Supplementary Materials for Inorganic Structures in Space Group *P*3*m*1. Coordinate Analysis and Systematic Prediction of New Ferroelectrics

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Abstract

ICSD Release 2007/1 contains 47 families of inorganic crystal structures, some single member only, within the 311 entries listed under polar space group *P*3*m*1. Coordinate analysis reveals, over a range of confidence levels, 12 such families to be candidate ferroelectrics. Selection is based on the detection of an approach to nonpolar supergroup symmetry, within specified limits, by the atomic arrangement as reported in a confirmed polar space group. The primary source of uncertainty in such predictions is the reliability of the underlying structural determination. The candidates include In_2ZnS_4, $TlSn_2F_5$, Cu_7Te_4, $NaMnSe_2$, $Na_2In_2(Mo_3O_8)(MoO_4)_2$, Nb_3Br_7S, Nb_3TeI_7, fencooperite, $Bi(HCOO)_3$, $Li(NpO_2)(CO_3)(H_2O)_2$, $LiPtD_{0.66}$ and $Ag_3(MoO_3F_3)(Ag_3(MoO_4)Cl)$. A total of 20 structures examined are likely to be nonpolar, a further 20 have reduced predictive properties and 3 others are more likely to retain *P*3*m*1 symmetry over a wide thermal range. Substantial uncertainties associated with many of the listed 163 CdI_2, 69 ZnS and 10 SiC polytype structures, together with their low potential for use as possible ferroelectrics, led to their exclusion from fuller analysis.

2. Contents

3. Equivalent positions in polar space group *P*3*m*1 and centrosymmetric supergroups $P\bar{3}m1$ and $P\bar{6}m2$

The coordinates of each atom or group of atoms in a structure that is capable of undergoing a phase transition from ferroelectric to paraelectric without integral change in lattice translations is relatable to a Wyckoff position in the resulting supergroup. All such coordinate relationships are given below explicitly in order to facilitate their use in examining the tables that follow without requiring access to a copy of the *International Tables for Crystallography*.[1]

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[1] The general 6(*e*) Wyckoff position of space group *P*3*m*1 has coordinates: (1) *x, y, z*; (2) $\bar{y}$, *x-y, z*; (3) $\bar{x}+y$, $\bar{x}$, *z*; (4) $\bar{y}$, $\bar{x}$, *z* ; (5) $\bar{x}+y$, *y*, *z*; (6) *x*, *x-y*, *z*, with a single special 3(*d*) position at $x, \bar{x}, z$; $x, 2x, z$; $2\bar{x}, \bar{x}\ z$ and three 1-fold positions at 1(*c*) ⅔, ⅓, *z*; 1(*b*) ⅓, ⅔, *z*; and 1(*a*) 0, 0, *z*. The centrosymmetric supergroups of space group *P*3*m*1 are $P\bar{3}m1$ and $P\bar{6}m2$.

The general 12(*j*) Wyckoff position of space group $P\bar{3}m1$ has coordinates: (1) *x, y, z*; (2) $\bar{y}$, *x-y, z*; (3) $\bar{x}+y$, $\bar{x}$, *z*; (4) $y, x, \bar{z}$; (5) *x-y*, $y, \bar{z}$; (6) $\bar{x}$, $\bar{x}+y$, $\bar{z}$; (7) $\bar{x}, \bar{y}, \bar{z}$; (8) $y, \bar{x}+y, \bar{z}$; (9) *x-y*, $x, \bar{z}$; (10) $\bar{y}, \bar{x}, z$; (11) $\bar{x}+y$, *y*, *z*; and (12) *x*, *x-y*, *z*. There are also three special 6-fold positions, one at 6(*i*): (1) *x*, $\bar{x}$, *z*; (2) *x*, 2*x*, *z*; (3) $2\bar{x}$, $\bar{x}$, *z*; (4) $\bar{x}$, *x*, $\bar{z}$; (5) 2*x*, *x*, $\bar{z}$; (6) $\bar{x}$, $2\bar{x}, \bar{z}$; a second at 6(*h*): (1) *x*, 0, ½; (2) 0, *x*, ½; (3) $\bar{x}$, $\bar{x}$, ½; (4) $\bar{x}$, 0, ½; (5) 0, $\bar{x}$, ½; (6) *x*, *x*, ½; and a third at 6(*g*): (1) *x*, 0, 0; (2) 0, *x*, 0; (3) $\bar{x}$, $\bar{x}$, 0; (4) $\bar{x}$, 0, 0; (5) 0, $\bar{x}$, 0; (6) *x*, *x*, ,0; two special 3-fold positions, one at 3(*f*): ½, 0, ½; 0, ½, ½; ½, ½, ½; the other at 3(*e*): ½, 0, 0; 0, ½, 0; ½, ½, 0; two special 2-fold positions, one at 2(*d*): ⅓, ⅔, *z* and ⅔,⅓, $\bar{z}$ and the other at 2(*c*), 0, 0, *z* and 0,0, $\bar{z}$; and two 1-fold special positions, at 1(*b*) 0, 0, ½ and at 1(*a*) 0, 0, 0.

The general 12(*o*) Wyckoff position of space group $P\bar{6}m2$ has coordinates: (1) *x, y, z*; (2) $\bar{y}$, *x-y, z*; (3) $\bar{x}+y$, $\bar{x}$, *z*; (4) *x, y*, $\bar{z}$; (5) $\bar{y}$, *x-y*, $\bar{z}$; (6) $\bar{x}+y$, $\bar{x}\ \bar{z}$; (7) $\bar{y}, \bar{x}, z$; (8) $\bar{x}+y$, *y*, *z*; (9) *x*, *x-y*, *z* (10) $\bar{y}, \bar{x}, \bar{z}$; (11) $\bar{x}+y$, *y*, $\bar{z}$; and (12) *x*, *x-y*, $\bar{z}$. There are also three special 6-fold positions, one at 6(*n*): (1) *x*, $\bar{x}$, *z*; (2) *x*, 2*x*, *z*; (3) $2\bar{x}$, $\bar{x}$, *z*; (4) *x*, $\bar{x}$, $\bar{z}$; (5) *x*, 2*x*, $\bar{z}$; (6) $2\bar{x}$, $\bar{x}, \bar{z}$; the second at 6(*m*): (1) *x, y*, ½; (2) $\bar{y}$, *x-y*, ½; (3) $\bar{x}+y$, $\bar{x}$, ½; (4) $\bar{y}, \bar{x}$, ½ ; (5) $\bar{x}+y$, *y*, ½; (6) *x*, *x-y*, ½; and the third at 6(*l*): (1) *x, y*, 0; (2) $\bar{y}$, *x-y*, 0; (3) $\bar{x}+y$, $\bar{x}$, 0; (4) $\bar{y}, \bar{x}$, 0 ; (5) $\bar{x}+y$, *y*, 0; (6) *x*, *x-y*, 0, two special 3-fold positions at 3(*k*): (1) *x*, $\bar{x}$, ½; (2) *x*, 2*x*, ½; (3) $2\bar{x}, \bar{x}$, ½; and 3(*j*): (1) *x*, $\bar{x}$, 0; (2) *x*, 2*x*, 0; (3) $2\bar{x}, \bar{x}$, 0, also three special 2-fold positions, one at 2(*i*): ⅔,⅓, *z* and ⅔,⅓, $\bar{z}$; the second at 2(*h*): ⅓, ⅔, *z* and ⅓, ⅔, $\bar{z}$; the third at 2(*g*): 0, 0, *z* and 0,0, $\bar{z}$; and six 1-fold positions, at 1(*f*): ⅔,⅓, ½; 1(*e*): ⅔,⅓, 0; 1(*d*): ⅓, ⅔, ½; 1(*c*): ⅓, ⅔, 0; 1(*b*): 0, 0, ½ and 1(*a*): 0,0, 0.

4. Tabular data for structures reported in space group *P*3*m*1 predicted as new ferroelectrics

Table S1(*a*)

Modified atomic positions for $In_{1.53}Zn_{4.1}S_8$ (Gnehm & Niggli, 1972) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [16312]
a = 3.857(2), c = 24.961(15) Å. $z^* = z + 0.0049$. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition														
	*P*3*m* 1	$P\bar{3}m1$	*x*	*y*	*z*	*z**	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	*occ.*	u_{iso}
S1	1(*a*)	1(*a*)	0.0	0.0	0	0.005	0.0	0.0	0.0	0.0	0.0	0.12	0.12	1	0.12
S2	1(*c*)		0.6666	0.3333	0.125(1)	0.130	0.6666	0.3333	0.123	0.0	0.0	0.17	0.17	1	0.09
		2(*d*)													
S8	1(*b*)		0.3333	0.6666	0.879(1)	0.884	0.3333	0.6666	0.877	0.0	0.0	0.17	0.17	1	0.12
S3	1(*a*)		0.0	0.0	0.251(1)	0.256	0.0	0.0	0.258	0.0	0.0	-0.04	0.04	1	0.04
		2(*c*)													
S7	1(*a*)		0.0	0.0	0.736(1)	0.741	0.0	0.0	0.742	0.0	0.0	-0.03	0.03	1	0.04
S4	1(*c*)		0.6667	0.3333	0.378(1)	0.383	0.6666	0.3333	0.379	0.0	0.0	0.10	0.10	1	0.04
		2(*d*)†													
S6	1(*c*)		0.6666	0.3333	0.620(1)	0.625	0.6667	0.3333	0.621	0.0	0.0	0.10	0.10	1	0.04
S5	1(*a*)	1(*b*)	0.0	0.0	0.5042(6)	0.5091	0.0	0.0	0.50	0.0	0.0	0.23	0.23	1	0.00
Zn1	1(*c*)		0.6667	0.3333	0.035(2)	0.040	0.6667	0.3333	0.030	0.0	0.0	0.25	0.25	0.5	0.22
		2(*d*)													
Zn7	1(*b*)		0.3333	0.6666	0.975(1)	0.980	0.3333	0.6666	0.970	0.0	0.0	0.25	0.25	0.6	0.15
Zn2,In1	1(*a*)		0.0	0.0	0.156(1)	0.161	0.0	0.0	0.161	0.0	0.0	0.00	0.00	0.6,0.4	0.04
		2(*c*)													
Zn6,In4	1(*a*)		0.0	0.0	0.834(1)	0.839	0.0	0.0	0.839	0.0	0.0	0.00	0.00	0.6,0.4	0.0
Zn3	1(*c*)		0.6667	0.3333	0.2864(5)	0.2913	0.6667	0.3333	0.3001	0.0	0.0	-0.22	0.22	1	0.10
		2(*d*)													
In3	1(*b*)		0.3333	0.6666	0.6862(5)	0.6911	0.3333	0.6666	0.6999	0.0	0.0	-0.22	0.22	0.09	0.14
Zn4,In2	1(*a*)		0.0	0.0	0.410(2)	0.415	0.0	0.0	0.438	0.0	0.0	-0.57	0.57	0.4.0.6	0.09
		2(*d*)†													
Zn5	1(*c*)		0.6667	0.3333	0.534(1)	0.539	0.6667	0.3333	0.562	0.0	0.0	-0.57	0.57	0.5	0.20

† Assuming appropriate corrections for the S4,S6 and Zn4/In2,Zn5 pair Wyckoff positions,

[2] Where each atom at x, y, z in space group $P3m1$ is considered as displaced from the location x_i', y_i', z_i' in a hypothetical supergroup, and $\Delta\xi_i = [(x_i - x_i')^2 + (y_i - y_i')^2 + (x_i - x_i')(y_i - y_i') + (z_i - z_i')^2]^{1/2}$ in a trigonal setting. Unlike Tables 1-10, from which the authors' original z-values were removed in order to conserve space, the supplementary tables generally retain the authors' z-values. Excluded values are readily determined from the relation $z^* = z$ + a constant given in each table.

Table S1(*b*)

Modified atomic positions for $In_{2.02}Zn_{6.58}S_{10}$ (Gnehm & Niggli, 1972) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å [16313]
$a = 3.838$, $c = 31.3$ Å; $z^* = z + 0.0036$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wyckoff positions													
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
S1	1(*c*)		0.6667	0.3333	0.0412(37)	0.6667	0.3333	0.0464	0	0	-0.16	0.16	1.	0.08
		2(*d*)												
S10	1(*b*)		0.3333	0.6667	0.9484(40)	0.3333	0.6667	0.9536	0	0	-0.16	0.16	1.	0.08
S2	1(*b*)		0.3333	0.6667	0.1540(37)	0.3333	0.6667	0.1498	0	0	0.13	0.13	1.	0.08
		2(*d*)												
S9	1(*c*)		0.6667	0.3333	0.8544(63)	0.6667	0.3333	0.8502	0	0	0.13	0.13	1.	0.08
S3	1(*c*)		0.6667	0.3333	0.2513(88)	0.6667	0.3333	0.2544	0	0	-0.10	0.10	1.	0.08
		2(*d*)												
S8	1(*b*)		0.3333	0.6667	0.7425(37)	0.3333	0.6667	0.7456	0	0	-0.10	0.10	1.	0.08
S4	1(*b*)		0.3333	0.6667	0.3488(40)	0.3333	0.6667	0.3490	0	0	-0.01	0.01	1.	0.08
		2(*d*)												
S7	1(*c*)		0.6667	0.3333	0.6508(39)	0.6667	0.3333	0.6510	0	0	-0.01	0.01	1.	0.08
S5	1(*c*)		0.6667	0.3333	0.4507(69)	0.6667	0.3333	0.4545	0	0	-0.12	0.12	1.	0.08
		2(*d*)												
S6	1(*b*)		0.3333	0.6667	0.5417(36)	0.3333	0.6667	0.5455	0	0	-0.12	0.12	1.	0.08
Zn1,In1	1(*b*)		0.3333	0.6667	0.0796(24)	0.3333	0.6667	0.0532	0	0	0.83	0.83	0.52,0.48	0.08
		2(*d*)†												
Zn8	1(*c*)		0.6667	0.3333	0.9732(28)	0.6667	0.3333	0.9468	0	0	0.83	0.83	1.	0.08
Zn2	1(*c*)		0.6667	0.3333	0.1791(29)	0.6667	0.3333	0.1799	0	0	-0.03	0.03	0.94	0.08
		2(*d*)†												
Zn7,In5	1(*b*)		0.3333	0.6667	0.8193(24)	0.3333	0.6667	0.8201	0	0	-0.03	0.03	0.58,0.42	0.08
Zn3	1(*b*)		0.3333	0.6667	0.2798(27)	0.3333	0.6667	0.2789	0	0	0.03	0.03	1.	0.08
		2(*d*)†												
Zn6,In4	1(*c*)		0.6667	0.3333	0.7220(27)	0.6667	0.3333	0.7211	0	0	0.03	0.03	0.69,0.31	0.08
In2	1(*a*)		0	0	0.5036(2)	0	0	0.5	0	0	0.11	0.11	0.66	0.08
Zn4	1(*c*)		0.6667	0.3333	0.3795(28)	0.6667	0.3333	0.3812	0	0	-0.05	0.05	1.	0.08
		2(*d*)†												
Zn5,In3	1(*b*)		0.3333	0.6667	0.6171(26)	0.3333	0.6667	0.6188	0	0	-0.05	0.05	0.85,0.15	0.08

† The Zn1/In1,Zn8 pair, exhibiting the largest mismatch, also the Zn2, Zn7/In5; Zn3, Zn6/In4 and Zn4, Zn5/In3 pairs requires equivalent site occupancy for the phase transition. Further investigation of the $In_{2.02}Zn_{6.58}S_{10}$ structure is hence necessary.

Table S2(*a*)

Modified atomic positions for $LiMnSe_2$ (Kim & Hughbanks, 1999), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [50817]
a = 4.1905(3), c = 6.6199(5) Å. $z^* = z - 0.0339$. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Mn†	1(*a*)	1(*b*)	0.	0.	0.6129(9)	0.5790	0.	0.0	0.5	0.	0.	0.52	0.52	0.15
Se1	1(*a*)	1(*a*)	0.	0.	0.	-0.0339	0.	0.	0.0	0.	0.	-0.22	0.22	0.13
Se2	1(*b*)	1(*d*)	0.3333	0.6667	0.4889(6)	0.4550	0.3333	0.6667	0.5	0.	0.	-0.30	0.30	0.13

† Li undetermined.

Table S2(*b*)

Modified atomic positions for $LiMnTe_2$ (Kim *et al.*, 1998), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [unlisted in ICSD]
a = 4.517(3), c = 7.187(3) Å. $z^* = z - 0.0324$. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	$z^\dagger$	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Mn††	1(*a*)	1(*b*)	0.	0.	0.6123(9)	0.5799	0.	0.0	0.5	0.	0.	0.57	0.57	0.15
Te1	1(*a*)	1(*a*)	0.	0.	0.	-0.0324	0.	0.	0.0	0.	0.	-0.23	0.23	0.14
Te2	1(*b*)	1(*d*)	0.3333	0.6667	0.4850(4)	0.4526	0.3333	0.6667	0.5	0.	0.	-0.34	0.34	0.15

† Authors' z-coordinates replaced by 1- z for consistency with Table 2.25(*a*).
†† Li undetermined.

Table S2(*c*)

Modified atomic positions for $NaMnTe_2$ (Kim *et al.*, 1998), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [unlisted in ICSD].
a = 4.5630(6), c = 7.542(2) Å. Origin displaced ⅔,⅓, z^* with $z^* = z - 0.105$, where $z = 1 - (z_{orig}) + 0.166$ and the coordinates z_{orig} were reported; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Mn	1(*a*)	1(*b*)	0	0	0.633(3)	0.528	0.	0.0	0.5	0.	0.	0.21	0.21	0.13
Te1	1(*a*)	1(*a*)	0	0	0 (2)	-0.105	0.	0.	0.0	0.	0.	-0.79	0.69	0.13
Te2	1(*b*)	1(*d*)	0.3333	0.6667	0.514(2)	0.409	0.3333	0.6667	0.5	0.	0.	-0.69	0.60	0.13
Na	1(*c*)	1(*e*)	0.6667	0.3333	0.271	0.166	0.6667	0.3333	0.0	0.	0.	1.25	1.25	0.15

Table S2(*d*)

Modified atomic positions for $CuScS_2$ (Dismukes *et al.*, 1971) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [15298]
a = 3.7333(5), c = 6.098(1) Å. $z^* = z + 0.0290$; with an origin translation of + ⅔, ⅓, 0.1103
$\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu	1(*a*)	1(*b*)	0	0	0.5229(3)	0.5519	0.	0.0	0.5	0.	0.	0.32	0.32	0.06
S1	1(*a*)	1(*a*)	0	0	-0.1137(4)	-0.0847	0.	0.	0.0	0.	0.	-0.52	0.52	0.06
S2	1(*b*)	1(*d*)	0.3333	0.6667	0.3645(4)	0.3935	0.3333	0.6667	0.5	0.	0.	-0.65	0.65	0.06
Sc	1(*c*)	1(*e*)	0.6667	0.3333	0.1103	0.1393	0.6667	0.3333	0.0	0.	0.	0.85	0.85	0.06

Table S2(*e*)

Modified atomic positions for II-$AgAlS_2$ (Range *et al.*, 1974) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [25356]†
a = 3.50, c = 6.84 Å. $z^* = z + 0.011$; with an origin translation of + ⅔, ⅓, 1-z. $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ag‡	1(*a*)	1(*b*)	0	0	0.455	0.466	0	0	0.5	0	0	-0.23	0.23	n/a†
S1	1(*a*)	1(*a*)	0	0	0.814	0.825	0	0	1.0	0	0	-1.20	1.20	n/a
S2	1(*b*)	1(*c*)	0.3333	0.6667	0.186	0.197	0.3333	0.6667	0	0	0	1.34	1.34	n/a
Al	1(*c*)	1(*e*)	0.6667	0.3333	0	0.011	0.6667	0.3333	0	0	0	0.08	0.08	n/a

† Phase III-Ag_3SI has Ag(u_{iso}) = 0.07 Å, see (Abrahams, 2006) Table 5.
‡ The coordinates show both Al and Ag as octahedrally coordinated, with 3 $d_{Ag\text{-}S}$ = 2.73, 3 at 3.18 Å.

