0554	0.3847	0.4847	0.	0.5	0.5	1.12	-2.32	-0.24	2.02	0.12
N1	9(*b*)	0.0619	-0.4596	0.5874	0.0333	-0.4687	0.5615	0.58	0.18	0.41	0.80	0 .18
N6‡	18(*f*) 9(*b*)	-0.0047	0.4778	0.4644	-0.0333	0.4687	0.4385	0.58	0.18	0.41	0.80	0.17
N2	9(*b*)	0.0584	-0.3630	0.6581	0.0661	-0.3839	0.6539	-0.16	0.42	0.07	0.37	0.21
N5‡	18(*f*) 9(*b*)	-0.0738	0.4049	0.3503	-0.0661	0.3839	0.3461	-0.16	0.42	0.07	0.37	0.20
N3‡	9(*b*)	0.3274	0.2651	0.1963	0.3287	0.2810	0.2197	-0.03	-0.32	-0.37	0.50	0.25
N4	18(*f*) 9(*b*)	-0.3300	-0.2969	0.7570	-0.3287	-0.2810	0.7803	-0.03	-0.32	-0.37	0.50	0.17
N5′	9(*b*)	0.0893	0.3414	0.4875	0.0822	0.3916	0.4734	0.14	1.01	0.22	1.11	0.20
N6′	18(*f*)† 9(*b*)	0.0751	0.4418	0.5407	0.0822	0.3916	0.5266	-0.14	1.01	0.22	0.97	0.17
Ow1	9(*b*),9(*e*)††	-0.1106	-0.3368	0.5157	0	0.5	0.5	-2.23	3.29	0.25	2.96	0.23
Ow2	9(*b*)	-0.2473	-0.4297	0.4150	-0.2410	-0.3734	0.3816	-0.13	-1.13	0.53	1.31	0.18
Ow3	18(*f*)† 9(*b*)	-0.2347	-0.3178	0.6517	-0.2410	-0.3734	0.6184	0.13	1.12	0.53	1.30	0.23

† Sign of x and y in the coordinates of O22, N6′ and Ow3 is incorrect for $R\bar{3}$; sign reversal leads to the given Δx, Δy and Δz magnitudes.

‡ Rhombohedral centering applied to N5′ and N6′ which were omitted from ICSD #35406, release 2005/1.

†† Note large Δy(C3), Δx(Ow1) and Δy(Ow1); also the inversion-center relationship between C3 and Ow1 sites, with $\Delta\xi = 0.52$ Å if each were identically occupied.

Table S47

Atomic positions for $H_{0.8}Ca_{1.77}Ce_{2.1}Cl_{0.73}Fe_{1.41}K_{0.19}Mn_{3.7}Na_{13.61}Nb_{0.92}O_{76}Si_{25}Y_{0.25}Zr_{3.17}$ at room temperature (Johnsen & Grice, 1999),[†] with hypothetical $x'y'z'$ coordinates and Δx, Δy, Δz and u_{eq} isplacements in Å. Assumed magnitudes are in italic, see §5.8.