Table S3

Modified atomic positions for $Na_2In_2(Mo_3O_8)(MoO_4)_2$ (Collins *et al.*, 1989), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [65821]

	Wykoff Position												
	$P3m1$	$P\bar{3}m1$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
In1	1(*a*)		0	0	0.2973	0	0	0.2928	0	0	0.05	0.05	0.07
		2(*c*)											
In2	1(*a*)		0	0	-0.28836(9)	0	0	-0.2928	0	0	0.05	0.05	0.08
Mo1	1 c		0.6667	0.3333	0.1310(1)	0.6667	0.3333	0.1266	0	0	0.04	0.04	0.08
		2(*d*)											
Mo2	1(*b*)		0.3333	0.6667	-0.1221(1)	0.3333	0.6667	-0.1266	0	0	0.05	0.05	0.08
Mo3	3(*d*)	3(*f*)	0.51592(7)	-0.51592(7)	-0.50258(8)	0.5	-0.5	-0.5			-0.03	0.03	0.11
Na1	1(*a*)		0	0	0.004(1)	0	0	0	0	0	0.05	0.05	0.15
Na2	1(*b*)		0.3333	0.6667	0.232(1)	0.3333	0.6667	0.228	0	0	0.05	0.05	0.14
		2(*d*)†											
Na3	1(*c*)		0.6667	0.3333	0.776(2)	0.6667	0.3333	0.772	0	0	0.05	0.05	0.15
O1	3(*d*)		0.342(1)	0.171(1)	0.6041(5)	0.3463	0.1732	0.6011	-0.02	-0.01	0.03	0.04	0.08
	a = 5.7856(8), c = 11.266(1) Å. $z^* = z + 0.0053$. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]												
		6(*i*)											
O5	3(*d*)		0.1753(7)	0.3506(8)	0.4020(5)	0.1732	0.3463	0.3989	0.01	0.02	0.03	0.04	0.09
O2	3(*d*)		0.1619(8)	0.3238(8)	0.8342(6)	0.1619	0.3239	0.8315	0.0	0.0	0.03	0.03	0.13
		6(*i*)											
O6	3(*d*)		0.324(2)	0.162(2)	0.1713(6)	0.3239	0.1619	0.1686	0.0	0.0	0.03	0.03	0.12
O3	1(*c*)		0.6667	0.3333	0.977(1)	0.6667	0.3333	0.975	0	0	0.02	0.02	0.12
		2(*d*)											
O7	1(*b*)		0.3333	0.6667	0.027(1)	0.3333	0.6667	0.025	0	0	0.02	0.02	0.13
O4	1(*b*)		0.3333	0.6667	0.5842(9)	0.3333	0.6667	0.6070	0	0	-0.26	0.26	0.06
		2(*d*)											
O8	1(*c*)		0.6667	0.3333	0.370(1)	0.6667	0.3333	0.3930	0	0	-0.26	0.26	0.09

† Occupancies for Na2, Na3 given as 0.62(2) and 0.42(2), respectively.

Table S4(*a*)

Modified atomic positions for $Ta_{1.34}Nb_{1.66}TeI_7$ (Smith & Miller, 2000), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [92517].
$a = 7.620(1)$, $c = 6.913(1)$ Å, $z^* = z + 0.0088$;† $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition														
	$P3m1$	$P\bar{3}m1$	x	y	z†	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
Ta,Nb	3(*d*)	3(*f*)	0.53406(7)	0.46594(7)	0.5	0.5088	0.5	0.5	0.5	0.26	-0.26	0.06	0.27	0.09	0.45,0.55
Te	1(*c*)		0.6667	0.3333	0.2019(4)	0.2107	0.6667	0.3333	0.2449	0	0	-0.24	0.24	0.10	1.
		2(*d*)													
I1	1(*b*)		0.3333	0.6667	0.7121(3)	0.7209	0.3333	0.6667	0.7551	0	0	-0.24	0.24	0.10	1.
I2	3(*d*)		0.3278(3)	0.6722(3)	0.7641(3)	0.7729	0.3292	0.6708	0.7432	-0.01	0.01	0.21	0.21	0.11	1.
		6(*i*)													
I3	3(*d*)		0.6695(2)	0.3305(2)	0.2777(3)	0.2865	0.6708	0.3292	0.2568	-0.01	0.01	0.21	0.21	0.11	1.

† Reported z-values replaced by z + ¼.

Table S4(*b*)

Modified atomic positions for $Ta_{0.86}Nb_{2.14}TeI_7$ (Smith & Miller, 2000), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [92518].
$a = 7.622(1)$, $c = 6.902(1)$ Å $z^* = z - 0.0085$;† $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition														
	$P3m1$	$P\bar{3}m1$	x	y	z†	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
Ta1,Nb	3(*d*)	3(*f*)	0.46638(6)	0.53362(6)	0.5	0.4915	0.5	0.5	0.5	-0.26	0.26	0.06	0.27	0.10	0.286,0.714
Te1	1(*b*)		0.3333	0.6667	0.7977(3)	0.7892	0.3333	0.6667	0.7555	0.0	0.0	0.23	0.23	0.10	1
		2(*d*)													
I1	1(*c*)		0.6667	0.3333	0.2868(3)	0.2783	0.6667	0.3333	0.2445	0.0	0.0	0.23	0.23	0.11	1.
I2	3(*d*)		0.16386(9)	0.83614(9)	0.2355(2)	0.2270	0.16457	0.83543	0.2566	-0.01	0.01	-0.20	0.20	0.11	1.
		6(*i*)													
I3	3(*d*)		0.83472(7)	0.16528(7)	0.7223(3)	0.7138	0.83543	0.16457	0.7434	-0.01	0.01	-0.20	0.20	0.12	1.

† Reported z-values replaced by z + ¼.

Table S5

Modified atomic positions for $C_2H_{3.38}Ba_6Cl_{1.62}Fe_3O_{31.38}Si_8$ (Grice, 2001), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [92798].
$a = 10.7409(5)$, $c = 7.0955(4)$ Å; $z^* = z + 0.0108$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition															
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
Ba1	3(*d*)	3(*j*)	0.82749(5)	0.17251(5)	0.	0.0108	0.82749	0.17251	0	0.	0.	0.08	0.08	1.	0.15
Ba2	3(*d*)	3(*k*)	0.51607(5)	0.48393(5)	0.5006(2)	0.5114	0.51607	0.48393	0.5	0.	0.	0.08	0.08	1.	0.12
Fe	3(*d*)	3(*j*)	0.4373(1)	0.5627(1)	0.0010(3)	0.0118	0.4373	0.5627	0	0.	0.	0.08	0.08	1.	0.10
Si1	1(*a*)		0.	0.	0.7218(8)	0.7326	0.	0.	0.7215	0.	0.	0.08	0.08	1.	0.08
		2(*g*)													
Si3	1(*a*)		0.	0.	0.2789(8)	0.2897	0.	0.	0.2785	0.	0.	0.08	0.08	1.	0.09
Si2	3(*d*)		0.1678(2)	0.3356(5)	0.7284(5)	0.7392	0.1674	0.3350	0.7290	0.	0.01	0.07	0.07	1.	0.10
		6(*n*)													
Si4	3(*d*)		0.1669(2)	0.8331(2)	0.2704(6)	0.2812	0.1674	0.8325	0.2710	-0.01	0.01	0.07	0.07	1.	0.11
C1	1(*c*)		0.6667	0.3333	0.181(5)	0.192	0.6667	0.3333	0.232	0.	0.	-0.28	0.28	1.	0.22
		2(*i*)													
C2	1(*c*)		0.6667	0.3333	0.716(5)	0.727	0.6667	0.3333	0.767	0.	0.	-0.28	0.28	1.	0.20
O1	1(*a*)	1(*b*)	0.	0.	0.498(3)	0.508	0.	0.	0.5	0.	0.	0.06	0.06	1.	0.22
O2	3(*d*)		0.0822(5)	0.1644(10)	0.797(1)	0.808	0.0821	0.1641	0.799	0.	0.	0.06	0.06	1.	0.14
		6(*n*)													
O5	3(*d*)		0.0819(5)	0.1638(9)	0.199(1)	0.210	0.0820	0.1641	0.201	0.	0.	0.06	0.06	1.	0.11
O3	6(*e*)		0.3316(8)	-0.0777(8)	0.804(1)	0.815	0.3305	-0.0773	0.804	0.01	0.	0.08	0.08	1.	0.15
		12(*o*)													
O6	6(*e*)		0.5933(7)	-0.0769(8)	0.196(1)	0.206	0.5922	-0.0773	0.196	0.01	0.	0.07	0.07	1.	0.14
O8	3(*d*)		0.5972(5)	0.4028(5)	0.176(3)	0.187	0.6669	0.3331	0.232	-0.75	0.75	-0.39	0.85	1.	0.25
		6(*n*)													
O9	3(*d*)		0.7366(4)	0.2634(4)	0.711(2)	0.722	0.6669	0.3338	0.768	0.75	-0.75	-0.40	0.85	1.	0.19
O4	3(*d*)	3(*k*)	0.167(1)	0.334(2)	0.505(2)	0.516	0.167	0.334	0.5	0.	0.	0.11	0.11	1.	0.24
O7	1(*b*)	1(*c*)	0.3333	0.6667	-0.006(3)	0.005	0.3333	0.6667	0	0.	0.	0.04	0.04	1.	0.13
O10	1(*b*)	1(*d*)	0.3333	0.6667	0.504(4)	0.515	0.3333	0.6667	0.5	0.	0.	0.11	0.11	1.000.	0.22
Cl,O	3(*d*)	3(*k*)	0.8361(4)	0.1639(4)	0.501(1)	0.512	0.8361	0.1639	0.5	0.	0.	0.09	0.09	**0.54,0.46**	0.18

Table S6

Modified atomic positions for $Bi(HCOO)_3$ (Stålhandske, 1969), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [151262].
a = 10.5663(1), c = 4.1193(2) Å. $z^* = z - 0.0543$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	Position											
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Bi1	1(*a*)	1(*a*)	0.	0.	0.	-0.0543	0.	0.	0	0.	0.	-0.22	0.22	0.24
Bi2	1(*c*)		0.6667	0.3333	0.3544(6)	0.3001	0.6667	0.3333	0.4036	0.	0.	-0.43	0.43	0.24
		2(*d*)												
Bi3	1(*b*)		0.3333	0.6667	0.5472(9)	0.4929	0.3333	0.6667	0.5964	0.	0.	-0.43	0.43	0.26
C1	3(*d*)		0.155(2)	0.845(2)	0.374(10)	0.320	0.167	0.833	0.310	-0.13	0.13	0.04	0.14	0.15
		6(*i*)												
C2	3(*d*)		0.822(2)	0.178(2)	0.754(8)	0.700	0.833	0.167	0.690	-0.12	0.12	0.04	0.13	0.13
C3	3(*d*)	3(*e*)	0.486(2)	0.514(2)	0.103(9)	0.049	0.5	0.5	0	-0.15	0.15	0.20	0.25	0.13
O1	3(*d*)		0.198(2)	0.802(2)	0.620(8)	0.566	0.184	0.858	0.588	0.03	-0.59	-0.09	0.58	0.17
		6(*i*)												
O4	3(*d*)		0.085(1)	0.915(1)	0.444(7)	0.390	0.092	0.858	0.412	-0.03	0.60	-0.09	0.59	0.14
O2	3(*d*)		0.864(2)	0.136(2)	0.974(7)	0.920	0.870	0.193	0.087	-0.07	-0.60	-0.47	0.79	0.16
		6(*i*)												
O5	3(*d*)		1.751(1)	0.249(1)	0.800(7)	1.746	1.740	0.193	-0.087	0.08	0.59	-0.47	0.79	0.14
O3	3(*d*)		0.527(2)	0.473(2)	0.340(7)	0.286	0.555	0.445	0.113	-0.30	0.30	0.71	0.77	0.16
		6(*i*)												
O6	3(*d*)		0.417(1)	0.583(1)	0.115(9)	0.061	0.445	0.555	-0.113	-0.30	0.30	0.72	0.78	0.12

Table S7

Modified atomic positions in $LiPtD_{0.66}$ (Nacken & Bronger, 1978) with hypothetical *x′, y′, z′* coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å.^{2} [200045].
a = 2.728, c = 4.226 Å, $z^* = z - 0.194$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z - z')c$.^{2}
Origin translation: + ⅓, ⅔, 0.

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$occ.$	u_{iso}
Pt	1(*a*)		0.3333	0.6667	0	-0.194	0.3333	0.6667	-0.25	0	0	0.24	0.24	1.	0.10
		2(*d*)													
Li	1(*b*)		0.6667	0.3333	0.5	0.306	0.6667	0.3333	-0.25	0	0	0.24	0.24	1.	0.05
D1	1(*a*)		0.3333	0.6667	-0.63	-0.824	0.3333	0.6667	-0.768	0	0	-0.24	0.24	0.33	0.21
		2(*d*)													
D2	1(*b*)		0.6667	0.3333	0.905	0.711	0.6667	0.3333	0.768	0	0	-0.24	0.24	0.33	0.23

5. Entries for structures reported in space group *P*3*m*1 that are as likely nonpolar

3.1 32*H* CdI_2 [6279]

Cu*K*α, 15° oscillation, zero-layer *a*-axis, Weissenberg photographs; 32 *I*(10*l*), visually estimated, 6-levels; extensive disorder scattering; manual match of structure to *I*(10*l*), a = 4.24, c = 107.97 Å (Prasad & Srivastava, 1970). Near-regular edge-sharing CdI_6 octahedra, $d_{Cd\text{-}I} \approx 2.975$ Å. All 32 independent I and 16 independent Cd atoms conform exactly to $P\bar{6}m2$ symmetry, the Cd atoms displaced c/64 as in Table S8 to form very nearly regular octahedra with $d_{Cd\text{-}I} = 2.97$ Å. If not displaced, the Cd coordination would be an unlikely planar trigonal. Both the symmetry conformation and displacement relationships together with the extensive but unexamined diffuse scattering indicate the need for further structural investigation and analysis.

3.2 $NaLiZnO_2$ [40458]

Prepared at 975 K, Mo*K*α diffractometry, 220 symmetry-independent *I*(*hkl*), absorption corrections, u_{ij}, R = 0.0406, wR = 0.0387 (Hoppe, 1983). All reported atomic coordinates, as modified in Table S9 by an origin translation of ⅓,⅔,-0.1381, see §1.6, approach supergroup $P\bar{3}m1$ symmetry within $\Delta\xi_{max} \lesssim 0.01$ Å. The structure hence does not differ significantly from centrosymmetry.

3.3 $16H_{12}$ CdI_2 [49572]

Cu*K*α 15° oscillation photographs, 18 6-level visual *I*(10*l*) estimates, manual structure

sequencing, c = 54.68 Å, homometric structure.[3] The $16H_{12}$, $22H_{10}$ and $22H_{11}$ structure determinations by Sarna *et al.* (1984) are among the later CdI_2 polytype reports. The asymmetric unit, composition Cd_8I_{16}, has near-regular edge-sharing CdI_6 octahedra and $d_{Cd\text{-}I}$ = 2.986 Å. Table S10 shows space group $P\bar{6}m2$ is exactly satisfied if I3 is in Wyckoff position 1(*a*) and both I11 and Cd2 are in 1(*c*), the reverse of that reported, leaving all $d_{Cd\text{-}I}$ unchanged. As in §3.1, structural reinvestigation is advisable.

3.4 $22H_{11}$ CdI_2 [49574]

Cu$K\alpha$ 15° oscillation photographs, 26 7-level visual $I(10l)$ estimates, manual fitting as for the $16H_{12}$ polytype, Sarna *et al.*, (1984). Atomic coordinates in Table S11 correspond to near-regular edge-sharing CdI_6 octahedra with $d_{Cd\text{-}I}$ = 2.985Å. All I atoms exactly satisfy supergroup $P\bar{6}m2$ symmetry, except for the I3, I21 and I5, I19 pairs, also all Cd atoms except for the Cd2, Cd19 and Cd3, Cd9 pairs under a *c*/44 displacement by all Cd atoms, *cf.* §3.1. Replacing the Wyckoff 1-fold position of one Cd in each of these pairs by the italic values in Table S11 eliminates the symmetry exceptions without changing the bonding about I or Cd. As in §3.1, substantial but uninvestigated diffuse scattering together with a close approach to supergroup symmetry indicates the need for structural reinvestigation.

3.5 12*L* ZnS polytype [107137]

Cu $K\alpha$, oscillation photographs, 7 visually estimated $I(10l)$, 4,4,2,2 sequence polytype with c = 37.488 Å (Kiflawi & Mardix, 1970). The coordinates as reported, see Table S12, give $d_{Zn11\text{-}S10}$ = 0.78 Å with remaining $d_{Zn\text{-}S}$ = 2.34 Å. All z(Zn)-, also all z(S)-coordinates on

[3] A non-congruent structure with identical X-ray intensity distribution.

replacement by z(S)-1/48, fully satisfy the symmetry of supergroup $P\bar{3}m1$ if the 7 pairs of 1-fold Wyckoff locations that are presently in violation are assumed incorrectly selected and brought into compliance. The assignment of Wyckoff locations consistent with both structure and supergroup remains to be fully investigated by current structural determination methods in order to elucidate the potential for nonpolarity, *cf.* §§3.1-3.3.

3.6 $Pb_2Nb_2O_7$ ($Pb_{17}Nb_{17}O_{59.5}$ per cell) [17039].

Mo$K\alpha$, graphite monochromator; absorption, anomalous dispersion and secondary extinction corrections; wR = 0.068 for 3,225 symmetry-equivalent, 836 independent $F_{obs}^2 > 2\sigma(F_{obs}^2)$ with R = 0.052 (Bernotat-Wulf & Hoffmann, 1981). The metal atoms form octahedra in this structure with double most polytype *a*- and *c*-axes at 7.472 and 28.351 Å. All 18 metal and 20 of the 28 independent O atoms approach the symmetry of supergroup $P\bar{3}m1$ within $\Delta\xi \lesssim u_{iso}$, except for the O9/O18, O14,/O15 pairs with $u_{iso} \approx 0.9$, 0.4 Å in addition to the O25/O28 pair for which $\Delta\xi \approx 0.6$ Å with $u_{iso} \approx 0.3$ Å, also atoms O24 and O27, see Table S13. The latter two may be related to unreported atoms *O24′* and *O27′*; further, the atoms designated as 'Nb6' and 'Pb6' may have been misidentified as Pb6 and Nb6. The authors note the appearance in $Pb_2Nb_2O_7$ of oxygen vacancies in addition to partially occupied Pb sites, as also found in other lead niobate polytypes. The results in Table S13 are suggestive of possible ferroelectricity but with an uncertainty level high enough that further experimental investigation is desirable.

3.7 6*H*-PbI_2 [24264]

Cu$K\alpha$, Weissenberg camera, 19 visually estimated I(10l), many noted as exhibiting

uncorrected absorption effects (Mitchell, 1959). Reassigning Pb2 in Table S14 from Wyckoff position 1(*a*) to 1(*b*) and *I*3 from 1(*b*) to 1(*a*) results in an exact match with supergroup $P\bar{3}m1$ symmetry, leaving all Pb atoms with unchanged octahedral bonding and $d_{\text{Pb-O}} \approx 3.21$ Å. The calculated powder pattern intensity distribution for the reported structure and that from the reassigned structure differ significantly but not enough to be rejected, hence the validity of the change awaits experimental confirmation. Four additional PbI_2 polytype structures were also reported by Mitchell (1959), but no others in space group $P31m$.

3.8 $(Cd_{0.5}Pb_{0.5})_3OSiO_4$ [36480]

Powder pattern at ~1015 K, triclinic to trigonal symmetry at $T_{\text{trans}} \approx 975$ K. Experimental $I(hkl)$ measurement method not stated, 19 $I(hkl) > 0$ with $R(I) = 0.18$ for a random, 0.24 for an ordered Cd and Pb distribution, u undetermined (Eysel & Breuer, 1983). Strongly distorted Cd/PbO_6 octahedra, SiO_4 forms more regular tetrahedra. All atoms except O4 and O6 approach supergroup $P\bar{6}m2$ symmetry with $\Delta\xi_j \lesssim 0.45$ Å; if both O4 and O6 were in Wyckoff locations 1(*b*) or 1(*c*), then $\Delta\xi$(O4,O6) = 0.25 Å, see Table S15. If u(O) is comparable with $\Delta\xi$(O) at 1015 K, the space group reported would be in question. Further investigation, including the polarity or otherwise of the *c* axis, is necessary.

3.9 $Cu_{0.8}Ag_{0.96}Te$ [41905]

Electron diffractometry, 277 photometric $|\Phi(h0l)^2|$, Patterson function, 36 atoms, 54 variable coordinates, $R = 0.184$ (Avilov *et al.*, 1974). Over half the independent atoms in the $Cu_{0.8}Ag_{0.96}Te$ unit cell, with $a = 8.54$ Å, occupy 3(*d*) rather than more common 1-fold

Wyckoff positions in this space group. Noting that 32 of the independent atoms presented in Table S16 have $\Delta\xi \lesssim 1.3$ Å with respect to supergroup $P\bar{3}m1$ symmetry, also the highly variable number of nearest neighbors (4-11) for each element, redetermination of the structure may well reveal a similar approach to higher symmetry by the remaining atoms for which $\Delta\xi$ appears unacceptably large. In that case, the conditions for ferroelectricity would be satisfied; property predictions for $Cu_{0.8}Ag_{0.96}Te$, however, must await definitive remeasurement.

3.10 $Cu_{1.81}Te$ [42156]

Electron diffraction determination, 121 photometric$|\Phi(h0l)^2|$, Patterson function, $R = 0.217$ (Baranova *et al.*, 1973). All 25 Cu and Ag of the total 35 independent atoms reported in $Cu_{0.8}Ag_{0.96}Te$, see §3.8, are related to comparable locations in this independent study of $Cu_{1.81}Te$ with its 36 independent atoms, with both sets occupying closely comparable unit cells. The comparison shows, *inter alia*, that Cu4 in $Cu_{1.81}Te$ corresponds to the location of Te1 in $Cu_{0.8}Ag_{0.96}Te$, leading to the possibility that an unrecognized atom may exist in $Cu_{1.81}Te$ at ~⅔,⅓, -0.07. The lack of atoms in $Cu_{1.81}Te$ near-symmetrically related to Cu4 or Cu15 may also be due to oversight, see *Cu4A* and *Cu 15A* in Table S17. Together with reversed *x* and *y* coordinates for one atom in the Te3/Te10, the Te4/Te9, and the Cu8/Cu22 pairs (matching Ag9 in Table S16), all atoms satisfy supergroup $P\bar{3}m1$ symmetry with $\Delta\xi \lesssim$ 1.4 Å; only 4 atoms appear to have $\Delta\xi \gtrsim 0.24$ Å. $Cu_{1.81}Te$ may hence also be a candidate for ferroelectricity but, as in §3.8, potential structural problems lower the confidence of any property prediction which must await definitive remeasurement.

3.11 $Cu_{0.45}In_{3.17}Se_5$ [54750]

Cu $K\alpha$, powder diffractometry, profile refinement, texture parameter, $R(I) = 0.0794$, $R(P) = 0.1309$, Gulay *et al*. (2004). The sites proposed for Cu, In1 and Se1 form similar distorted tetrahedra; all atoms approach the symmetry of supergroup $P\bar{6}m2$ within $\Delta\xi \lesssim 0.20$ Å except for Se2 in a highly distorted octahedron and $\Delta\xi$(Se2) ≈ 1.67 Å. The remaining atoms occupy strongly distorted tetrahedra or octahedra. The unique location assigned Se2 is problematic with an arbitrary change in z(Se2) from the 0.1806 reported to 0.075, see Table S18, resulting in all $\Delta\xi \lesssim 0.19$ Å. The magnitudes of u range from 0.09 to 0.17 Å, hence are comparable with such a $\Delta\xi_{max}$. The possibility of space group misassignment suggests the advisability of further measurement.

3.12 $BaTiO_{2.67}$ [54785]

High-resolution transmission electron microscopy; selected area electron diffraction. The atomic coordinates and site occupancies for reduced trigonal barium titanate proposed by Woodward *et al*. (2004) in Table S19 are unrefined and differ from the symmetry of supergroup $P\bar{3}m1$ only in the assumed occupancy of the O3 site. A full structure determination is necessary to understand the properties of this reduced material.

3.13 Pseudo-hexagonal BN [56315/6]

Synchrotron X-radiation, $\lambda = 0.5$ Å, twin-domain crystal, 618 F_{obs}, $R = 0.053$, $wR = 0.104$ in $F\bar{4}3m$; with 9 F_{obs} omitted, $R = 0.020$, $wR = 0.045$ in a cell with 'hexagonal' c-axis = $\sqrt{3}.a_{cubic}$, Kupčik *et al.*, (1994). Although the 'hexagonal' symmetry was noted to be 'pseudo', a model in space group $P3m1$ was examined but R could not be reduced below

~0.2, with coordinates as in Table S20. A twinned model in space group $F\bar{4}3m$ was successfully refined to give the *R* and *wR* values above. Further investigation is necessary to determine the symmetry in an untwinned sample and to confirm the likelihood of nonpolarity.

3.14 $Si_6H_3(OH)_3$ [56605]

Mo*K*α, single crystal diffractometry, *x* and *y* coordinates of two Si and one O atom refined with 18 *F*(*hk*0), *R* = 0.083; *z*(Si), *z*(O) and *x*,*y*,*z*(H) values assumed (Dettlaff-Weglikowska *et al.*, 1997). Excluding H, the symmetry of supergroup $P\bar{6}m2$ is satisfied with $\Delta\xi_{max} \lesssim 0.7$ Å, see Table S21(*a*). The author's assumed location for H1, in a 3(*d*) position with 1/3 occupancy, has $\Delta\xi$(H1) ≈ 0.5 Å and also satisfies $P\bar{6}m2$ symmetry as in Table S21(*b*). However, the resulting $d_{Si1\text{-}H1}$ = 2.22 Å lies significantly outside the 1.49-1.51 Å range reported by Howard *et al.* (1992) for $d_{Si\text{-}H}$ although the assumed but disordered H2 position with $d_{Si2\text{-}H2}$ = 1.54 Å agrees satisfactorily, as does $\Delta\xi$(H2) ≈ 1.2 Å suggesting a possible approach to supergroup symmetry. If the refined atomic coordinates can be confirmed, with improved H1 location, then the criteria for ferroelectricity would be met. The confidence level of such a prediction, however, remains low until the detailed structure is redetermined or dielectric measurements demonstrate the exhibition or otherwise of ferroelectricity.

3.15 $Al_{48}Ca_4Cr_7$ [57537]

Prepared at 1573 K from the elements. MoKα, diffractometry, 2266 independent $F^2_{obs} \geqslant \sigma(F^2_{obs})$, u_{iso} for each atom, unvaried site occupancies, *R* = 0.086 (Czech *et al.* 1984). Spectroscopic analysis agrees closely with the formula $Al_{48}Ca_4Cr_7$. The structure in Table

S22, however, gives rise to the formula $Al_{51}Ca_4Cr_7$ for all sites fully occupied. An occupancy of 78.6% at each Al site corresponds to the analytic formula, but the content might be variable not only at Al but also at the Cr and Ca sites. 18 of the 21 independent atoms listed in Table S22 approach the symmetry of supergroup $P\bar{6}m2$ with $\Delta\xi_{max} \lesssim 1.4$ Å; Al4, Al6 and Cr1, Cr2 appear to violate such symmetry. The possibility that one or more undetermined Cr atoms are present, near-symmetrically related to Cr1 and Cr2, also that x and y(Al13) might be reversed together with other site occupancy changes, remains to be investigated. The approach to higher symmetry and the widely variable nearest-neighbor distribution about each Al and Ca, with none closer than 3 Å about Al12, are consistent with the possibility that other sites may be overlooked. It is hence possible that the criteria for ferroelectricity with rather high T_C are satisfied in $Al_{48}Ca_4Cr_7$ but further experimental measurement is necessary before property predictions for this alloy can be made with confidence.

3.16 $Ca_{0.95}Li_{1.05}Sn$ [58911, 107334]

Mo$K\alpha$, precession and Weissenberg films, 224 independent F_{obs}, Ca and Sn from Patterson projections, least-squares refinement, single unreported u_{iso}; Li location assumed, $R = 0.102$, (Müller & Voltz, 1974). All atomic positions have $\Delta\xi \lesssim 0.07$ Å, with respect to the symmetry of supergroup $P\bar{6}m2$, except for $\Delta\xi$(Li6) ≈ 0.45 Å, see Table S23; however, $d_{Li6\text{-}Ca1}$ is only 1.3 Å. If z(Li6) = 0.5, then $d_{Li6\text{-}Ca1} = 1.8$ Å with all $\Delta\xi \lesssim 0.01$ Å. Uncertainties in the Li atom locations hence preclude property predictions. A second ICSD entry, 107334, includes possible locations for three additional but low occupancy Li atom sites but is in error and is now cancelled (Allmann, 2007).

3.17 $YBa_2Cu_3O_{6.5}$ [68420]

Superconducting $YBa_2Cu_3O_7$ prepared at 1225 K; electron microscopy; two new trigonal phases; formula $YBa_2Cu_3O_{6.5}$ determined thermogravimetrically; phase I, space group $P\bar{3}1m$; phase II, $P31m$ (Li *et al*., 1989), each with 'the same unit cell size and atomic positions'. HREM images suggest an exchange between Y and Cu3 sites in phase II. Equal occupancy as in Table S24 gives space group $P\bar{3}1m$, with all $\Delta\xi = 0$, unequal occupancy leads to $P3m1$ as suggested by the authors. Further investigation is necessary to clarify the structural and physical properties.

3.18 BiTeI [79364]

Cu$K\alpha$, powder diffractometry, texture parameter, full-profile refinement, u_{ij} for each atom, $R_I = 0.054$, $R_{Pr} = 0.129$, $R_{WP} = 0.144$ (Shevelkov *et al.*, 1995). Assuming the Te and I atoms share the 2(*d*) site, as in Table S25, then all $\Delta\xi$ would be less than u_{iso} and the symmetry more likely $P\bar{3}1m$. Although the authors identified BiTeBr as in space group $P\bar{3}1m$, they excluded isostructural BiTeI from centrosymmetry since refinement attempts led to R_I = 0.141 whereas for BiTeBr, R_I = 0.0.042. In view of the study by Keramidas *et al.* (1993) reporting the space group of BiTeI as $P3$ with $R = 0.075$, see §2.3 in Abrahams (2000) for a comparison of the two studies, further structural investigation is advisable.

3.19 $YH_{0.667}$ [152861]

$YH_{2/3}$, structure based on FLAPW computations,[4] $P3m1$ symmetry assumed in modelling relationship between H atom ordering and Fermi surface; (Garces *et al.*, 2005). Residual *c*-

[4] Full-potential linearized assessed plane wave (Blaha *et al*., 2001).

glide plane from parental hcp-Y($P6_3/mmc$) structure notably present, see Table S26. Chosen model approaches $P\bar{6}m2$ symmetry, with all $\Delta\xi \lesssim 0.5$ Å if H3 and H4 each occupy Wyckoff position 2(*g*) or 2(*h*). Had the structure been experimentally determined, with the H3 and H4 sites appropriately occupied, the criteria for ferroelectricity would have been satisfied; confirmation requires either such a determination or definitive dielectric measurements.

3.20 $Eu_8I_9(CN)(NCN)_3$ [172030]

Prepared at 695 K, Mo$K\alpha$ diffractometer, 1587 independent $F_{obs} \geqslant 2\sigma(F_{obs})$, absorption corrections, U^{ij}, R = 0.0344, wR^2 = 0.0647 (Liao & Dronskowski, 2006). Atomic displacement magnitudes required to satisfy supergroup $P\bar{6}m2$ symmetry range from $\Delta\xi$ = 0.07 to 1.58 Å, see Table S27. The largest value, however, violates the criteria for ferroelectricity at ambient temperatures; in addition, both C2 and N3 are required to occupy Wyckoff location 1(*c*) in the higher space group, resulting in a linear cyanamid ion. The survey of nine such ions by Kožíšek *et al.* (2002) shows all are nonlinear, with 168.3 $\leq \angle$ N-C-N $\leq$ 173.8(1)°, hence one or more lighter atoms may be misassigned due to the 4 independent Eu and 3 I atoms present; additional structural study is indicated.

6. Tabular data for structures reported in space group *P*3*m*1 that are as likely nonpolar

Table S8

Modified atomic positions for 32*H*-CdI_2 (Prasad & Srivastava, 1970), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [6279].
$a = 4.24$, $c = 107.97$ Å; $z^* = z + 0.00$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	position										
	*P*3*m*1	$P\bar{6}m2$	*x*	*y*	*z*	*x′*	*y′*	*z′*	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
I1	1(*a*)	1(*a*)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	n/a
I2	1(*a*)		*0.3333*	*0.6666*	0.125	*0.3333*	*0.6666*	0.125	0.0	-0.0	0.01	0.01	n/a
		2(*h*)*											
I17	1(*b*)		0.3333	0.6666	0.875	0.3333	0.6666	0.875	0.0	-0.0	0.01	0.01	n/a
I3	1(*a*)		*0.3333*	*0.6666*	0.25	*0.3333*	*0.6666*	0.25	0.0	-0.0	0.01	0.01	n/a
		2(*h*)*											
I15	1(*b*)		0.3333	0.6666	0.75	0.3333	0.6666	0.75	0.0	-0.0	0.01	0.01	n/a
I4	1(*a*)		0.0	0.0	0.375	0.0	0.0	0.375	0.0	0.0	0.0	0.0	n/a
		2(*g*)											
I6	1(*a*)		0.0	0.0	0.625	0.0	0.0	0.625	0.0	0.0	0.0	0.0	n/a
I5	1(*a*)	1(*b*)	0.0	0.0	0.5	0.0	0.0	0.5	0.0	0.0	0.0	0.0	n/a
I7	1(*a*)		*0.6666*	*0.3333*	0.7188	*0.6666*	*0.3333*	0.7188	0.0	-0.0	0.01	0.01	n/a
		2(*g*)*											
I23	1(*c*)		0.6666	0.3333	0.2813	0.6666	0.3333	0.2813	0.0	-0.0	0.01	0.01	n/a
I8	1(*a*)		*0.6666*	*0.3333*	0.9063	*0.6666*	*0.3333*	0.9063	0.0	-0.0	0.01	0.01	n/a
		2(*i*)*											
I20	1(*c*)		0.6666	0.3333	0.0938	0.6666	0.3333	0.0938	0.0	-0.0	0.01	0.01	n/a
I9	1(*b*)		0.3333	0.6666	0.0625	0.3333	0.6666	0.0625	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I18	1(*b*)		0.3333	0.6666	0.9375	0.3333	0.6666	0.9375	0.0	0.0	0.0	0.0	n/a
I10	1(*b*)		0.3333	0.6666	0.1875	0.3333	0.6666	0.1875	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I16	1(*b*)		0.3333	0.6666	0.8125	0.3333	0.6666	0.8125	0.0	0.0	0.0	0.0	n/a
I11	1(*b*)		0.3333	0.6666	0.3125	0.3333	0.6666	0.3125	0.0	-0.0	0.0	0.0	n/a
		2(*h*)											
I14	1(*b*)		0.3333	0.6666	0.6875	0.3333	0.6666	0.6875	0.0	-0.0	0.0	0.0	n/a
I12	1(*b*)		0.3333	0.6666	0.4375	0.3333	0.6666	0.4375	0.0	-0.0	0.0	0.0	n/a
		2(*h*)											
I13	1(*b*)		0.3333	0.6666	0.5625	0.3333	0.6666	0.5625	0.0	-0.0	0.0	0.0	n/a
I19	1(*c*)		0.6666	0.3333	0.0313	0.6666	0.3333	0.0312	0.0	-0.0	-0.01	0.01	n/a
		2(*i*)											
I32	1(*c*)		0.6667	0.3333	0.9686	0.6667	0.3333	0.9686	0.0	-0.0	-0.01	0.01	n/a
I21	1(*c*)		0.6666	0.3333	0.1563	0.6666	0.3333	0.1563	0.0	-0.0	0.01	0.01	n/a
		2(*i*)											
I31	1(*c*)		0.6667	0.3333	0.8438	0.6667	0.3333	0.8438	0.0	-0.0	0.01	0.01	n/a
I22	1(*c*)		0.6666	0.3333	0.2188	0.6666	0.3333	0.2188	0.0	-0.0	0.01	0.01	n/a
		2(*i*)											
I30	1(*c*)		0.6667	0.3333	0.7813	0.6667	0.3333	0.7812	0.0	-0.0	0.01	0.01	n/a

I24	1(*c*)		0.6666	0.3333	0.3438	0.6666	0.3333	0.3438	0.0	-0.0	0.01	0.01	n/a
		2(*i*)											
I29	1(*c*)		0.6667	0.3333	0.6563	0.6667	0.3333	0.6562	0.0	-0.0	0.01	0.01	n/a
I25	1(*c*)		0.6666	0.3333	0.4063	0.6666	0.3333	0.4063	0.0	-0.0	0.01	0.01	n/a
		2(*i*)											
I28	1(*c*)		0.6667	0.3333	0.5938	0.6667	0.3333	0.5938	0.0	-0.0	0.01	0.01	n/a
I26	1(*c*)		0.6666	0.3333	0.4688	0.6666	0.3333	0.4688	0.0	-0.0	0.01	0.01	n/a
		2(*i*)											
I27	1(*c*)		0.6667	0.3333	0.5313	0.6667	0.3333	0.5312	0.0	-0.0	0.01	0.01	n/a
Cd1[†]	1(*a*)		0.0	0.0	0.0781	0.0	0.0	0.0625	0.0	0.0	1.68	1.68	n/a
		2(*g*)											I
Cd8	1(*a*)		0.0	0.0	0.9531	0.0	0.0	0.9375	0.0	0.0	1.68	1.68	n/a
Cd2	1(*a*)		0.0	0.0	0.2031	0.0	0.0	0.1875	0.0	0.0	1.68	1.68	n/a
		2(*g*)											
Cd7	1(*a*)		0.0	0.0	0.8281	0.0	0.0	0.8125	0.0	0.0	1.68	1.68	n/a
Cd3	1(*a*)		*0.6667*	*0.3333*	0.3281	*0.6667*	*0.3333*	0.3125	0.0	0.0	1.68	1.68	n/a
		2(*i*)*											
Cd15	1(*c*)		0.6667	0.3333	0.7031	0.6667	0.3333	0.6875	0.0	0.0	1.68	1.68	n/a
Cd6	1(*a*)		*0.3333*	*0.6666*	0.7656	*0.3333*	*0.6666*	0.7500	0.0	0.0	1.68	1.68	n/a
		2(*h*)*											
Cd11	1(*b*)		0.3333	0.6666	0.2656	0.3333	0.6666	0.2500	0.0	0.0	1.68	1.68	n/a
Cd4	1(*a*)		0.0	0.0	0.4531	0.0	0.0	0.4375	0.0	0.0	1.68	1.68	n/a
		2(*g*)											
Cd5	1(*a*)		0.0	0.0	0.5781	0.0	0.0	0.5625	0.0	0.0	1.68	1.68	n/a
Cd9	1(*b*)	1(*c*)	0.3333	0.6666	0.0156	0.3333	0.6666	0.0	0.0	0.0	1.68	1.68	n/a
Cd13	1(*b*)	1(*d*)	0.3333	0.6666	0.5156	0.3333	0.6666	0.5	0.0	0.0	1.68	1.68	n/a
Cd10			*0.6667*	*0.3333*	0.1406	*0.6667*	*0.3333*	0.1250	0.0	0.0	1.68	1.68	n/a
		2(*i*)*											
Cd16	1(*c*)		0.6667	0.3333	0.8906	0.6667	0.3333	0.8750	0.0	0.0	1.68	1.68	n/a
Cd12	1(*b*)		0.3333	0.6666	0.3906	0.3333	0.6666	0.3750	0.0	0.0	1.68	1.68	n/a
		2(*h*)											
Cd14	1(*b*)		0.3333	0.6666	0.6406	0.3333	0.6666	0.6250	0.0	0.0	1.68	1.68	n/a

* Wyckoff 1-fold positions inconsistent with $P\bar{6}m2$ replaced by values in italic.