a = 14.192(1), c = 29.983(3) Å. $z^* = z + 0.0029$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position $R3$, $R\bar{3}$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Mn1/Y	9(*b*)	0.3937(1)	0.0640(1)	0.8357(1)	0.4025	0.0774	0.8335	-0.12	-0.19	0.07	0.28	0.11
	18(*f*)											
Ca/Ce1/Na1	9(*b*)	0.0908(1)	0.6661(2)	0.1687(1)	0.0774	0.6749	0.1665	0.19	-0.12	-0.02	0.17	0.13
Fe1/Mn2/Zr	9(*b*)	0.1741(2)	0.8108(2)	0.8331(1)	0.1815	0.8209	0.8311	-0.11	-0.14	-0.03	0.22	0.11
	18(*f*)											
Fe2	9(*b*)	0.811(2)	0.169(2)	0.1709 (5)	0.8185	0.1791	0.1689	-0.11	-0.14	-0.03	0.22	0.15
Nb1	3(*a*)	0	0	0.1322(1)	0	0	0.1296	0	0	0.08	0.08	0.11
	6(*c*)											
Nb2[‡]	*3(a)*	*0*	*0*	*0.873*	*0*	*0*	*0.8704*	*0*	*0*	*0.08*	*0.08*	n/r
Si1	3(*a*)	0	0	0.9234(2)	0	0	0.9352	0	0	-0.35	0.35	0.10
	6(*c*)											
Si2[‡]	*3(a)*	*0*	*0*	*0.053*	*0*	*0*	*0.0648*	*0*	*0*	*-0.35*	*0.35*	0.16
Na2	9(*b*)	0.4375(15)	0.5538(11)	0.3225 (3)	0.4416	0.5608	0.3218	-0.06	-0.10	0.02	0.14	0.17
	18(*f*)											
Na3	9(*b*)	0.5544(8)	0.4323(7)	0.6789(2)	0.5584	0.4392	0.6782	-0.06	-0.10	0.02	0.14	0.21
Na4/Ce2	9(*b*)	0.5651(7)	0.4371(7)	0.1242(2)	0.5623	0.4338	0.1206	0.04	0.05	0.11	0.14	0.25
	18(*f*)											
Na5/Ce3/K1	9(*b*)	0.4405(1)	0.5696(1)	0.8829(1)	0.4377	0.5662	0.8794	0.04	0.05	0.10	0.13	0.12
Zr2/Nb2	9(*b*),9(*e*)	0.5119(1)	0.5052(1)	0.0029	0.5	0.5	0	0.17	0.07	0.09	0.21	0.09
Si3	9(*b*)	0.4154(3)	0.6081(3)	0.0880(1)	0.4031	0.5962	0.0866	0.17	0.17	0.04	0.23	0.10
	18(*f*)											
Si4	9(*b*)	0.6092(3)	0.4158(3)	0.9149(1)	0.5969	0.4038	0.9134	0.17	0.17	0.04	0.30	0.11
Si5	9(*b*)	0.1286(4)	0.8745(4)	0.0916(1)	0.1268	0.8766	0.0907	0.03	-0.03	0.03	0.04	0.11
	18(*f*)											
Si6	9(*b*)	0.8751(4)	0.1212(3)	0.9102(1)	0.8732	0.1234	0.9093	0.03	-0.03	0.03	0.04	0.11
Si7	9(*b*)	0.7278(3)	0.6591(3)	0.0732(2)	0.7206	0.6618	0.0699	0.10	-0.04	0.10	0.13	0.10
	18(*f*)											
Si10	9(*b*)	0.0561(3)	0.7134(3)	0.9334(2)	0.0588	0.7206	0.9301	-0.04	-0.10	0.10	0.16	0.10
Si8	9(*b*)	0.7153(3)	0.0583(3)	0.0732(2)	0.7243	0.0628	0.0702	-0.13	-0.06	0.09	0.19	0.10
	18(*f*)											
Si9	9(*b*)	0.2667(3)	-0.0673(3)	0.9328(2)	0.2757	-0.0628	0.9298	-0.13	-0.06	0.09	0.19	0.10
O1	9(*b*)	0.2651(9)	0.7213(9)	0.0902(2)	0.2751	0.7310	0.0911	-0.14	-0.14	-0.03	0.24	0.14
	18(*f*)											
O4	9(*b*)	0.7150(7)	0.2593(7)	0.9081(3)	0.7249	0.2690	0.9089	-0.14	-0.14	-0.03	0.24	0.14
O2	9(*b*)	0.4637(7)	0.5743(6)	0.1279(2)	0.4478	0.5527	0.1248	0.23	0.31	0.09	0.48	0.14
	18(*f*)											
O5	9(*b*)	0.5681(7)	0.4690(8)	0.8784(3)	0.5522	0.4473	0.8753	0.23	0.31	0.09	0.48	0.17