† All atoms exactly match space group $P\bar{6}m2$ if $c/64 = 1.68$ Å is subtracted from each reported value of z(Cd).

Table S9

Modified atomic coordinates in $NaLiZnO_2$ (Hoppe, 1983) with hypothetical $x'\,y'\,z'$ coordinates the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å, for $\Delta x = (x - x')$, $\Delta y = (y - y')$ and $\Delta z = (z - z')$.[3] [40458]

a = 3.304(1), c = 5.820(3) Å, $z^* = z - 0.1381$, origin translated ⅓, ⅔, 0, see §1.6.

	Wykoff	Position													
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}	*occ.*
Na	1(*a*)	1(*b*)	0.	0.	0.5001(18)	0.	0.	0.5	0	0	0.0	0.0	0.11	1.
Zn1,Li1	1(*b*)		0.3333	0.6667	-0.1381	0.3333	0.6667	-0.1359	0	0	-0.01	0.01	0.06	0.435,0.565
		2(*d*)†												
Zn2,Li2	1(*c*)		0.6667	0.3333	0.1337(2)	0.6667	0.3333	0.1359	0	0	-0.01	0.01	0.09	0.565,0.435
O1	1(*c*)		0.6667	0.3333	0.7774(14)	0.6667	0.3333	0.7754	0	0	0.01	0.01	0.07	1
		2(*d*)												
O2	1(*b*)		0.3333	0.6667	0.2267(18)	0.3333	0.6667	0.2246	0	0	0.01	0.01	0.06	1

† Occupancy of Wykoff location 2(*d*) above the expected phase transition requires identical occupation by Zn and Li in the two 1-fold positions below T_C.

Table S10

Modified atomic positions for $16H_{12}$-CdI_2 (Sarna *et al.*, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [49572].
$a = 4.24$, $c = 54.67999$ Å; $z^* = z + 0.0000$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wyckoff Position												
	$P3m1$	$P\bar{6}m2$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
I 1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	n/a
I 9	1(*c*)	1(*f*)	0.6667	0.3333	0.5	0.6667	0.3333	0.5	0	0	0	0	n/a
I 2	1(*b*)		0.3333	0.6667	0.0625	0.33	0.67	0.0625	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I 16	1(*b*)		0.3333	0.6667	0.9375	0.33	0.67	0.9375	0.0	0.0	0.0	0.0	n/a
I 3*	1(*a*)		*0.0*	*0.0*	0.1250	*0.0*	*0.0*	0.6250	0.0	0.0	0.0	0.0	n/a
		2(*g*)											
I 15	1(*a*)		0	0	0.875	0	0	0.875	0.0	0.0	0.0	0.0	n/a
I 7	1(*c*)		0.6667	0.3333	0.375	0.6667	0.3333	0.375	0.0	0.0	0.0	0.0	n/a
		2(*i*)											
I 11*	1(*c*)		*0.6667*	*0.3333*	0.625	*0.6667*	*0.3333*	0.125	0.0	0.0	0.0	0.0	n/a
I 4	1(*b*)		0.3333	0.6667	0.1875	0.3333	0.6667	0.1875	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I 14	1(*b*)		0.3333	0.6667	0.8125	0.3333	0.6667	0.8125	0.0	0.0	0.0	0.0	n/a
I 5	1(*a*)		0	0	0.2500	0	0	0.2500	0.0	0.0	0.0	0.0	n/a
		2(*g*)											
I 13	1(*a*)		0	0	0.7500	0	0	0.7500	0.0	0.0	0.0	0.0	n/a
I 6	1(*b*)		0.3333	0.6667	0.3125	0.3333	0.6667	0.3125	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I 12	1(*b*)		0.3333	0.6667	0.6875	0.3333	0.6667	0.6875	0.0	0.0	0.0	0.0	n/a
I 8	1(*b*)		0.3333	0.6667	0.4375	0.3333	0.6667	0.4375	0.0	0.0	0.0	0.0	n/a
		2(*h*)											
I 10	1(*b*)		0.3333	0.6667	0.5625	0.3333	0.6667	0.5625	0.0	0.0	0.0	0.0	n/a
Cd 1	1(*c*)		0.6667	0.3333	0.09375	0.6667	0.3333	0.09375	0.0	0.0	0.0	0.0	n/a
		2(*i*)											
Cd 8	1(*c*)		0.6667	0.3333	0.90625	0.6667	0.3333	0.90625	0.0	0.0	0.0	0.0	n/a
Cd 2*	1(*c*)		*0.6667*	*0.3333*	0.15625	*0.6667*	*0.3333*	0.1875	0.0	0.0	0.0	0.0	n/a
		2(*i*)											
Cd 7	1(*c*)		0.6667	0.3333	0.78125	0.6667	0.3333	0.8125	0.0	0.0	0.0	0.0	n/a
Cd 3	1(*c*)		0.6667	0.3333	0.34375	0.6667	0.3333	0.34375	0.0	0.0	0.0	0.0	n/a
		2(*i*)											
Cd 6	1(*c*)		0.6667	0.3333	0.65625	0.6667	0.3333	0.65625	0.0	0.0	0.0	0.0	n/a
Cd 4	1(*a*)		0	0	0.46875	0	0	0.46875	0.0	0.0	0.0	0.0	n/a
		2(*g*)											
Cd 5	1(*a*)		0	0	0.53125	0	0	0.53125	0.0	0.0	0.0	0.0	n/a

* Wyckoff 1-fold positions inconsistent with $P\bar{6}m2$ replaced by values in italic.

Table S11

Modified atomic positions for $22H_{11}$-CdI_2 (Sarna *et al.*, 1984), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [49574].

$a = 4.24$, $c = 75.1899$ Å; $z^* = z + 0.0000$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wyckoff Position											
	$P3m1$	$P\bar{6}m2$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
I1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0
I2	1(*b*)		0.3333	0.6667	0.04545	0.3333	0.6667	0.04545	0	0	0	0
		2(*h*)										
I22	1(*b*)		0.3333	0.6667	0.95455	0.3333	0.6667	0.95455	0	0	0	0
I3	1(*b*)		*0.3333*	*0.6667*	0.09091	*0.3333*	*0.6667*	0.09091	0	0	0	0
		2(*h*)										
I21	1(*b*)		*0.3333*	*0.6667*	0.9091	*0.3333*	*0.6667*	0.9091	0	0	0	0
I4	1(*b*)		0.3333	0.6667	0.13636	0.3333	0.6667	0.13636	0	0	0	0
		2(*h*)										
I20	1(*b*)		0.3334	0.6667	0.86364	0.3334	0.6667	0.86364	0	0	0	0
I5	1(*c*)		*0.3333*	*0.6667*	0.18182	*0.3333*	*0.6667*	0.18182	0	0	0	0
		2(*h*)										
I19	1(*a*)		*0.3333*	*0.6667*	0.81818	*0.3333*	*0.6667*	0.81818	0	0	0	0
I6	1(*b*)		0.3334	0.6667	0.22727	0.3334	0.6667	0.22727	0	0	0	0
		2(*h*)										
I18	1(*b*)		0.3334	0.6667	0.77273	0.3334	0.6667	0.77273	0	0	0	0
I7	1(*a*)		0.0	0.0	0.27273	0.0	0.0	0.27273	0	0	0	0
		2(*g*)										
I17	1(*a*)		0.0	0.0	0.72727	0.0	0.0	0.72727	0	0	0	0
I8	1(*b*)		0.3333	0.6667	0.31818	0.3333	0.6667	0.31818	0	0	0	0
		2(*h*)										
I16	1(*b*)		0.3333	0.6667	0.68182	0.3333	0.6667	0.68182	0	0	0	0
I9	1(*a*)		0.0	0.0	0.36364	0.0	0.0	-0.6364	0	0	0	0
		2(*g*)										
I15	1(*a*)		0.0	0.0	0.63636	0.0	0.0	0.6364	0	0	0	0
I10	1(*b*)		0.3333	0.6667	-0.5909	0.3333	0.6667	-0.5909	0	0	0	0
		2(*h*)										
I14	1(*b*)		0.3333	0.6667	0.5909	0.3333	0.6667	0.5909	0	0	0	0
I11	1(*a*)		0.0	0.0	0.40909	0.0	0.0	-0.5454	0	0	0	0
		2(*g*)										
I13	1(*a*)		0.0	0.0	0.54545	0.0	0.0	0.5454	0	0	0	0
I12	1(*b*)	1(*d*)	0.3333	0.6667	0.5	0.3333	0.6667	0.5	0	0	0	0
Cd1[†]	1(*c*)		0.6667	0.3333	0.02273	0.6667	0.3333	0.0454	0	0	-1.70	1.70
		2(*i*)										
Cd11	1(*c*)		0.6667	0.3333	0.93182	0.6667	0.3333	0.9545	0	0	-1.71	1.71
Cd2	1(*a*)		*0.6667*	*0.3333*	0.11364	*0.6667*	*0.3333*	0.1364	0	0	-1.71	1.71
		2(*i*)										
Cd10	1(*c*)		0.6667	0.3333	0.84091	0.6667	0.3333	0.8636	0	0	-1.71	1.71
Cd3	1(*a*)		*0.6667*	*0.3333*	0.20455	*0.6667*	*0.3333*	0.2273	0	0	-1.71	1.71
		2(*i*)										
Cd9	1(*c*)		0.6667	0.3333	0.75	0.6667	0.3333	0.7727	0	0	-1.71	1.71
Cd4	1(*c*)		0.6667	0.3333	0.29545	0.6667	0.3333	0.3182	0	0	-1.71	1.71
		2(*i*)										
Cd8	1(*c*)		0.6667	0.3333	0.65909	0.6667	0.3333	0.6818	0	0	-1.71	1.71
Cd5	1(*c*)		0.6667	0.3333	0.38636	0.6667	0.3333	0.4091	0	0	-1.71	1.71
		2(*i*)										
Cd7	1(*c*)		0.6667	0.3333	0.56818	0.6667	0.3333	0.5909	0	0	-1.71	1.71
Cd6	1(*c*)	1(*f*)	0.6667	0.3333	0.47727	0.6667	0.3333	0.5000	0	0	-1.71	1.71

[†] Note the apparent z(Cd) displacement by all Cd atoms of $c/44$ from $P\bar{6}m2$ symmetry in this $22H_{11}$ polytype under appropriate Wyckoff position correction for the Cd2,Cd10 and Cd3,Cd9 pairs.

Table S12

Modified atomic positions for 12*L*-ZnS (Kiflawi & Mardix, 1970), with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [107137].
a = 3.823, c = 37.488 Å; z(S)* = z - 0.0208; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	Position												
	$P3m1$	$P\bar{3}m1$[†]	x	y	z	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Zn1	1(*a*)	1(*a*)	0.0	0.0	0.0	0.0	-0.1667	0.1667	0.0	0	0	0	0	n/a
Zn4	1(*a*)		*0.6667*	*0.3333*	0.25	0.25	*0.6667*	*0.3333*	0.25	0	0	0	0	n/a
		2(*d*)												
Zn10	1(b)		0.3333	0.6667	0.75	0.75	0.3333	0.6667	0.75	0	0	0	0	
Zn2	1(b)		0.3333	0.6667	0.0833	0.0833	0.3333	0.6667	0.0833	0	0	0	0	n/a
		2(*d*)												
Zn12[‡]	1(c)		0.6667	0.3333	*0.9167*	*0.9167*	0.6667	0.3333	0.**9**167	0	0	0	0	
Zn6	1(b)		0.3333	0.6667	0.4167	0.4167	0.3333	0.6667	0.4167	0	0	0	0	n/a
		2(*d*)												
Zn8	1(c)		0.6667	0.3333	0.5833	0.5833	0.6667	0.3333	0.5833	0	0	0	0	
Zn3	1(c)		0.6667	0.3333	0.1667	0.1667	0.6667	0.3333	0.1667	0	0	0	0	n/a
		2(*d*)												
Zn11	1(*a*)		*0.3333*	*0.6667*	0.8333	0.8333	*0.3333*	*0.6667*	0.8333	0	0	0	0	
Zn5	1(c)		0.6667	0.3333	0.3333	0.3333	0.6667	0.3333	0.3333	0	0	0	0	n/a
		2(*d*)												
Zn9	1(*a*)		*0.3333*	*0.6667*	0.6667	0.6667	*0.3333*	*0.6667*	0.6667	0	0	0	0	
Zn7	1(*a*)	1(*b*)	0.0	0.0	0.5	0.5	0.0	0.0	0.5	0	0	0	0	n/a
S1[*]	1(*a*)		*0.3333*	*0.6667*	0.0625	0.0417	*0.3333*	*0.6667*	0.0416	0	0	0	0	n/a
		2(*d*)												
S12	1(c)		0.6667	0.3333	0.9792	0.9584	0.6667	0.3333	0.9584	0	0	0	0	n/a
S4	1(*a*)		0.0	0.0	0.3125	0.2917	0.0	0.0	0.2916	0	0	0	0	n/a
		2(*c*)												
S9	1(*a*)		0.0	0.0	0.7292	0.7084	0.0	0.0	0.7084	0	0	0	0	n/a
S2	1(*b*)		0.3333	0.6667	0.1458	0.1250	0.3333	0.6667	0.1250	0	0	0	0	n/a
		2(*d*)												
S11	1(*a*)		*0.6667*	*0.3333*	0.8958	0.8750	*0.6667*	*0.3333*	0.8750	0	0	0	0	
S6	1(*b*)		0.3333	0.6667	0.4792	0.4584	0.3333	0.6667	0.4584	0	0	0	0	n/a
		2(*d*)												
S7	1(*a*)		*0.6667*	*0.3333*	0.5625	0.5417	*0.6667*	*0.3333*	0.5416	0	0	0	0	n/a
S3	1(*c*)		0.6667	0.3333	0.2292	0.2084	0.6667	0.3333	0.2084	0	0	0	0	n/a
		2(*d*)												
S10	1(*b*)		0.3333	0.6667	0.8125	0.7917	0.3333	0.6667	0.7916	0	0	0	0	n/a
S5	1(*c*)		*0.3333*	*0.6667*	0.3958	0.3750	*0.3333*	*0.6667*	0.3750	0	0	0	0	n/a
		2(*d*)												
S8	1(*c*))		0.6667	0.3333	0.6458	0.6250	0.6667	0.3333	0.6250	0	0	0	0	n/a

[*] All reported z(S) replaced by z(S) – 1/48, giving atom pairs related by z' and 1-z', hence $\Delta z = 0$.

[†] Supergroup $P\bar{6}m2$ is an alternative choice for an appropriate selection of 1-fold Wyckoff positions.

[‡] z[Zn12] assumed as 0.9169 instead of reported 0.8169; Wyckoff positions for the Zn4,Zn10; Zn3,Zn11 and Zn5,Zn9 pairs, also S1,S12; S2,S11; S6,S7 and S5,S8 pairs inconsistent with $P\bar{3}m1$ replaced by values in italic.

Table S13

Atomic positions for $Pb_2Nb_2O_7$† at room temperature (Bernotat-Wulf & Hoffmann, 1981) with hypothetical *x'y'z'* coordinates in space group *P*3*m*1 and the Δx, Δy, Δz and $\Delta\xi$ displacements in Å. [17039]

a = 7.472(1), c = 28.351(3) Å; $z^* = z - 0.0025$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	*P*3*m*1	$P\bar{3}m1$	*x*	*y*	*z*	*z**	*x'*	*y'*	*z'*	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
Nb1	**3(*d*)**	**3(*e*)**	**0.4937(4)**	**0.5063(4)**	**0.0000**	**-0.0025**	**0.5**	**0.5**	**0.0**	**-0.09**	**0.05**	**-0.07**	**0.10**	**0.12**
Nb2	**1(*c*)**		**0.6666**	**0.3333**	**0.1135(3)**	**0.1110(3)**	**0.6666**	**0.3333**	**0.1090**	**0.**	**0.**	**0.06**	**0.06**	**0.12**
		2(*d*)												
Nb9	**1(*b*)**		**0.3333**	**0.6666**	**0.8955(3)**	**0.8930(3)**	**0.3333**	**0.6666**	**0.8910**	**0.**	**0.**	**0.06**	**0.06**	**0.09**
Nb3	**3(*d*)**		**0.8329(3)**	**0.1671(3)**	**0.2196(2)**	**0.2171(2)**	**0.8334**	**0.1666**	**0.2182**	**0.01**	**0.0**	**-0.03**	**0.03**	**0.07**
		6(*i*)												
Nb8	**3(*d*)**		**0.1661(6)**	**0.8339(6)**	**0.7833(3)**	**0.7808(3)**	**0.1666**	**0.8334**	**0.7818**	**-0.0**	**0.0**	**-0.03**	**0.03**	**0.15**
Nb4	**1(*a*)**		**0.0**	**0.0**	**0.3348(3)**	**0.3323(3)**	**0.0**	**0.0**	**0.3283**	**0.0**	**0.0**	**0.11**	**0.11**	**0.10**
		2(*c*)												
Nb7	**1(*a*)**		**0.0**	**0.0**	**0.6783(3)**	**0.6757(3)**	**0.0**	**0.0**	**0.6717**	**0.0**	**0.0**	**0.11**	**0.11**	**0.10**
Nb5	**1(*c*)**		**0.6666**	**0.3333**	**0.458(1)**	**0.4559(1)**	**0.6666**	**0.3333**	**0.4455**	**0.0**	**0.0**	**0.29**	**0.29**	**0.07**
		2(*d*)												
Pb6/Nb6	**1(*b*)**		**0.3333**	**0.6666**	**0.5674(1)**	**0.5649(1)**	**0.3333**	**0.6666**	**0.5545**	**0.0**	**0.0**	**0.29**	**0.29**	**0.08**
Pb1	**1(*a*)**	**1(*a*)**	**0.0**	**0.0**	**0.9955(3)**	**0.9930(3)**	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**	**-0.20**	**0.20**	**0.19**
Pb2	**3(*d*)**		**0.1676(2)**	**0.8324(2)**	**0.1071(1)**	**0.1046(1)**	**0.1690**	**0.8310**	**0.1072**	**0.02**	**0.01**	**-0.07**	**0.07**	**0.15**
		6(*i*)												
Pb9	**3(*d*)**		**0.8296(5)**	**0.1704(5)**	**0.8927(3)**	**0.8902(3)**	**0.8310**	**0.1690**	**0.8928**	**-0.01**	**0.01**	**-0.07**	**0.07**	**0.20**
Pb3	**1(*b*)**		**0.3333**	**0.6666**	**0.2200(2)**	**0.2175(2)**	**0.3333**	**0.6666**	**0.2188**	**0.**	**0.**	**-0.04**	**0.04**	**0.17**
		2(*d*)												
Pb8	**1(*c*)**		**0.6666**	**0.3333**	**0.7824(1)**	**0.7799(1)**	**0.6666**	**0.3333**	**0.7812**	**0.**	**0.**	**-0.04**	**0.04**	**0.09**
Pb4	**3(*d*)**		**0.4919(3)**	**0.5081(3)**	**0.3372(2)**	**0.3347(2)**	**0.4930**	**0.5070**	**0.3328**	**0.02**	**0.01**	**0.05**	**0.06**	**0.18**
		6(*i*)												
Pb7	**3(*d*)**		**0.5059(2)**	**0.4941(2)**	**0.6721(1)**	**0.6692(1)**	**0.5070**	**0.4930**	**0.6672**	**-0.01**	**0.01**	**0.05**	**0.05**	**0.07**
Nb6/Pb6	**3(*d*)**		**0.8284(5)**	**0.1716(5)**	**0.5674(1)**	**0.5623(2)**	**0.8307**	**0.1693**	**0.5577**	**-0.02**	**0.02**	**0.13**	**0.13**	**0.17**
		2(*d*)												
Pb5	**3(*d*)**		**0.1670(3)**	**0.8330(3)**	**0.4495(1)**	**0.4470(1)**	**0.1693**	**0.8307**	**0.4423**	**-0.02**	**0.02**	**0.13**	**0.13**	**0.15**
O1	**3(*d*)**		**0.458(3)**	**0.542(3)**	**0.7701(10)**	**0.7676(10)**	**0.459**	**0.541**	**0.7683**	**0.01**	**0.01**	**-0.02**	**0.03**	**0.12**
		6(*i*)												
O13	**3(*d*)**		**0.539(2)**	**0.461(2)**	**0.2316(8)**	**0.2310(8)**	**0.541**	**0.459**	**0.2317**	**0.02**	**0.01**	**-0.02**	**0.03**	**0.11**
O2	**3(*d*)**		**0.46(2)**	**0.54(2)**	**0.9319(9)**	**0.9294(9)**	**0.46**	**0.54**	**0.9333**	**0.0**	**0.0**	**-0.12**	**0.12**	**0.11**
		6(*i*)												
O11	**3(*d*)**		**0.54(2)**	**0.46(2)**	**0.0654(8)**	**0.0629(8)**	**0.54**	**0.46**	**0.0667**	**0.0**	**0.0**	**-0.11**	**0.11**	**0.1**
O3	**3(*d*)**		**0.126(3)**	**0.874(3)**	**0.2000(9)**	**0.1994(9)**	**0.128**	**0.872**	**0.2024**	**0.01**	**0.01**	**-0.09**	**0.09**	**0.12**
		6(*i*)												
O7	**3(*d*)**		**0.871(3)**	**0.129(3)**	**0.7971(10)**	**0.7946(10)**	**0.872**	**0.128**	**0.7976**	**0.01**	**0.01**	**-0.09**	**0.09**	**0.12**
O4	**3(*d*)**		**0.127(3)**	**0.873(3)**	**0.3635(10)**	**0.3610(10)**	**0.126**	**0.874**	**0.3617**	**-0.01**	**-0.01**	**-0.02**	**0.03**	**0.14**
		6(*i*)												
O6	**3(*d*)**		**0.875(4)**	**0.125(4)**	**0.6402(14)**	**0.6377(14)**	**0.874**	**0.126**	**0.6383**	**0.01**	**-0.01**	**-0.02**	**0.02**	**0.2**
O5	**3(*d*)**		**0.877(2)**	**0.123(2)**	**0.2821(9)**	**0.2796(9)**	**0.875**	**0.125**	**0.2822**	**-0.03**	**-0.01**	**-0.07**	**0.08**	**0.12**
		6(*i*)												
O16	**3(*d*)**		**0.127(3)**	**0.873(3)**	**0.7176(12)**	**0.7151(12)**	**0.125**	**0.875**	**0.7178**	**0.01**	**-0.01**	**-0.08**	**0.08**	**0.16**
O8	**3(*d*)**		**0.791(2)**	**0.209(2)**	**0.1458(7)**	**0.1452(7)**	**0.792**	**0.208**	**0.1465**	**0.01**	**0.01**	**-0.04**	**0.04**	**0.08**
		6(*i*)												
O12	**3(*d*)**		**0.207(2)**	**0.793(2)**	**0.8528(8)**	**0.8522(8)**	**0.208**	**0.792**	**0.8535**	**-0.01**	**0.01**	**-0.04**	**0.04**	**0.09**

O9	**3(*d*)**		**0.788(6)**	**0.212(6)**	**0.506124(**	**0.5055(24)**	**0.831**	**0.169**	**0.4743**	**-0.32**	**0.32**	**0.88**	**0.94**	**0.29**
		6(*h*)												
O18	**3(*d*)**		**0.126(4)**	**0.874(4)**	**0.5575(14)**	**0.5569(14)**	**0.169**	**0.831**	**0.5257**	**-0.32**	**0.32**	**0.88**	**0.94**	**0.18**
O10	**3(*d*)**		**0.789(3)**	**0.211(3)**	**0.9852(11)**	**0.9846(11)**	**0.791**	**0.209**	**0.9864**	**0.01**	**0.01**	**-0.05**	**0.05**	**0.15**
		6(*g*)												
O17	**3(*d*)**		**0.206(3)**	**0.794(3)**	**0.0125(11)**	**0.0119(11)**	**0.209**	**0.791**	**0.0136**	**-0.02**	**0.03**	**-0.05**	**0.05**	**0.14**
O14	**3(*d*)**		**0.549(5)**	**0.451(5)**	**0.4291(19)**	**0.4285(19)**	**0.504**	**0.496**	**0.4204**	**0.34**	**-0.34**	**0.23**	**0.41**	**0.25**
		6(*i*)												
O15	**3(*d*)**		**0.542(4)**	**0.458(2)**	**0.5883(15)**	**0.5877(15)**	**0.496**	**0.504**	**0.5796**	**0.34**	**-0.34**	**0.23**	**0.41**	**0.2**
O19	**1(*b*)**		**0.3333**	**0.6666**	**0.1301(29)**	**0.1295(29)**	**0.3333**	**0.6666**	**0.1344**	**0**	**0**	**-0.14**	**0.14**	**3.5**
		2(*d*)												
O23	**1(*c*)**		**0.6666**	**0.3333**	**0.8613(49)**	**0.8607(49)**	**0.6666**	**0.3333**	**0.8656**	**0**	**0**	**-0.14**	**0.14**	**5.6**
O20	**1(*b*)**		**0.3333**	**0.6666**	**0.3047(40)**	**0.3041(40)**	**0.3333**	**0.6666**	**0.3056**	**0**	**0**	**-0.04**	**0.04**	**6.3**
		2(*d*)												
O21	**1(*c*)**		**0.6666**	**0.3333**	**0.6936(36)**	**0.6930(36)**	**0.6666**	**0.3332**	**0.6944**	**0.0**	**-0.0**	**-0.04**	**0.04**	**0.21**
O22	**1(*a*)**		**0.0**	**0.0**	**0.0728(47)**	**0.0722(47)**	**0.0**	**0.0**	**0.0816**	**0.0**	**0.0**	**-0.27**	**0.27**	**0.27**
		2(*c*)												
O26	**1(*a*)**		**0.0**	**0.0**	**0.9096(40)**	**0.9090(40)**	**0.0**	**0.0**	**0.9184**	**0.0**	**0.0**	**-0.27**	**0.27**	**0.24**
O24	**1(*b*)**		**0.3333**	**0.6666**	**0.4881(40)**	**0.4875(40)**	**0.3333**	**0.6666**	**0.4881**	**0**	**0**	**-0.02**	**0.02**	**4.3**
		2(*d*)												
O24′ ‡	**1(*b*)**		***0.6666***	***0.3333***	***0.5119***	***0.5113***	***0.6666***	***0.3333***	***0.5119***	***0***	***0***	***-0.02***	**0.02**	**n/a**
O25	**1(*b*)**		**0.3333**	**0.6666**	**0.6468(49)**	**0.6462(49)**	**0.3333**	**0.6666**	**0.6672**	**0**	**0**	**-0.60**	**0.60**	**6.3**
		2(*d*)												
O28	**1(*c*)**		**0.6667**	**0.3333**	**0.3124(45)**	**0.3118(45)**	**0.6667**	**0.3333**	**0.3328**	**0.0**	**0.0**	**-0.60**	**0.60**	**0.28**
O27	**1(*a*)**		**0**	**0**	**0.4249(50)**	**0.4243(50)**	**0**	**0**	**0.4249**	**0**	**0**	**-0.02**	**0.02**	**5.0**
		2(*c*)												
O27′ ‡	**1(*a*)**		***0***	***0***	***0.5751***	***0.5757***	***0***	***0***	***0.5751***	***0***	***0***	***-0.02***	**0.02**	**n/a**

† $Pb_{17}Nb_{17}O_{59.5}$ per unit cell.

‡ Atoms O24′ and O27′ in italic assumed present but not reported by the authors.

Table S14

Atomic positions for 6*H*-PbI_2 at room temperature (Mitchell, 1959) with hypothetical *x'y'z'* coordinates in space group $P3m1$ and the Δx, Δy, Δz and $\Delta\xi$ displacements in Å. [24264]
a = 4.557, c = 20.937 Å. $z^* = z + 0.0000$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position											
	$P3m1$	$P\bar{3}m1$	x	y	$z = z^*$	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Pb1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	n/a
Pb2	1(*b*)†		*0.3333*	*0.6667*	0.3333	*0.3333*	*0.6667*	0.3333	0	0	0	0	n/a
		2(*d*)											
Pb3	1(*c*)		0.6667	0.3333	0.6667	0.6667	0.3333	0.6667	0	0	0	0	n/a
I1	1(*b*)		0.3333	0.6667	0.088	0.3333	0.6667	0.088	0	0	0	0	n/a
		2(*d*)											
I6	1(*c*)		0.6667	0.3333	0.912	0.6667	0.3333	0.912	0	0	0	0	n/a
I2	1(*c*)		0.6667	0.3333	0.245	0.6667	0.3333	0.245	0	0	0	0	n/a
		2(*d*)											
I5	1(*b*)		0.3333	0.6667	0.755	0.3333	0.6667	0.755	0	0	0	0	n/a
I3	1(*a*)		*0*	*0*	0.421	*0*	*0*	0.421	0	0	0	0	n/a
		2(*d*)											
I4	1(*a*)		0	0	0.579	0	0	0.579	0	0	0	0	n/a

† Modified Wyckoff position for Pb2 from 1(*a*), and I3 from 1(*b*), in italic leaves all three Pb atoms with unchanged octahedral bonding and $d_{Pb\text{-}I}$ = 3.21 Å.

Table S15

Modified atomic positions for $(Cd_{0.5}Pb_{0.5})_3OSiO_4$ (Eysel & Breuer, 1983) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [36480].
a = 7.133, c = 5.99 Å; $z^* = z + 0.013$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Cd1,Pb1	3(*d*)	3(*j*)	0.5	-0.5	0	0.013	0.5	-0.5	0	0	0	0.08	0.08	0.5.0.5
Cd2,Pb2	3(*d*)	3(*k*)	0.833	-0.833	0.5	0.513	0.833	-0.833	0.5	0	0	0.08	0.08	0.5,0.5
Si1	1(*a*)	1(*a*)	0	0	0	0.013	0	0	0	0	0	0.08	0.08	1.
Si2	1(*b*)	1(*d*)	0.3333	0.6667	0.5	0.513	0.3333	0.6667	0.5	0	0	0.08	0.08	1.
O1	1(*c*)		0.6667	0.3333	0.26	0.273	0.6667	0.3333	0.26	0	0	0.08	0.08	1.
		2(*i*)												
O2	1(*c*)		0.6667	0.3333	0.74	0.753	0.6667	0.3333	0.74	0	0	0.08	0.08	1.
O3	3(*d*)	3(*k*)	0.46	-0.46	0.42	0.433	0.46	-0.46	0.5	0	0	-0.40	0.40	1.
O4	1(*b*)		0.3333	0.6667	0.77	0.783	0.3333	0.6667	0.75	0	0	0.20	0.20	1.
		2(*h*)												
O6†	1(*b*)		0.3333	0.6667	0.27	0.283	0.3333	0.6667	0.25	0	0	0.20	0.20	1.
O5	3(*d*)	3(*j*)	0.875	-0.875	0.91	0.923	0.875	-0.875	1.0	0	0	-0.46	0.46	1.

† The O6 coordinates were reported in Wyckoff position 1(*a*), see §3.7.

Table S16

Modified atomic positions for $Cu_{0.8}Ag_{0.96}Te$ (Avilov *et al.*, 1974) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [41905].
$a = 8.54(1)$, $c = 21.7(1)$ Å; $z^* = z - 0.041$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	Position												
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Cu1	1(*a*)		0	0	0.105	0.064	0	0	0.109	0	0	-0.98	0.98	1.
		2(*c*)												
Cu15	1(*a*)		0	0	0.887	0.846	0	0	0.891	0	0	-0.98	0.98	0.55
Cu2†	3(*d*)		0.19	0.81	*0.5*	*0.459*	0.207	0.793	*0.542*	-0.09	0.15	*-0.80*	0.81	1.
		6(*i*)												
Cu9	3(*d*)		0.777	0.223	0.416	0.375	0.793	0.207	0.458	-0.15	0.19	-0.78	0.80	0.65
Cu3	1(*b*)		0.3333	0.6667	0.145	0.104	0.3333	0.6667	0.162	0	0	-1.26	1.26	0.75
		2(*d*)												
Cu13‡	1(*c*)		0.6667	0.3333	0.822	0.781	0.6667	0.3333	0.838	0	0	-1.24	1.24	1.
Cu4†	3(*d*)	3(*e*)	0.505	0.495	*0.1*	*0.059*	*0.5*	*0.5*	*0*	*0*	*0*	*-0.19*	0.19	0.85
Cu5	3(*d*)		0.145	0.855	0.202	0.161	0.180	0.820	0.217	-0.30	0.30	-1.22	1.26	0.55
		6(*i*)												
Cu12	3(*d*)		0.785	0.215	0.768	0.727	0.820	0.180	0.783	-0.30	0.30	-1.22	1.26	0.65
Cu6	1(*b*)		0.3333	0.6667	0.277	0.236	0.3333	0.6667	0.214	0	0	0.48	0.48	0.5
		2(*d*)												
Cu14	1(*c*)		0.6667	0.3333	0.849	0.808	0.6667	0.3333	0.786	0	0	0.48	0.48	0.75
Cu7	1(*a*)		0	0	0.305	0.264	0	0	0.308	0	0	-0.95	0.95	1.
		2(*c*)												
Cu11	1(*a*)		0	0	0.688	0.647	0	0	0.691	0	0	-0.95	0.95	1.
Cu8	1(*b*)		0.3333	0.6667	0.376	0.335	0.3333	0.6667	0.386	0	0	-1.11	1.11	0.85
		2(*d*)												0.65
Cu10‡	1(*c*)		0.6667	0.3333	0.605	0.564	0.6667	0.3333	0.614	0	0	-1.10	1.10	0.8
Ag1	3(*d*)	3(*e*)	0.503	0.497	0.019	-0.022	0.5	0.5	0	0.03	-0.03	-0.48	0.48	0.9 0
Ag2	3(*d*)		0.834	0.166	0.031	-0.010	0.834	0.166	0.089	0	0	-2.15	2.15	1.
		6(*i*)												
Ag9	3(*d*)		0.165	0.835	0.852	0.811	0.165	0.835	0.911	0	0	-2.17	2.17	1.
Ag3	3(*d*)		0.501	0.499	0.307	0.266	0.5	0.5	0.255	0.01	-0.01	0.24	0.24	1.
		6(*i*)												
Ag8	3(*d*)		0.505	0.495	0.798	0.757	0.5	0.5	0.745	0.04	-0.04	0.26	0.26	0.8
Ag4	3(*d*)		0.17	0.83	0.349	0.208	0.202	0.798	0.171	-0.27	0.27	0.80	0.84	1.
		6(*i*)												
Ag10	3(*d*)		0.765	0.235	0.908	0.867	0.798	0.202	0.829	-0.28	0.278	0.82	0.87	1.
Ag5	1(*a*)		0	0	0.526	0.485	0	0	0.363	0	0	2.65	2.65	1.
		2(*c*)												
Ag7	1(*a*)		0	0	0.791	0.759	0	0	0.637	0	0	2.65	2.65	
Ag6	1(*c*)		0.6667	0.3333	0.617	0.576	0.6667	0.3333	0.554	0	0	0.48	0.48	1.
		2(*d*)												
Te6	1(*b*)		0.3333	0.6667	0.509	0.468	0.3333	0.6667	0.446	0	0	0 48	0.48	1.
Te1	1(*b*)		0.3333	0.6667	0.021	-0.020	0.3333	0.6667	-0.080	0	0	1.30	1.30	1.
		2(*d*)												
Te3	1(*c*)		0.6667	0.3333	0.197	0.140	0.6667	0.3333	0.080	0	0	1.30	1.30	1.
Te4	3(*d*)		0.814	0.186	0.291	0.250	0.814	0.186	0.259	0	0	-0.20	0.2	*0.5.*
		6(*i*)												
Te4′††	3(*d*)		*0.186*	*0.814*	*0.773*	*0.732*	*0.186*	*0.814*	*0.741*	*0*	*0*	*-0.20*	0.2	*0.5*
Te2	3(*d*)		0.832	0.168	0.141	0.100	0.836	0.164	0.084	-0.03	0.03	0.35	0.35	1.
		6(*i*)												
Te10	3(*d*)		0.16	0.84	0.974	0.933	0.164	0.836	0.916	-0.03	0.03	0.37	0.37	1.
Te5	3(*d*)		0.505	0.495	0.444	0.403	0.5	0.5	0.384	0.04	-0.04	0.41	0.41	1.
		6(*i*)												
Te9	3(*d*)		0.505	0.495	0.676	0.635	0.5	0.5	0.616	0.04	-0.04	0.41	0.41	1.
Te7	3(*d*)		0.825	0.175	0.518	0.477	0.840	0.160	0.449	-0.13	0.13	0.61	0.62	1.
		6(*i*)												
Te8	3(*d*)		0.145	0.855	0.62	0.579	0.160	0.840	0.551	-0.13	0.13	0.61	0.62.	1

† Coordinate(s) assumed in error and changed to value(s) in italic.
‡ Wyckoff location changed from 1(*b*) to 1(*c*).
†† Te4′ assumed at Te4(x, y, z) with value(s) in italic and each site half occupied.