O3	9(*b*) 18(*f*)	0.1127(9)	0.9150(9)	0.3724(2)	0.0948	0.9050	0.3701	0.26	0.14	0.07	0.36	0.14
O6	9(*b*)	0.9232(9)	0.1050(9)	0.6322(2)	0.9052	0.0950	0.6299	0.26	0.14	0.07	0.36	0.15
O7	9(*b*) 18(*f*)	0.0511(7)	0.2895(8)	0.0610(3)	0.0558	0.2920	0.0594	-0.07	-0.04	0.05	0.11	0.13
O12	9(*b*)	-0.0605(6)	0.7055(7)	0.9422(3)	-0.0558	0.7080	0.9406	-0.07	-0.04	0.05	0.11	0.12
O8	9(*b*) 18(*f*)	0.0637(7)	0.7607(7)	0.0631(3)	0.0528	0.7772	0.0599	0.15	-0.23	0.10	0.23	0.14
O11	9(*b*)	0.2592(7)	0.0418(8)	0.9433(4)	0.2756	0.0528	0.9401	-0.23	-0.16	0.10	0.35	0.16
O9	9(*b*) 18(*f*)	0.1595(9)	0.8563(1)	0.1409(2)	0.1535	0.8468	0.1383	0.09	0.13	0.08	0.21	0.14
O13	9(*b*)	0.8526(10)	0.1628(9)	0.8643(2)	0.8465	0.1532	0.8617	0.09	0.14	0.08	0.22	0.14
O10	9(*b*) 18(*f*)	0.0594(9)	0.9341(10)	0.0869(2)	0.0708	0.9491	0.0927	-0.16	-0.21	-0.17	0.36	0.16
O14	9(*b*)	0.9178(6)	0.0359(6)	0.9015(3)	0.9292	0.0509	0.9073	-0.16	-0.21	-0.17	0.36	0.15
O15	9(*b*) 18(*f*)	0.0444(9)	0.7748(9)	0.2948(4)	0.0328	0.7756	0.2922	0.16	-0.01	0.08	0.17	0.15
O21	9(*b*)	-0.0211(8)	0.2236(8)	0.7103(4)	-0.0328	0.2244	0.7077	0.17	-0.01	0.08	0.18	0.13
O16	9(*b*) 18(*f*)	0.0259(8)	0.2662(10)	0.2961(5)	0.0309	0.2611	0.2943	-0.07	0.07	0.05	0.09	0.16
O20	9(*b*)	0.2559(8)	0.2251(8)	0.7075(4)	0.2611	0.2302	0.7057	-0.07	-0.07	0.05	0.13	0.14
O17	9(*b*) 18(*f*)	0.9529(8)	0.2560(8)	0.2136(4)	0.9589	0.2596	0.2108	-0.09	-0.05	0.08	0.15	0.12
O23	9(*b*)	0.0350(9)	0.7369(9)	0.7921(4)	0.0411	0.7404	0.7892	-0.09	-0.05	0.09	0.15	0.14
O18	9(*b*) 18(*f*)	0.7656(9)	0.0268(8)	0.2147(4)	0.7517	0.0358	0.2114	0.20	-0.13	0.10	0.20	0.13
O22	9(*b*)	0.0448(9)	0.2980(9)	0.7920(4)	0.0358	0.2841	0.7887	0.13	0.20	0.10	0.30	0.13
O19	9(*b*) 18(*f*)	0.8193(9)	0.1674(9)	0.2837(2)	0.8229	0.1771	0.2795	-0.05	-0.14	0.13	0.21	0.14
O24	9(*b*)	0.1734(8)	0.8133(8)	0.7247(2)	0.1771	0.8229	0.7205	-0.05	-0.14	0.13	0.21	0.13
O26	3(*a*),3(*a*)	0	0	0.9762(4)	0	0	0	0	0	-0.71	0.71	0.12
Cl1	3(*a*) 6(*c*)	0	0	0.2689(4)	0	0	0.2544	0	0	0.43	0.43	0.17
Cl2	3(*a*)	0	0	0.7601(4)	0	0	0.7456	0	0	0.43	0.43	0.17
Na6	9(*b*) 18(*f*)	0.2738(7)	0.7515(8)	0.6881(2)	*0.2619*	*0.7507*	*0.6891*	*0.17*	*0.01*	*-0.03*	*0.18*	0.23
Na7[††]	*9(b)*	*0.75*	*0.25*	*0.31*	*0.7381*	*0.2493*	*0.3109*	*0.17*	*0.01*	*-0.03*	*0.18*	n/r
O25	9(*b*) 18(*f*)	0.2652(9)	0.7276(10)	0.8337(2)	*0.2651*	*0.7278*	*0.8339*	*0.01*	*-0.01*	*-0.01*	*0.01*	0.16
O27	*9(b)*	*0.735*	*0.272*	*0.166*	*0.7349*	*0.2722*	*0.1661*	*0.01*	*-0.01*	*-0.01*	*0.01*	n/r

[†] Equivalent coordinates at values reported ±(⅔,⅓,⅓) are also used in the table.