Table S17

Modified atomic positions for $Cu_{1.81}Te$ (Baranova *et al*., 1973) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [42156].
a = 8.37(1), c = 21.6(2) Å, $z^* = z + 0.0045$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	occ.	u_{iso}
Cu1	3(*d*)	3(*e*)	0.5	0.5	0	0.005	0.5	0.5	0	0.0	0.0	0.11	0.11	0.5	0.16
Cu2	1(*c*)		0.6667	0.3333	0.045	0.050	0.6667	0.3333	0.052	0.0	0.0	-0.04	0.04	1.	0.16
		2(*d*)													
Cu23	1(*b*)		0.3333	0.6667	0.94	0.945	0.3333	0.6667	0.948	0.0	0.0	-0.06	0.06	1.	0.16
Cu3	3(*d*)		0.835	0.165	0.061	0.066	0.836	0.164	0.064	-0.01	0.01	0.04	0.04	1.	0.16
		6(*i*)													
Cu21	3(*d*)		0.163	0.837	0.932	0.937	0.164	0.836	0.936	-0.01	0.01	0.02	0.02	1.	0.16
Cu4	1(*b*)		0.3333	0.6667	0.062	0.067	0.3333	0.6667	0.067	0.0	0.0	0.0	0.0	1.	0.16
		2(*d*)													
Cu4A†	*1(c)*		*0.6667*	*0.3333*	*0.938*	*0.933*	*0.6667*	*0.3333*	*0.933*	*0.0*	*0.0*	*0.0*	*0.0*	n/a	n/a
Cu5	1(*a*)		0	0	0.225	0.229	0	0	0.2235	0.0	0.0	0.12	0.12	1.	0.16
		2(*c*)													
Cu19	1(*a*)		0	0	0.778	0.783	0	0	0.7765	0.0	0.0	0.14	0.14	1.	0.16
Cu6	3(*d*)		0.496	0.504	0.225	0.229	0.4955	0.5045	0.223	0.01	-0.01	0.13	0.13	1.	0.16
		6(*i*)													
Cu20	3(*d*)		0.505	0.495	0.779	0.784	0.5045	0.4955	0.777	0.01	-0.01	0.15	0.15	1.	0.16
Cu7	3(*d*)		0.162	-0.162	0.254	0.259	0.1635	0.8365	0.2615	-0.01	0.01	-0.05	0.05	0.5	0.16
		6(*i*)													
Cu17	3(*d*)		0.835	0.165	0.731	0.736	0.8365	0.1635	0.7385	-0.01	0.01	-0.05	0.05	1.	0.16
Cu8	3(*d*)		0.825	0.175	0.27	0.275	0.8265	0.1735	0.275	-0.03	-0.03	0.0	0.03	1.	0.16
		6(*i*)													
Cu22	3(d)		*0.172*	*0.828*	0.72	*0.725*	*0.1735*	*0.8265*	0.725	*-0.03*	*-0.03*	*0.0*	*0.03*	1.	0.16
Cu9	1(*b*)		0.3333	0.6667	0.271	0.276	0.3333	0.6667	0.287	0	0	-0.24	0.24	1.	0.16
		2(*d*)													
Cu16	1(*c*)		0.6667	0.3333	0.697	0.702	0.6667	0.3333	0.713	0	0	-0.24	0.24	1.	0.16
Cu10	1(*a*)		0	0	0.327	0.332	0	0	0.3275	0.0	0.0	0.10	0.1	1.	0.16
		2(*c*)													
Cu14	1(*a*)		0	0	0.672	0.677	0	0	0.6725	0.0	0.0	0.10	0.1	1.	0.16
Cu11	1(*c*)		0.6667	0.3333	0.368	0.373	0.6667	0.3333	0.318	0.0	0.0	1.19	1.19	1.	0.16
		2(*d*)													
Cu18	1(*b*)		0.3333	0.6667	0.732	0.737	0.3333	0.6667	0.682	0.0	0.0	1.19	1.19	1.	0.16
Cu12	3(*d*)		0.83	0.17	0.499	0.504	0.835	0.165	0.4395	-0.04	0.04	1.39	1.39	0.5	0.16
		6(*i*)													
Cu13	3(*d*)		0.16	0.84	0.62	0.625	0.165	0.835	0.5605	-0.04	0.04	1.39	1.39	1.	0.16
Cu15	3(*d*)		0.495	0.505	0.675	0.680	0.5	0.5	0.680	-0.04	0.04	0	0.04	1.	0.16
		6(*i*)													
Cu15A†	*3(d)*		*0.505*	*0.495*	*0.315*	*0.320*	*0.5*	*0. 5*	*0.320*	*0.04*	*-0.04*	*0*	*0.04*	*1.*	*0.16*
Cu24	1(*a*)	1(*a*)	0	0	0.998	0.003	0	0	0	0.0	0.0	0.06	0.06	1.	0.16
Te1	1(*a*)		0	0	0.114	0.119	0	0	0.1145	0.0	0.0	0.10	0.1	1.	0.16
		2(*c*)													
Te12	1(*a*)		0	0	0.885	0.890	0	0	0.8855	0.0	0.0	0.10	0.1	1.	0.16

Te2	3(*d*)		0.505	0.495	0.115	0.120	0.505	0.495	0.1155	0.0	0.0	0.10	0.1	1.	0.16
		6(*i*)													
Te11	3(*d*)		0.495	0.505	0.884	0.889	0.495	0.505	0.8845	0.0	0.0	0.10	0.1	1.	0.16
Te3	3(*d*)		0.835	0.165	0.39	0.395	0.830	0.170	0.391	0.04	-0.04	0.09	0.10	1.	0.16
		6(*i*)													
Te10‡	3(*d*)		*0.175*	*0.825*	0.609	0.614	*0.170*	*0.830*	0.609	-0.04	0.04	0.11	0.12	1.	0.16
Te4	1(*b*)		0.3333	0.6667	0.392	0.397	0.3333	0.6667	0.3915	0.0	0.0	0.12	0.12	1.	0.16
		2(*d*)													
Te9‡	1(*b*)		*0.6667*	*0.3333*	0.609	0.614	*0.6667*	*0.3333*	0.6085	0.0	0.0	0.12	0.12	1.	0.16
Te5	1(*a*)		0	0	0.442	0.447	0	0	0.442	0.0	0.0	0.11	0.11	1.	0.16
		2(*c*)													
Te8	1(*a*)		0	0	0.558	0.563	0	0	0.558	0.0	0.0	0.11	0.11	1.	0.16
Te6	3(*d*)		0.505	0.495	0.442	0.447	0.504	0.496	0.4425	0.01	-0.01	0.10	0.10	1.	0.16
		6(*i*)													
Te7	3(*d*)		0.497	0.503	0.557	0.562	0.496	0.504	0.5575	0.01	-0.01	0.10	0.10	1.	0.16

† Entries fully in italic are for atoms assumed present.

‡ Entries with *x* and *y* coordinates only in italic assume a reversal of values in the original report. Note Cu8 and Cu22 location comparability with that of Ag2 and Ag9 in Table S16.

Table S18

Modified atomic positions for $Cu_{0.45}In_{3.17}Se_5$ (Gulay *et al*., 2004) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [54750].
a = 4.0263(2), c = 16.2992(7) Å; $\Delta z = z - 0.0786$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
Cu,In1	1(*a*)		0.	0.	0.0736	0.	0.	0.0761	0.	0.	-0.04	0.04	0.13	0.45, 0.339(8)
		2(*g*)												
Se1	1(*a*)		0.	0.	-0.0786	0.	0.	-0.0761	0.	0.	-0.04	0.04	0.11	1.
In2	1(*b*)		0.3333	0.6667	0.3774	0.3333	0.6667	0.3891	0.	0.	-0.19	0.19	0.17	0.523(5)
		2(*h*)												
In5	1(*b*)		0.3333	0.6667	0.5992	0.3333	0.6667	0.6109	0.	0.	-0.19	0.19	0.09	0.308(6)
In3	1(*c*)		0.6667	0.3333	0.8506	0.6667	0.3333	0.8401	0.	0.	0.17	0.17	0.17	1.
		2(*i*)												
In4	1(*c*)		0.6667	0.3333	0.1704	0.6667	0.3333	0.1599	0.	0.	0.17	0.17	0.15	1.
Se2†	1(*b*)	1(*c*)	0.3333	0.6667	-0.0036	0.3333	0.6667	0.	0.	0.	-0.06	0.06	0.16	1.
Se5	1(*a*)	1(*b*)	0.	0.	0.5109	0.	0.	0.5	0.	0.	0.19	0.19	0.16	1.
Se3	1(*c*)		0.6667	0.3333	0.6794	0.6667	0.3333	0.6791	0.	0.	0.0	0.0	0.15	1.
		2(*i*)												
Se4	1(*c*)		0.6667	0.3333	0.3212	0.6667	0.3333	0.3209	0.	0.	0.0	0.0	0.13	1.

† With Se2(x,y,z) arbitrarily changed from ⅓, ⅔, 0.1806 to = ⅓, ⅔, 0.075 see §3.10.

Table S19

Atomic positions for $BaTiO_{2.67}$ (Woodward *et al*., 2004) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [54785].
$a = 5.7$, $c = 7.0$ Å.; $z^* = z$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Ba1	1(*a*)	1(*a*)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.
Ba2	1(*b*)		0.3333	0.6667	0.6667	0.3333	0.6667	0.6667	0.	0.	0.	0.	1.
		2(*d*)											
Ba3	1(*c*)		0.6667	0.3333	0.3333	0.6667	0.3333	0.3333	0.	0.	0.	0.	1.
Ti1	1(*a*)	1(*b*)	0.	0.	0.5	0.	0.	0.5	0.	0.	0.	0.	1.
Ti2	1(*b*)		0.3333	0.6667	0.1667	0.3333	0.6667	0.1667	0.	0.	0.	0.	1.
		2(*d*)											
Ti3	1(*c*)		0.6667	0.3333	0.8333	0.6667	0.3333	0.8333	0.	0.	0.	0.	1.
O1	3(*d*)	3(*e*)	0.5	0.	0.	0.5	0.	0.	0.	0.	0.	0.	1.
O2	3(*d*)		0.8333	0.6667	0.6667	0.8333	0.6667	0.6667	0.	0.	0.	0.	1.
		6(*i*)											
O3	3(*d*)		0.1667	0.3333	0.3333	0.1667	0.3333	0.3333	0.	0.	0.	0.	0.667

Table S20

Modified atomic positions for BN (Kupčik *et al.*, 1994) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [56315].
$a = 2.563(1)$, $c = 6.278(1)$ Å; $z^* = z - 1/24 = z - 0.0417$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	Position											
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
B1	1(*a*)	1(*a*)	0	0	0	-0.0417	0	0	0	0	0	-0.26	0.26
B2	1(*c*)		0.6667	0.3333	0.3333	0.2916	0.6667	0.3333	0.3333	0	0	-0.26	0.26
		2(*d*)											
B3	1(*b*)		0.3333	0.6667	0.6667	0.6250	0.3333	0.6667	0.6667	0	0	-0.26	0.26
N1	1(*a*)	1(*b*)	0	0	0.25	0.2083	0	0	0.5	0	0	-1.83	1.30
N2	1(*c*)		0.6667	0.3333	0.5833	0.5416	0.6667	0.3333	0.3333	0	0	1.31	0.78
		2(*d*)											
N3	1(*b*)		0.3333	0.6667	0.9167	0.8750	0.3333	0.6667	0.6667	0	0	1.31	0.26

Table S21(*a*)

Modified atomic positions for $Si_3H_3(OH)_3)_{0.333}$ (Dettlaff-Weglikowska *et al.*, 1997) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [56605].
$a = 3.8$, $c = 6.04$ Å; $z^* = z - 0.1233$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

Wykoff Position

	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
Si1	1(*b*)	1(*c*)	0.3333	0.6667	0	-0.123	0.3333	0.6667	0	0	0	-0.74	0.74	0.5	0.15
Si2	1(*c*)	1(*e*)	0.6667	0.3333	0.135	0.012	0.6667	0.3333	0	0	0	0.07	0.07	0.5	0.15
O	1(*b*)	1(*d*)	0.3333	0.6667	-0.265	-0.388	0.3333	0.6667	-0.5	0	0	0.68	0.68	1.	0.15

Table S21(*b*)

Modified atomic positions for $Si_3H_3(OH)_3)_{0.333}$ (Dettlaff-Weglikowska *et al.*, 1997) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [56605].
$a = 3.8$, $c = 6.04$ Å; $z^* = z - 0.085$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

Wykoff Position

	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
Si1	1(*b*)	1(*c*)	0.3333	0.6667	0	-0.0850	0.3333	0.6667	0	0	0	-0.51	0.51	0.5	0.15
Si2	1(*c*)	1(*e*)	0.6667	0.3333	0.135	0.0500	0.6667	0.3333	0	0	0	0.30	0.30	0.5	0.15
O	1(*b*)	1(*d*)	0.3333	0.6667	-0.265	-0.3500	0.3333	0.6667	-0.5	0	0	0.91	0.91	1.	0.15
H1	3(*d*)	3(*k*)	0.1956	-0.1956	-0.335	-0.4200	0.1956	-0.1956	-0.5	0	0	0.48	0.48	0.333	0.15
H2	1(*c*)	1(*f*)	0.6667	0.3333	0.39	0.3050	0.6667	0.3333	0.5	0	0	-1.17	1.17	1.	0.15

Table S22

Modified atomic positions for $Al_{51}Ca_4Cr_7$ **(**Czech, *et al.*, 1984) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [57537].
$a = 10.281$, $c = 11.579(3)$ Å, $z^* = z + 0.0023$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Al1	3(*d*)	3(*j*)	0.2457(3)	0.7543	0.9225(6)	0.9248	0.2457	0.7543	1.0	0.	0.	-0.87	0.87	0.01
Al2	3(*d*)	3(*k*)	0.7592(3)	0.2408	0.4412(5)	0.4435	0.7592	0.2408	0.5	0.	0.	-0.65	0.65	0.09
Al3	3(*d*)		0.5129(3)	0.4871	0.3156(5)	0.3179	0.5432	0.4568	0.3239	-0.31	0.31	-0.07	0.32	0.06
		6(*n*)												
Al14	3(*d*)		0.5734(3)	0.4266	0.6678(6)	0.6701	0.5432	0.4568	0.6761	0.31	-0.31	-0.07	0.32	0.11
Al5	3(*d*)	3(*k*)	0.9089(3)	0.0911	0.4131(6)	0.4154	0.9089	0.0911	0.5	0.	0.	-0.98	0.98	0.08
Al8	3(*d*)		0.7550(3)	0.2450	0.8789(6)	0.8812	0.7888	0.2112	0.8256	-0.35	0.35	0.64	0.73	0.10
		6(*n*)												
Al9	3(*d*)		0.8226(4)	0.1774	0.2277(6)	0.2300	0.7888	0.2112	0.1743	0.35	-0.35	0.64	0.73	0.12
Al10	3(*d*)		0.4236(4)	0.5764	0.1273(7)	0.1296	0.4236	0.5764	0.1133	0.	0.	0.19	1.34	0.13
		6(*n*)												
Al13[†]	3(*d*)		*0.4222(3)*	*0.5778*	*0.9007(5)*	*0.9030*	*0.4222*	*0.5778*	*0.8867*	*0.*	*0.*	0.19	1.29	0.08
Al11	3(*d*)		0.0914(4)	0.9086	0.6195(8)	0.6219	0.1302	0.8699	0.6754	-0.40	0.40	-0.62	0.74	0.13
		6(*n*)												
Al12	3(*d*)		0.1689(5)	0.8311	0.2689(9)	0.2712	0.1301	0.8698	0.3246	0.40	-0.40	-0.62	0.74	0.13
Al7	6(*e*)	6(*l*)	0.9974(5)	0.7313(5)	0.0258(5)	0.0235	0.9974	0.7313	0.0	0.0	0.	0.27	0.27	0.10
Al4	6(*e*)		0.5988(4)	0.6643(5)	0.5142(4)	0.5165	0.6250	0.6744	0.3751	-0.27	-0.10	1.64	1.67	0.09
		12(*o*)												
Al6	6(*e*)		0.3155(4)	0.3488(4)	0.7640(4)	0.7663	0.3256	0.3750	0.6249	-0.10	-0.28	1.64	1.67	0.11
Ca1	1(*a*)		0	0	0.8544(8)	0.8567	0	0	0.8415	0.	0.	0.18	0.18	0.14
		2(*g*)												
Ca2	1(*a*)		0	0	0.1714(8)	0.1737	0	0	0.1585	0.	0.	0.18	0.18	0.15
Ca3	1(*b*)		0.3333	0.6667	0.6825(8)	0.6848	0.3333	0.6667	0.6578	0.	0.	0.31	0.31	0.14
		2(*h*)												
Ca4	1(*b*)		0.3333	0.6667	0.3669(6)	0.3692	0.3333	0.6667	0.3422	0.	0.	0.31	0.31	0.01
Cr1	1(*c*)	1(*f*)	0.6667	0.3333	0.2711(7)	0.2734	0.6667	0.3333	0.5	0.	0.	-2.62	2.62	0.08
Cr2	3(*d*)	3(*k*)	0.8357(1)	0.1643	0.6162(0)	0.6185	0.8357	0.1643	0.5	0.	0.	1.37	1.37	0.01
Cr3	3(*d*)	3(*j*)	0.4972(2)	0.5028	0.9290(2)	0.9313	0. 4972	0.5028	1.0	-0.03	0.03	-0.79	0.79	0.10

[†] Assuming the x and y coordinates for Al13, also the sign of z, are reversed from those reported as in italic.

Table S23

Modified atomic positions for $Ca_{0.95}Li_{1.05}Sn$ **(**Müller & Voltz, 1974) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [58911,107334].
$a = 4.94(1)$, $c = 10.90(2)$ Å, $z^* = z + 0.0049$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position															
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$\Delta\xi^\dagger$	*occ.*
Ca1,Li1	1(*a*)		0	0	0.334	0.339	0	0	0.333	0	0	0.07	0.07	0.01	0.95,0.05
		2(*g*)													
Ca2,Li2	1(*a*)		0	0	0.668	0.673	0	0	0.667	0	0	0.07	0.07	0.01	0.95,0.05
Ca3,Li3	1(*a*)	1(*a*)	0	0	0.999	0.004	0	0	1.000	0	0	0.04	0.04	0.01	0.95,0.05
Li4	1(*b*)		0.3333	0.6667	0.214	0.219	0.3333	0.6667	0.213	0	0	0.07	0.07	0.01	1.
		2(*h*)													
Li5	1(*b*)		0.3333	0.6667	0.788	0.793	0.3333	0.6667	0.787	0	0	0.07	0.07	0.01	1.
Li6[†]	1(*c*)	1(*f*)	0.6667	0.3333	0.454	0.459	0.6667	0.3333	0.5	0	0	-0.45	0.45	0.01	1.
Sn1	1(*b*)	1(*d*)	0.3333	0.6667	0.500	0.505	0.3333	0.6667	0.5	0	0	0.05	0.05	0.00	1.
Sn2	1(*c*)		0.6667	0.3333	0.146	0.151	0.6667	0.3333	0.146	0	0	0.05	0.05	0.01	1.
		2(*i*)													
Sn3	1(*c*)		0.6667	0.3333	0.853	0.858	0.6667	0.3333	0.853	0	0	0.05	0.05	0.01	1.

[†] As reported, z(Li6) = 0.454 giving $d_{Li6\text{-}Ca1}$ = 1.3 Å. If z(Li6) = 0.5, then $d_{Li6\text{-}Ca1}$ = 1.8 Å, $z^* = z$ and all resulting $\Delta\xi' \approx 0.01$ Å.

Table S24

Atomic positions for $YBa_2Cu_3O_{6.5}$ **(**Li *et al.*, 1989) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [68420].
$a = 5.4$, $c = 6.6$ Å, $z^* = z$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	Δxyz	*occ.*
Y,Cu3	1(*b*)		0.3333	0.6667	0.8333	0.3333	0.6667	0.8333	0	0	0	0	1. 0
		2(*d*)†											
Cu3,Y	1(*c*)		0.6667	0.3333	0.1667	0.6667	0.3333	0.1667	0	0	0	0	1.
Ba1	1(*b*)		0.3333	0.6667	0.3333	0.3333	0.6667	0.3333	0	0	0	0	1.
		2(*d*)											
Ba2	1(*c*)		0.6667	0.3333	0.6667	0.6667	0.3333	0.6667	0	0	0	0	1.
Cu1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	1.
Cu2	1(*a*)	1(*b*)	0	0	0.5	0	0	0.5	0	0	0	0	1.
O1	3(*d*)	3(*e*)	0	0.5	0	0	0.5	0	0	0	0	0	0.72
O2	3(*d*)		0.3333	0.1667	0.3333	0.3333	0.1667	0.3333	0	0	0	0	0.72
		6(*i*)											
O3	3(*d*)		0.1667	0.3333	0.6667	0.1667	0.3333	0.6667	0	0	0	0	0.72

† Site exchange between Y and Cu3 sites is noted in Li *et al.*'s (1989) text, but not in Table II.

Table S25

Modified atomic positions for BiTeI **(**Shevel′kov *et al.*, 1995) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and $u_{\rm iso}$ displacements in Å. [79364].
a = 4.3392(1), c = 6.854(1) Å, $z^* = z + 0.0187$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition													
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$u_{\rm iso}$
Bi	1(*a*)	1(*a*)	0	0	0	0.0187	0	0	0	0	0	0.13	0.13	0.12
T1	1(*c*)		0.6667	0.3333	0.6928(2)	0.7115	0.6667	0.3333	0.7209	0	0	-0.06	0.06	0.16
		2(*d*)												
I	1(*b*)		0.3333	0.6667	0.2510(2)	0.2697	0.3333	0.6667	0.2791	0	0	-0.06	0.06	0.14

Table S26

Modified atomic positions for $YH_{0.667}$ **(**Garces, *et al*., 2005) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [152861].
a = 3.6817, c = 17.4710 Å; $z^* = z - 0.01664$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
Y1	1(*a*)	1(*a*)	0.	0.	0.00389	-0.01277	0.	0.	0.	0.	0.	-0.22	0.22
Y2	1(*b*)	1(*d*)	0.3333	0.6667	0.50389	0.48723	0.3333	0.6667	0.5	0.	0.	-0.22	0.22
Y3	1(*b*)		0.3333	0.6667	0.82944	0.81278	0.3333	0.6667	0.83140	0.	0.	-0.32	0.32
		2(*h*)											
Y5	1(*b*)		0.3333	0.6667	0.16666	0.14999	0.3333	0.6667	0.16860	0.	0.	-0.33	0.33
Y4	1(*a*)		0.	0.	0.32944	0.31278	0.	0.	0.33140	0.	0.	-0.33	0.33
		2(*g*)											
Y6	1(*a*)		0.	0.	0.66666	0.64999	0.	0.	0.66860	0.	0.	-0.33	0.33
H1	1(*b*)	1(*c*)	0.3333	0.6667	0.03775	0.02109	0.3333	0.6667	0	0.	0.	0.37	0.37
H2	1(*a*)	1(*b*)	0.	0.	0.53775	0.52109	0.	0.	0.5	0.	0.	0.37	0.37
H3	1(*a*)		0.	0.	0.79558	0.77892	0.	0.	0.75	0.	0.	0.50	0.50
		2(*g*)/2(*h*)[†]											
H4	1(*b*)		0.3333	0.6667	0.29558	0.27892	0.3333	0.6667	0.25	0.	0.	0.51	0.51

[†] Both H3 and H4 assumed to occupy either the 2(*g*) or the 2(*h*) supergroup locations in the event of a phase transition.

Table S27

Modified atomic positions for $Eu_8I_9(CN)(NCN)_3$ **(**Liao & Dronskowski, 2006) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [172030].
a = 10.6132(9), c = 7.7832(9) Å; $z^* = z - 0.02713$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Eu1	3(*d*)	3(*k*)	-0.13593(4)	0.13593(4)	0.61082(9)	0.58369	-0.13593	0.13593	0.5	0.	0.	0.65	0.65	0.13
Eu2	1(*b*)	1(*d*)	0.3333	0.6667	0.5356(2)	0.5085	0.3333	0.6667	0.5	0.	0.	0.07	0.07	0.15
Eu3	3(*d*)	3(*j*)	-0.53385(4)	0.53385(4)	1.14057(12)	1.11344	-0.53385	0.53385	1.0	0.	0.	0.88	0.88	0.16
Eu4	1(*a*)	1(*a*)	0.0000	0.0000	1.21148(16)	1.18435	0.0000	0.0000	1.0	0.	0.	1.43	1.43	0.14
I1	3(*d*)	3(*j*)	0.13092(5)	-0.13092(5)	0.91033(13)	0.88320	0.13092	-0.13092	1.0	0.	0.	-0.91	0.91	0.15
I2	3(*d*)	3(*j*)	-0.20315(6)	0.20315(6)	0.21507(15)	0.18794	-0.20315	0.20315	0	0.	0.	1.46	1.25	0.17
I3	3(*d*)	3(*k*)	-0.48217(6)	0.48217(6)	0.67255(19)	0.64542	-0.48217	0.48217	0.5	0.	0.	1.13	1.13	0.19
N1	3(*d*)	3(*k*)	0.2296(7)	-0.2296(7)	0.3237(18)	0.2966	0.2296	-0.2296	0.5	0.	0.	-1.58	1.58	0.15
N2	3(*d*)	3(*k*)	0.1046(7)	-0.1046(7)	0.4414(15)	0.4143	0.1046	-0.1046	0.5	0.	0.	-0.67	0.67	0.13
N3	1(*b*)	1(*c*)	0.3333	0.6667	1.007(4)	0.980	0.3333	0.6667	1.0	0.	0.	-0.16	0.16	0.19
C1	3(*d*)	3(*k*)	0.1633(8)	-0.1633(8)	0.387(2)	0.360	0.1633	-0.1633	0.5	0.	0.	-1.09	1.09	0.13
C2	1(*b*)	1(*c*)	0.3333	0.6667	0.870(3)	0.843	0.3333	0.6667	1.0	0.	0.	-1.22	1.22	0.14

7. Entries for structures with reduced predictive properties

4.1 $CdGaInS_4$ [2465, 20785]

Photometric I_{obs}, R = 0.127, uncertainties and u_{iso} not reported (Mekhtiev *et al.,* 1977). S3 location reported at ⅓, ⅓, 0.611 inappropriate for $P3m1$ and modified by ICSD to ⅓, ⅔, 0.611. Distorted tetrahedra, $d_{Cd\text{-}S}$ = 2.48, 3×2.45; $d_{In\text{-}S}$ = 2.46, 3×2.72 and $d_{Ga\text{-}S}$ = 2.34, 3×2.37Å, agree moderately with Shannon's (1976) $d_{Cd,In,Ga\text{-}S}$ = 2.62, 2.46, 2.31 Å only for $d_{Ga\text{-}S}$. Relationships among z-coordinates are suggestive of an approach to supergroup $P\bar{6}m2$, see Table S28. Kyazimov & Amiraslanov (1983) report a = 3.869(3), c = 24.668(14) Å for the 'double-packet' $CdGaInS_4$ polytype in space group $P\bar{3}m1$, R = 0.112, $d_{Cd\text{-}S} = 6 \times 2.617$, $d_{In\text{-}S}$ = 2.437, 3×2.390, $d_{Ga\text{-}S}$ = 2.437, 3×2.390Å with $d_{Cd\text{-}S}$ notably closer to Shannon's (1972) octahedral $d_{Cd\text{-}S}$ = 2.79 Å than tetrahedral length. Structural reinvestigation of both $CdGaInS_4$ variants is appropriate.

4.2 $12H_6$-CdI_2 [6066]

Cu$K\alpha$ oscillation photography, 15 visual estimated $I(01l)$, determined in $P3m1$ with all atoms in 1-fold Wyckoff positions, n_iz coordinates with z = 1/24 for n the i-th integer between 0 and 23, ionic separations of ~1.7 Å (Chadha, 1974), see Table S29. Edge-sharing CdI_6 octahedra close to regular, with $d_{Cd\text{-}I}$ = 2.985 Å. Jain & Trigunyat (1977) suggested a centrosymmetric arrangement in space group $P\bar{3}m1$ is more likely. Table S29 shows that if I6, I8 and Cd1 each occupy Wyckoff position 1(b), with Cd5 and Cd6 in 1(c) instead of 1(b), then all original interatomic distances remain unchanged but with a resulting arrangement that exactly satisfies space group $P31c$. Further, for each atom at x_1,y_1,z_1 another exists at $x_2,y_2,-z_1$, hence this acentric space group is nonpolar. Palosz's (1980)

proposed description of 12H_6-polytypes with MX_2 composition suggests space group $R\bar{3}m$H, see also Iglesias (2006).

4.3(*a*) 24*L*-ZnS [15738]

Cu *K*α oscillation photographs, 19 visual *I*(21*l*), birefringence study (Brafman *et al.*, 1967), layer sequence taken as 7, 5, 5, 7 (Mardix *et al.*, 1967) in this 24*L* structure with c = 75.12 Å. All 24 independent Zn atom coordinates exactly satisfy the symmetry of space group $P\bar{6}m2$; each of the 24 independent S_i atoms occupy a 1-fold Wyckoff location identical to that of the *i*th Zn, with $z(S_i) = z(Zn_i)+1/32$, see Table S30(*a*). Each Zn atom consequently occupies near-regular tetrahedra of S atoms sharing corners and edges, with $d_{Zn\text{-}S} \approx 2.346$ Å. Each S atom similarly occupies a near-regular tetrahedron of Zn atoms, *cf.* §3.4. As in the latter case, further structural investigation of 24*L*-ZnS would be appropriate. The *c* axis in the ZnS polytypes ranges from 43.8 to 112.7 Å

4.3(*b*) 12*L*-ZnS [107137]

Cu *K*α, oscillation photographs, 7 visual *I*(10*l*), 4,4,2,2 sequence polytype (Kiflawi & Mardix, 1970). All $z(Zn_i)$-coordinates, also all $z'(S_i)$ coordinates where $z'(S_i) = z(S_i)$-1/48, see Table S30(*b*), together with individual changes in 3 paired sets of Zn and 4 paired sets of S in 1-fold Wyckoff locations, satisfy the symmetry of supergroup $P\bar{3}m1$. The possibility of symmetry misassignment, as in §§3.4 and 4.3(*a*), suggests a need for reexamination by modern structural refinement methods.

4.4 $Zn_{4.1}In_{1.53}S_8$ 8*H*8 [16312]

Nb-filtered Mo *K*α; 666 independent F_{obs}; uncorrected absorption and extinction; R = 0.189,

Gnehm & Niggli (1972). ZnS polytype variant, all atoms in 1-fold Wyckoff locations, nonstoichiometric composition. All Zn sites form distorted tetrahedra with $2.31 \lesssim d_{\text{Zn-S}} \lesssim 2.49$ Å, three shared with In. The In3 site, ~10% occupied, reportedly contains no Zn and forms a strongly distorted octahedron with 3 $d_{\text{In-S}} = 2.55$ and 3 at 2.77 Å; Shannon's (1976) radii give $d_{\text{Zn(IV)-S}} \approx 2.44$, $d_{\text{In(VI)-S}} \approx 2.64$ Å. Table S31 shows that, if the choice of 1-fold Wyckoff location assigned to an atom in each S4/S6, Zn4,In2/Zn5 pair were in error, then all atomic coordinates would satisfy supergroup $P\bar{3}m1$ with $\Delta\xi \lesssim 0.57$ Å and $\Delta\xi_i$ generally comparable to or smaller than $u_{\text{iso}(i)}$ for most atoms. Structural reinvestigation is hence advisable; should the pseudosymmetry indicated in Table S31 be thereby supported, the material would be a ferroelectric candidate.

4.5 K_2NaUCl_6 [20914]

Powder diffractometer, Cu $K\alpha$, 16 lines, 7 or more doubled (Aurov *et al.*, 1983). All metal atoms in locations assigned by Winkler (1954) to α-K_2LiAlF_6 structure in Table S34, with the six Cl atoms omitted as in Table S32. Placing K4 in Wyckoff position 1(*c*) and K6 in 1(*b*) instead of both in 1(*a*) locations, as indicated by the Table S32 values in italic, results in all coordinates exactly satisfying supergroup $P\bar{3}m1$ symmetry. However, the report by Graulich *et al.* (1998) that the K_2LiAlF_6 structure has a unit cell with doubled *c* axis, space group $R\bar{3}m$ and $R = 0.0453$, most likely eliminates the possibility of ferroelectricity in this material.

4.6 $KNaSO_4$ [26014]

Mineral aphthitalite, Mo$K\alpha$ diffractometry, $\mu R < 0.1$, no absorption corrections, 373 $F_{\text{obs}} >$

$3\sigma(F_{obs})$, U^{ij} for all atoms, R = 0.046, (Okada *et al.*, 1980). No atom present differs significantly from supergroup $P\bar{3}m1$ symmetry, see Table S33, with largest $\Delta\xi$ = 0.09 Å for O3 and O4 and thermal amplitudes of ~0.2 to ~0.3 Å.

4.7 I-K_2LiAlF_6 [27672]

Cu$K\alpha$ photometric powder intensities, diffuse scattering, phase transition from $R\bar{3}m$ to $P3m1$ at $T_C \approx$ 743 K; 26 independent $I(hkl)$, with structure derived in Table S34, $R \approx 0.12$ (Winkler, 1954). Except for 4 K and 4 F atoms, each with $|\Delta\xi| \approx 1.10$ Å, all other $\Delta\xi$ exactly satisfy supergroup $P\bar{3}1m$ symmetry. If the structure were correct, the criteria for ferroelectricity would be satisfied. However, Graulich *et al.* (1998) refined this high-temperature phase, with 252 independent $F_{obs} > 4\sigma(F_{obs})$ in a unit cell with doubled c axis, to R = 0.045 in space group $R\bar{3}m$, *cf.* §4.5.

4.8 $LiYMo_3O_8$ family [28525, 28526, 30579]

Cu$K\alpha$, powder diffractometer, 39 resolved $LiYMo_3O_8$ lines, 5 $LiScMo_3O_8$ lines; final $R(F^2)$ = 0.10 for $LiYMo_3O_8$; identical coordinates assumed for $LiScMo_3O_8$ (de Benedittis & Katz, 1965). McCarroll (1977) redetermined a and c for $LiYMo_3O_8$, also the six isomorphous Li$R$$Mo_3O_8$ materials with R = Sc, In, Sm, Gd, Yb and Lu, confirming the basic structure in Table S35. The coordinates for R = Y give $d_{Li\text{-}O2}$ = 1.39 Å whereas Shannon's (1976) radii give 1.99 Å. Reassigning O1 in Table S35 to Wyckoff position 1(c) instead of 1(a) results in $\Delta\xi \lesssim 0.30$ Å for all atoms, with respect to supergroup $P\bar{6}m2$ symmetry, the powder pattern remaining very close to that reported. Full structural redetermination is necessary to confirm the atomic assignment or dielectric investigation to determine whether or not

$LiYMo_3O_8$ and other members of this family are nonpolar or ferroelectric at room temperature.

4.9 β-CuI [30363, 84217, 78429, 80230]

CuI undergoes a phase transition at T_{trans} = 643(2) K from γ-CuI in $F\bar{4}3m$ to trigonal β-CuI; the latter, with space group $P\bar{3}1m$, initially coexists with CuI-IV in $R\bar{3}m$ before transforming to α-CuI in $Fm\bar{3}m$ at 673(8) K and melting at 878 K (Keen & Hull, 1995). Electron diffraction in combination with model building in space group $P3m1$, for CuI at ~385 K (most likely in the γ-phase) led to the results in Table S36(*a*), with R = 0.186 (Kurdyumova & Baranova, 1961). In contrast, Sakuma (1988) reported the structure of β-CuI in N_2 at 673 K, based on Ni-filtered CuK_α powder diffractometry and refined to R = 0.086 in $P3m1$; the departure from supergroup $P\bar{6}m2$ symmetry is $\Delta\xi \lesssim 0.9$ Å see Table S36(*b*). Keen & Hill (1994), in a high-resolution neutron powder diffraction study at 655 K, found the best fit in $P\bar{3}m1$ with Cu disordered over two sites, see Table S36(*c*). Keen & Hill's (1995) thermal dependence study of the CuI structure between 300 and 878 K confirms the formation of β-CuI at 647 K in space group $P\bar{3}m1$, see Table S36(*d*).

4.10 $BaVO_{2.5}$ [32657]

Preparation by laser heating to 2275 K; Mo$K\alpha$ diffractometry, corrections not stated, 501 $F(hkl)$, u_{ij}(Ba), B(V, O), R = 0.063 (de Beaulieu & Müller-Buschbaum, 1982). Atomic coordinates in Table S37 show all $\Delta\xi \lesssim u_{iso}$ with respect to corresponding locations in

supergroup $P\bar{3}1m$, hence $P\bar{3}1m$ is the more likely space group at the unstated, probably ambient, determination temperature.

4.11 $Na(Cu_{0.67}Fe_{0.22}Zn_{0.11})_2S_2$ [39255]

Mo$K\alpha$ diffractometry, 296 $I(hkl)$, u_{ij}, final R = 0.105 (Kaplunnik, *et al.*, 1990). An origin translation of ⅔,⅓, -0.2332, as in Table S38, results in $\Delta\xi \lesssim 0.03$ Å for all atoms, with respect to supergroup $P\bar{3}m1$ symmetry. Bond lengths are not changed thereby, the resulting powder pattern remaining identical with that for the structure reported except all $I(hkl)$ are transformed to $I(khl)$. The structure hence most likely exhibits inversion symmetry.

4.12 $Cr_{0.68}Se$–T' [42703]

Chemical transport; Cu$K\alpha_1$ powder photography; T'-phase "conveniently but not exclusively described in space group $P3m1$" (Wehmeier *et al*., 1970). Table S39 shows that $Cr_{0.68}Se$ satisfies supergroup $P\bar{3}m1$ symmetry exactly with one 1(a) site fully and the other 1(a) site 36% occupied by Cr. The T'-phase is one of six known Cr_xSe phases.

4.13 Ferrihydrite - $Fe_{10}O_{14}(OH)_2$ [56287, unlisted]

Co$K\alpha$, graphite monochromator, powder diffraction, low-resolution pattern, two broad maxima, 15 lines extracted. Coordinates proposed in Table S40 (Eggleton & Fitzpatrick, 1988) yield $d_{Fe1\text{-}Fe2} = d_{Fe3\text{-}Fe4} = 0.47$ Å with all other bonded $d_{Fe\text{-}Fe} < 1.90$ Å; if Fe3 and Fe6 were in Wyckoff 1(c) locations instead of 1(a) as reported, then all atoms would satisfy the symmetry of supergroup $P\bar{3}m1$ with $\Delta\xi_{max} \lesssim 0.31$ Å. Recent modelling of the pair

distribution function (Michel *et al.*, 2007) by direct Fourier transformation of the total X-ray scattering shows 20% of the Fe atoms to be tetrahedrally, 80% octahedrally, coordinated in a unit cell with double the *a*-axis in Table S40 and space group $P6_3mc$.

4.14 $CoGaInS_4$ [86413,86414, 69015]

CVD preparation at 1135 K, (*a*) Mo*K*α diffractometer, 589 independent $I_{obs} > 3\sigma(I_{obs})$, absorption corrections, B^j_{iso}, disordered metal site occupancies, best model in $P3m1$, R = 0.053, wR = 0.087; (*b*) neutron powder diffractometer, 190 independent I_{obs} (σ not given), wR = 0.044, $P3m1$ (Depero *et al.*, 1991). Application of a ⅓,⅔,0 origin translation to the X-ray coordinates in Table S41(*a*), also to the neutron coordinates in Table S41(*b*), changes no interatomic distances but reveals all atomic locations as no further than 0.02 or 0.14 Å respectively from satisfying the symmetry of space group $P\bar{3}1m$. Since $u_{iso} \approx 0.14$ Å, the space group used by Depero *et al.* (1991) is hence most likely misassigned. An earlier Mo*K*α diffractometer study by Haeuseler *et al.*, (1990), with ψ-scan absorption corrections, 652 independent $F_{obs} \geqslant 2\sigma(F_{obs})$, u^j_{11}, u^j_{33} and a different origin gave R = 0.051 in space group $P3m1$ with R = 0.030, wR = 0.036 in $P\bar{3}1m$, see Table S41(*c*).

4.15 $LaNdO_{1.75}S$ [86550]

Mo*K*α diffractometer, 230 independent I_{obs}, R = 0.065 (Kuz'micheva *et al.*, 1980). All atoms in Table S42 clearly satisfy the symmetry of supergroup $P\bar{3}1m$ within $\Delta\xi \lesssim 0.12$ Å, assuming equal occupation of the La and Nd sites by both atoms. The $\Delta\xi$ displacements are comparable with the reported u_{iso} thermal displacement magnitudes and the scattering

difference between ordered and disordered metal atoms in the 1(*b*) and 1(*c*) sites is probably below experimental detectability, hence the space group at room temperature has most likely been misassigned. Further structural investigation is advisable.