[‡] Si2 reported at 0, 0, 0.8757 is only 1.43 Å from Si1, hence is replaced in table as shown.

[††] *Na7, Nb2* and *O27* were not reported (n/r) but assumed in order to complete the relationship approaching $R\bar{3}$. Previously undetected or reported atoms and operations are given in italic.[4]

Table S48

Atomic positions for $AlCa_3Cd_{17}$ at room temperature (Cordier *et al.*, 1999), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å

$a = 22.134(7)$, $c = 27.108(3)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z - z')$

	Wyckoff Position	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3, R\bar{3}$											
Al1	3(*a*)	0	0	0.939(4)	0.040	0.021	0.945	0.89	-0.46	-0.16	0.79	0.10
	18(*f*)											
Al3	9(*b*)	0.920(3)	0.959(3)	0.0480(12)	0.960	0.979	0.054	-0.89	-0.44	-0.16	0.93	0.10
Al2	3(*a*)	0	0	0.436(4)	0.008	-0.039	0.4678	-0.18	0.86	-0.86	0.04	0.10
	18(*f*)											
Al4	9(*b*)	0.983(3)	0.077(3)	0.5003(12)	0.991	0.039	0.5322	-0.18	0.84	-0.86	0.93	0.10
Ca1	9(*b*)	0.370(2)	0.930(3)	0.6242(11)	0.370	0.932	0.6268	0.00	-0.04	-0.07	0.08	0.05
	18(*b*)											
Ca3	9(*b*)	0.630(4)	0.066 (3)	0.3706(16)	0.630	0.068	0.3732	0.00	-0.04	-0.07	0.08	0.05
Ca2	3(*a*)	0.038(3)	0.263(2)	0.4662(11)	0.038	0.261	0.4646	0.00	0.05	0.04	0.06	0.05
	18(*b*)											
Ca4	9(*b*)	0.962(4)	0.742(3)	0.5371(16)	0.962	0.739	0.5354	0.00	0.07	0.05	0.08	0.05
Ca6	9(*b*)	0.837 (3)	0.856(3)	0.6665(13)	0.839	0.861	0.6652	-0.04	-0.11	0.04	0.14	0.05
	18(*b*)											
Ca8	9(*b*)	0.159(3)	0.133(3)	0.3361(12)	0.161	0.139	0.3348	-0.04	-0.13	0.04	0.16	0.05
Ca5	9(*b*)	0.495(3)	0.196(3)	0.4957(13)	0.502	0.197	0.4934	-0.15	-0.02	0.06	0.17	0.05
	18(*b*)											
Ca7	9(*b*)	0.490(3)	0.802(3)	0.5090(13)	0.498	0.803	0.5067	-0.18	-0.02	0.06	0.17	0.05
Cd1	3(*a*)	0	0	0.1580(9)	0	0	0.1578	0	0	0.01	0.01	0.11
	6(*c*)											
Cd3	3(*a*)	0	0	0.8455(10)	0	0	0.8453	0	0	0.01	0.01	0.09
Cd2	3(*a*)	0	0	0.6686(9)	0	0	0.6688	0	0	-0.01	0.01	0.11
	6(*c*)											
Cd4	3(*a*)	0	0	0.3311(10)	0	0	0.3312	0	0	-0.01	0.01	0.09
Cd5	9(*b*)	0.6408(19)	0.6956(19)	0.3525(0)	0.5921	0.6182	0.3486	1.08	1.71	0.11	2.44	0.09
	18(*b*)											
Cd20	9(*b*)	0.4567(13)	0.4591(12)	0.6554(8)	0.4079	0.3818	0.6514	1.08	1.71	0.11	2.44	0.11
Cd6	9(*b*)	0.9782(19)	0.3585(19)	0.5214(13)	0.9808	0.3632	0.5215	-0.06	-0.10	-0.01	0.14	0.09
	18(*b*)											
Cd8	9(*b*)	0.0166(22)	0.6321(25)	0.4784(14)	0.0192	0.6368	0.4785	-0.06	-0.10	-0.01	0.14	0.09
Cd7	9(*b*)	0.3506(23)	0.3019(26)	0.6473(13)	0.3864	0.2717	0.6136	-0.79	0.67	0.91	1.17	0.09
	18(*b*)											
Cd11	9(*b*)	0.5778(17)	0.7586(17)	0.420(1)	0.6136	0.7283	0.3864	-0.79	0.67	0.91	1.17	0.09
Cd9	9(*b*)	0.7470(13)	-0.0952(13)	0.2470(8)	0.7727	-0.1599	0.2614	-0.57	1.43	-0.39	1.31	0.09
	18(*b*)											
Cd39	9(*b*)	0.2245(13)	-0.0418(12)	0.2757(8)	0.1599	-0.0675	0.2614	1.43	0.57	0.39	1.83	0.09
Cd10	9(*b*)	0.7517(14)	0.9026(13)	0.7520(9)	0.7504	0.9055	0.7514	0.03	-0.06	0.02	0.06	0.09
	18(*b*)											
Cd12	9(*b*)	0.2509(17)	0.0916(15)	0.2492(9)	0.2496	0.0945	0.2486	0.03	-0.06	0.02	0.06	0.09

Cd13	9(*b*)	0.7440(17)	-0.0557(20)	0.6439(10)	0.6821	0.0313	0.6040	1.37	-1.92	1.08	2.02	0.11
	18(*b*)											
Cd40	9(*b*)	0.5638(14)	0.6202(14)	0.4359(8)	0.6508	0.6821	0.3960	-1.92	-1.37	1.08	3.06	0.09
Cd14	9(*b*)	0.4031(18)	0.2684(21)	0.473(1)	0.4046	0.2706	0.4726	-0.03	-0.05	0.01	0.07	0.11
	18(*b*)											
Cd22	9(*b*)	0.5939(13)	0.7273(17)	0.5278(9)	0.5954	0.7294	0.5274	-0.03	-0.05	0.01	0.07	0.08
Cd15	9(*b*)	0.0954(14)	0.9811(14)	0.2786(8)	0.0982	0.9810	0.2776	-0.06	0.00	0.03	0.07	0.11
	18(*b*)											
Cd23	9(*b*)	0.8990(11)	0.0192(11)	0.7235(8)	0.9018	0.0190	0.7225	-0.06	0.00	0.03	0.07	0.08
Cd16	9(*b*)	0.1066(14)	0.9789(15)	0.7841(8)	0.1066	0.9790	0.7839	0.01	-0.00	0.01	0.01	0.11
	18(*b*)											
Cd24	9(*b*)	0.8934(12)	0.0209(12)	0.2163(8)	0.8934	0.0210	0.2161	0.01	-0.00	0.01	0.01	0.08
Cd17	9(*b*)	0.0363(17)	0.2904(18)	0.5883(9)	0.0289	0.2875	0.5868	0.16	0.06	0.04	0.20	0.11
	18(*b*)											
Cd25	9(*b*)	0.9786(12)	0.7155(15)	0.4147(8)	0.9711	0.7125	0.4132	0.17	0.07	0.04	0.22	0.08
Cd18	9(*b*)	0.6912(17)	0.6122(18)	0.4104(9)	0.6983	0.6179	0.4146	-0.16	-0.13	-0.11	0.27	0.11
	18(*b*)											
Cd26	9(*b*)	0.2946(12)	0.3764(15)	0.5812(8)	0.3017	0.3821	0.5854	-0.16	-0.13	-0.14	0.29	0.08
Cd19	9(*b*)	0.1270(12)	0.7949(13)	0.4972(8)	0.1268	0.7926	0.4958	0.01	0.05	0.04	0.06	0.11
	18(*b*)											
Cd27	9(*b*)	-0.1266(11)	-0.7903(11)	-0.4944(7)	-0.1268	-0.7926	-0.4958	0.01	0.05	0.04	0.06	0.08
Cd21	9(*b*)	0.9188(13)	0.3827(16)	0.6893(8)	0.9090	0.3366	0.6456	0.22	1.02	1.18	1.64	0.08
	18(*b*)											
Cd37	9(*b*)	0.1009(22)	0.7096(23)	0.3981(10)	0.0910	0.6634	0.3544	0.22	1.02	1.18	1.64	0.09
Cd28	9(*b*)	0.5448(11)	0.5436(10)	0.3484(7)	0.5530	0.5863	0.3930	-0.18	-0.95	-1.21	1.60	0.05
	18(*b*)											
Cd38	9(*b*)	0.4388(21)	0.3710(21)	0.5624(10)	0.4470	0.4137	0.6070	-0.18	-0.95	-1.21	1.60	0.09
Cd29	9(*b*)	0.5428(15)	0.7699(15)	0.6151(8)	0.5493	0.7739	0.6125	-0.14	-0.09	0.07	0.22	0.09
	18(*b*)											
Cd31	9(*b*)	0.4442(14)	0.2222(13)	0.3901(8)	0.4507	0.2261	0.3875	-0.14	-0.09	0.07	0.21	0.09
Cd30	9(*b*)	0.2269(16)	0.1142(14)	0.4442(8)	0.2156	0.1087	0.4462	0.25	0.12	-0.05	0.33	0.11
	18(*b*)											
Cd32	9(*b*)	0.7957(14)	0.8968(13)	0.5519(9)	0.7844	0.8913	0.5538	0.25	0.12	-0.05	0.33	0.09
Cd33	9(*b*)	0.6070(13)	0.8029(10)	0.7983(8)	0.6062	0.8053	0.8016	0.02	-0.05	-0.09	0.10	0.09
	18(*b*)											
Cd35	9(*b*)	0.3946(11)	0.1924(13)	0.1950(8)	0.3938	0.1947	0.1984	0.02	-0.05	-0.09	0.10	0.09
Cd34	9(*b*)	0.2649(10)	0.1364(10)	0.6422(7)	0.2692	0.1336	0.6366	-0.09	0.06	0.15	0.17	0.09
	18(*b*)											
Cd36	9(*b*)	0.7265(13)	0.8692(13)	0.3689(8)	0.7308	0.8664	0.3634	-0.09	0.06	0.15	0.17	0.09
Cd42	9(*b*)	0.7975(11)	0.4476(11)	0.4476(7)	0.7953	0.4439	0.4434	0.05	0.08	0.11	0.16	0.11
	18(*b*)											
Cd48	9(*b*)	0.2068(14)	0.5598(12)	0.5609(9)	0.2047	0.5561	0.5566	0.05	0.08	0.12	0.17	0.11
Cd43	9(*b*)	0.2029(12)	0.0525(11)	0.5545(8)	0.1902	0.0466	0.5492	0.28	0.13	0.15	0.39	0.11
	18(*b*)											
Cd45	9(*b*)	0.8226(13)	0.9593(13)	0.4562(8)	0.8098	0.9534	0.4508	0.28	0.13	0.15	0.39	0.11
Cd44	9(*b*)	0.5183(13)	0.7174(12)	0.7127(8)	0.5218	0.7169	0.7146	-0.08	0.01	0.05	0.09	0.11
	18(*b*)											
Cd46	9(*b*)	0.4748(14)	0.2835(14)	0.2836(8)	0.4782	0.2831	0.2854	-0.08	0.01	0.05	0.09	0.11
Cd41	9(*b*)	0.1215(12)	0.1056(12)	0.6040(7)	0.1321	0.1115	0.6111	-0.23	-0.13	-0.19	0.37	0.11
	18(*b*)											
Cd47	9(*b*)	0.8574(11)	0.8826(11)	0.3817(7)	0.8679	0.8885	0.3889	-0.23	-0.13	-0.19	0.37	0.11