4.16 $Cs_3Sb_2I_9$ [89694, 89695]

Mo*K*α diffractometry, 246 independent $I_{obs} \geqslant 3\sigma(I_{obs})$ at 283 K, absorption corrections, B^{ij}, refinement in $P\bar{3}1m$ gave R = 0.059 *vs.* 0.054 in $P31m$, a choice termed ambiguous (Arakcheeva *et al.*, 1999). The absence of second harmonic generation (SHG) favored $P\bar{3}1m$ at 0.98 probability. Structural results in $P31m$, see Table S43 confirm the symmetry of supergroup $P\bar{3}1m$ is satisfied by all atoms, with $\Delta\xi_{max} \lesssim 0.18$ Å and each $\Delta\xi$ less than its atomic thermal displacement. $P\bar{3}1m$ symmetry is thus expected, thermally, to be more stable in agreement with the observation of zero SHG, hence $P31m$ may be eliminated.

4.17 $Ba(Fe_{0.5}Ta_{0.5})O_3$ [99484]

Fe*K*α powder diffractometry, 2θ range 24-156°, non-cubic from Mössbauer spectra, R_p = 0.045, R_{wp} = 0.061 (Li *et al.*, 2004). The structure, determined in space group $P3m1$, is reported as related to the end member in cubic $Pm\bar{3}m$; comparable fits were also found in rhombohedral space groups. The final coordinates, see Table S44, exactly fit $P3c1$ within the experimental accuracy but which was not investigated; the symmetry of supergroup $P\bar{3}c1$ is also satisfied, with $\Delta\xi_{max} \lesssim 0.10$ Å. The atomic thermal displacements were not reported but, with u_{iso} comparable to the probable $\Delta\xi_{max}$ magnitudes, the room temperature space group is most likely misassigned. Further structural investigation, including the polarity of $Ba(Fe_{0.5}Ta_{0.5})O_3$ or otherwise, is advisable before making other deductions.

4.18 AlCuMg [109103]

Preparation at 975 K; photometered Cu$K\alpha$ precession photographs; atomic coordinates not explicit, ICSD values in Table S45; agreement indicators not given, stacking faults formed primary interest (Komura, 1962). All 10 Al,Cu sites are equally shared, each with 6 Al,Cu neighbors at 2.57 Å and 6 Mg at 3.02 Å; each of the 10 Mg sites has 12 nearest Al,Cu neighbors at 3.02 Å.. The *z*-coordinates in Table S45 are nonpolar, each atomic +*z* value corresponding to an equivalent atom with a 1-*z* coordinate, of which 12 atoms *exactly* satisfy $P\bar{6}\,m2$ symmetry. The Wyckoff *x, y* locations originally assigned to the remaining 4 pairs of atoms differ widely from such symmetry. If these four of the total 20 independent atoms in AlCuMg verifiably depart from supergroup symmetry, such symmetry would not be expected. A full structural redetermination is necessary to clarify the properties of AlCuMg.

4.19(*a*) $CeCuSnD_{0.33}$ family [152855]

Neutron powder diffractometry, λ = 1.470 Å; SRPXD, λ = 0.50000 Å; combined ND and XRD Rietveld analysis, U_{iso}, R_p = 0.0638, Rw_p = 0.141 (Maehlen *et al.*, 2005). The largest departure from supergroup $P\bar{3}\,1m$ symmetry by any atom is $\Delta\xi$(Ce) ≈ 0.26 Å, see Table S46(*a*), assuming both Cu and both Sn sites are each equally occupied as in isostructural $CuLaSnD_{0.47}$, see §S46(*b*), also that an undetected D2 site exists with occupancy identical to that of the D1 site. The criteria for ferroelectricity in $CeCuSnD_{0.33}$, with u_{iso} ≈ 0.10 Å for Ce, Cu and Sn, $\Delta\xi$(Cu) = 0.26 Å and $\sigma[\Delta\xi(Cu)]$ ≈ 0.02 Å, would then be satisfied. However, although $d_{Ce1\text{-}D2} = d_{Ce1\text{-}D1}$ = 2.62 Å is satisfactory, the short $d_{Sn1\text{-}Cu1}$ = 0.17 Å and $d_{Sn2\text{-}Cu2}$ = 0.61 Å place the determination, hence any resulting predictions, in question.

4.19(*b*) $CuLaSnD_{0.47}$ [152857]

Experimental procedures as in §2.47(*a*) with R_p = 0.1053, Rw_p = 0.1483 (Maehlen *et al.,* 2005). The largest departure from supergroup $P\bar{3}1m$ symmetry by any atom in isostructural $CuLaSnD_{0.47}$, assuming an undetected D2 site with ~23% atom occupancy, is 0.06 Å by Cu with u_{iso}(Cu) ≈ 0.08 Å, see Table S46(*b*). With all other $\Delta\xi_i < u_{iso(i)}$, the structure at ambient temperature does not differ significantly from $P\bar{3}1m$ symmetry. The short $d_{Sn1\text{-}Cu1}$ = 0.34 Å and $d_{Sn2\text{-}Cu2}$ = 0.44 Å here, as in §S46(*a*), suggests further structural investigation before any property predictions are made.

4.20 Ni_2H [201088]

Electron diffraction investigation, ~30 photometrically measured $F(h0l)$, R = 0.145 Khodyrev *et al.* (1978). All three independent atoms in Ni_2H are located within 0.01 Å of positions consistent with supergroup $P\bar{3}1m$ symmetry and $u_{iso} \gg \Delta\xi$ for each atom, see Table S47. The space group is hence most likely misassigned.

8. Tabular data for structures with reduced predictive properties

Table S28

Modified atomic positions for $CdGaInS_4$ **(**Mekhtiev *et al.*, 1977) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [2465].
$a = 3.915(5)$, $c = 12.725(5)$, $z^* = z - 0.015$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wyckoff position		x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
	$P3m1$	$P\bar{6}m2$[†]											
Cd	1(*a*)	1(*b*)	0	0	0.537	0.522	0	0	0.5	0	0	0.28	0.28
In	1(*b*)		0.3333	0.6667	0.804	0.789	0.3333	0.6667	0.759	0	0	0.38	0.38
		2(*h*)											
Ga	1(*b*)		0.3333	0.6667	0.286	0.271	0.3333	0.6667	0.241	0	0	0.38	0.38
S1	1(*b*)		0.3333	0.6667	0.102	0.087	0.3333	0.6667	0.246	0	0	-0.04	0.04
		2(*h*)/2(*i*)											
S4	1(*c*)		0.6667	0.3333	0.923	0.908	0.6667	0.3333	1	0	0	-0.03	0.03
S2	1(*a*)		0	0	0.342	0.327	0	0	0.0	0	0	-0.49	0.50
		2(*g*)/2(*h*)											
S3	1(*b*)[†]		0.3333	0.3333	0.611	0.596	0.3333	0.6667	0.754	0	0	-0.49	0.48

[†] The coordinates reported for In and Ga are consistent with supergroup $P\bar{6}m2$, those for S1 and S4 with supergroup $P\bar{3}m1$ and those for S2 and S3 with neither. A different choice of Wyckoff position for one S in both such pairs of atoms would result in an approach to the symmetry of $P\bar{6}m2$.

Table S29 $16H_6$-CdI_2

Modified atomic positions for $CdGaInS_4$ **(**Chadha, 1974) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [6066].
$a = 4.24$, $c = 41.010$ Å, $z^* = z`$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position												
	*P*3*m*1	*P*31*c*	*x*	*y*	*z*	*x′*	*y′*	*z′*	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{iso}
I1	1(*a*)		0	0	0	0	0	0	0	0	0	0	n/a
		2(*a*)											
I3	1(*b*)		0	0	0.5	0	0	0.5	0	0	0	0	n/a
I2	1(*a*)		0	0	0.3333	0	0	0.3333	0	0	0	0	n/a
		2(*a*)											
I5	1(*a*)		0	0	0.8333	0	0	0.8333	0	0	0	0	n/a
I4	1(*a*)		0	0	0.6667	0	0	0.6667	0	0	0	0	n/a
		2(*a*)†											
111	1(*c*)		*0.*	*0.*	0.16667	*0.*	*0.*	0.16667	0	0	0	0	n/a
I6	1(*b*)		*0.3333*	*0.6667*	0.0833	*0.3333*	*0.6667*	0.0833	0	0	0	0	n/a
		2(*b*)†											
I9	1(*c*)		0.6667	0.3333	0.5833	0.6667	0.3333	0.5833	0	0	0	0	n/a
I8	1(*b*)		*0.3333*	*0.6667*	0.4167	*0.3333*	*0.6667*	0.4167	0	0	0	0	n/a
		2(*b*)†											
I10	1(*c*)		0.6667	0.3333	0.9167	0.6667	0.3333	0.9167	0	0	0	0	n/a
I7	1(*c*)		0.6667	0.3333	0.25	0.6667	0.3333	0.25	0	0	0	0	n/a
		2(*b*)											
I12	1(*b*)		0.3333	0.6667	0.75	0.3333	0.6667	0.75	0	0	0	0	n/a
Cd1	1(*b*)		*0.3333*	*0.6667*	0.20833	*0.3333*	*0.6667*	0.20833	0	0	0	0	n/a
		2(*b*)†											
Cd2	1(*c*)		0.6667	0.3333	0.70833	0.6667	0.3333	0.70833	0	0	0	0	n/a
Cd3	1(*b*)		0.3333	0.6667	0.04167	0.3333	0.6667	0.04167	0	0	0	0	n/a
		2(*b*)†											
Cd5	1(*c*)		*0.6667*	*0.3333*	0.54167	*0.6667*	*0.3333*	0.54167	0	0	0	0	n/a
Cd4	1(*b*)		0.3333	0.6667	0.3750	0.3333	0.6667	0.3750	0	0	0	0	n/a
		2(*b*)†											
Cd6	1(*c*)		*0.6667*	*0.3333*	0.8750	*0.6667*	*0.3333*	0.8750	0	0	0	0	n/a

† 1-fold Wyckoff positions changed from those reported, with no change in interatomic distances, are in italic.

Table S30(*a*)

Modified atomic positions for 24*L*-ZnS **(**Mardix *et al*., 1967) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [15738].
$a = 3.82$, $c = 75.12$ Å. Each $z(S_i) = z(Zn_i) + 1/32$, $z^* = z$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position												
	$P3m1$	$P\bar{6}m2$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Zn1	1(*a*)	1(*a*)	0.0	0.0	0.0	0.0	0.0	0.0	0	0	0	0	n/a
Zn2	1(*b*)		0.3333	0.6667	0.04167	0.3333	0.6667	0.04167	0	0	0	0	n/a
		2(*h*)											
Zn24	1(*b*)		0.3333	0.6667	0.95833	0.3333	0.6667	0.95833	0	0	0	0	n/a
Zn3	1(*c*)		0.6667	0.3333	0.08333	0.6666	0.3333	0.0833	0	0	0	0	n/a
		2(*i*)											
Zn23	1(*c*)		0.6666	0.3333	0.91667	0.6667	0.3333	0.9166	0	0	0	0	n/a
Zn4	1(*a*)		0.0	0.0	0.12500	0.0	0.0	0.125	0	0	0	0	n/a
		2(*g*)											
Zn22	1(*a*)		0.0	0.0	0.8750	0.0	0.0	0.875	0	0	0	0	n/a
Zn5	1(*b*)		0.3333	0.6667	0.16667	0.3333	0.6667	0.16667	0	0	0	0	n/a
		2(*h*)											
Zn21	1(*b*)		0.3333	0.6667	0.83333	0.3333	0.6667	0.83333	0	0	0	0	n/a
Zn6	1(*c*)		0.6667	0.3333	0.20833	0.6667	0.3333	0.20833	0	0	0	0	n/a
		2(*i*)											
Zn20	1(*c*)		0.6666	0.3333	0.79167	0.6666	0.3333	0.79167	0	0	0	0	n/a
Zn7	1(*a*)		0.0	0.0	0.25000	0.0	0.0	0.25	0	0	0	0	n/a
		2(*g*)											
Zn19	1(*a*)		0.0	0.0	0.75000	0.0	0.0	0.75	0	0	0	0	n/a
Zn8	1(*b*)		0.3333	0.6667	0.29167	0.3333	0.6667	0.29167	0	0	0	0	n/a
		2(*h*)											
Zn18	1(*b*)		0.3333	0.6667	0.70833	0.3333	0.6667	0.70833	0	0	0	0	n/a
Zn9	1(*a*)		0.0	0.0	0.33333	0.0	0.0	0.3333	0	0	0	0	n/a
		2(*g*)											
Zn17	1(*a*)		0.0	0.0	0.66667	0.0	0.0	0.6666	0	0	0	0	n/a
Zn10	1(*c*)		0.6667	0.3333	0.37500	0.6666	0.3332	0.375	0	0	0	0	n/a
		2(*i*)											
Zn16	1(*c*)		0.6666	0.3333	0.62500	0.6667	0.3334	0.625	0	0	0	0	n/a
Zn11	1(*b*)		0.3333	0.6667	0.41667	0.3333	0.6667	0.4166	0	0	0	0	n/a
		2(*h*)											
Zn15	1(*b*)		0.3333	0.6667	0.58333	0.3333	0.6667	0.5833	0	0	0	0	n/a
Zn12	1(*a*)		0.0	0.0	0.45833	0.0	0.0	0.4583	0	0	0	0	n/a
		2(*g*)											
Zn14	1(*a*)		0.0	0.0	0.54167	0.0	0.0	0.5416	0	0	0	0	n/a
Zn13	1(c)	1(*f*)	0.6666	0.3333	0.5	0.6666	0.3333	0.5	0	0	0	0	n/a
S1	1(*a*)	1(*a*)	0	0	0.03125	0	0	0.0	0	0	0	0	n/a
S2	1(*b*)		0.3333	0.6667	0.07292	0.3333	0.6667	0.04167	0	0	0	0	n/a
		2(*h*)											
S24	1(*b*)		0.3333	0.6667	0.98958	0.3333	0.6667	0.95833	0	0	0	0	n/a
S3	1(*c*)		0.6667	0.3333	0.11458	0.6667	0.3333	0.08333	0	0	0	0	n/a
		2(*i*)											
S23	1(*c*)		0.6667	0.3333	0.94792	0.6667	0.3333	0.91667	0	0	0	0	n/a
S4	1(*a*)		0	0	0.15625	0	0	0.12500	0	0	0	0	n/a
		2(*g*)											
S22	1(*a*)		0	0	0.90625	0	0	0.87500	0	0	0	0	n/a

S5	1(*b*)		0.3333	0.6667	0.19792	0.3333	0.6667	0.166670	0	0	0	n/a
		2(*h*)										
S21	1(*b*)		0.3333	0.6667	0.86458	0.3333	0.6667	0.8333 0	0	0	0	n/a
S6	1(*c*)		0.6667	0.3333	0.22395	0.6667	0.3333	0.208330	0	0	0	n/a
		2(*i*)										
S20	1(*c*)		0.6667	0.3333	0.82292	0.6667	0.3333	0.791670	0	0	0	n/a
S7	1(*a*)		0	0	0.28125	0	0	0.2500 0	0	0	0	n/a
		2(*g*)										
S19	1(*a*)		0	0	0.78125	0	0	0.750000	0	0	0	n/a
S8	1(*b*)		0.3333	0.6667	0.32292	0.3333	0.6667	0.291670	0	0	0	n/a
		2(*h*)										
S18	1(*b*)		0.3333	0.6667	0.73958	0.3333	0.6667	0.708330	0	0	0	n/a
S9	1(*a*)		0	0	0.36458	0	0	0.333330	0	0	0	n/a
		2(*g*)										
S17	1(*a*)		0	0	0.69792	0	0	0.666670	0	0	0	n/a
S10	1(*c*)		0.6667	0.3333	0.40625	0.6667	0.3333	0.375000	0	0	0	n/a
		2(*i*)										
S16	1(*c*)		0.6667	0.3333	0.65625	0.6667	0.3333	0.625000	0	0	0	n/a
S11	1(*b*)		0.3333	0.6667	0.44792	0.3333	0.6667	0.416670	0	0	0	n/a
		2(*h*)										
S15	1(*b*)		0.3333	0.6667	0.61458	0.3333	0.6667	0.583330	0	0	0	n/a
S12	1(*a*)		0	0	0.48958	0	0	0.458330	0	0	0	n/a
		2(*g*)										
S14	1(*a*)		0	0	0.57292	0	0	0.541670	0	0	0	n/a
S13	1(*c*)	1(*f*)	0.6667	0.3333	0.53125	0.6667	0.3333	0.500000	0	0	0	n/a

Table S30(*b*)

Modified atomic positions for 12*L*-ZnS **(**Kiflawi & Mardix, 1970) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [107137].
a = 3.823, c = 37.488 Å. All reported z(S) replaced by z(S) – 1/48, $z^* = z$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Zn1	1(*a*)	1(*a*)	0.0	0.0	0.0	-0.1667	0.1667	0.0	0	0	0	0	n/a
Zn4	1(*a*)		0	0	0.25	0	0	0.25	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
Zn10	1(*b*)		0.3333	0.6667	0.75	0.3333	0.6667	0.75	0	0	0	0	
Zn2	1(*b*)		0.3333	0.6667	0.0833	0.3333	0.6667	0.0833	0	0	0	0	n/a
		2(*d*)											
Zn12†	1(*c*)		0.6667	0.3333	0.9167	0.6667	0.3333	0.9167	0	0	0	0	
Zn6	1(*b*)		0.3333	0.6667	0.4167	0.3333	0.6667	0.4167	0	0	0	0	n/a
		2(*d*)											
Zn8	1(*c*)		0.6667	0.3333	0.5833	0.6667	0.3333	0.5833	0	0	0	0	
Zn3	1(*c*)		0.6667	0.3333	0.1667	0.6667	0.3333	0.1667	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
Zn11	1(*a*)		0.0	0.0	0.8333	0.0	0.0	0.8333	0	0	0	0	
Zn5	1(*c*)		0.6667	0.3333	0.3333	0.6667	0.3333	0.3333	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
Zn9	1(*a*)		0.0	0.0	0.6667	0.0	0.0	0.6667	0	0	0	0	
Zn7	1(*a*)	1(*b*)	0.0	0.0	0.5	0.0	0.0	0.5	0	0	0	0	n/a
S1	1(*a*)		0.0	0.0	0.0417	0.0	0.0	0.0416	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
S12	1(*c*)		0.6667	0.3333	0.9584	0.6667	0.3333	0.9584	0	0	0	0	n/a
S4	1(*a*)		0.0	0.0	0.2917	0.0	0.0	0.2916	0	0	0	0	n/a
		2(g)											
S9	1(*a*)		0.0	0.0	0.7084	0.0	0.0	0.7084	0	0	0	0	n/a
S2	1(*b*)		0.3333	0.6667	0.1250	0.3333	0.6667	0.1250	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
S11	1(*a*)		0.0	0.0	0.8750	0.0	0.0	0.8750	0	0	0	0	
S6	1(*b*)		0.3333	0.6667	0.4584	0.3333	0.6667	0.4584	0	0	0	0	n/a
		2(*c*)/2(*d*)‡											
S7	1(*a*)		0.0	0.0	0.5417	0.0	0.0	0.5416	0	0	0	0	n/a
S3	1(*b*)		0.6667	0.3333	0.2084	0.6667	0.3333	0.2084	0	0	0	0	n/a
		2(*d*)											
S10	1(*b*)		0.3333	0.6667	0.7917	0.3333	0.6667	0.7916	0	0	0	0	n/a
S5	1(*c*)		0.6667	0.3333	0.3750	0.6667	0.3333	0.3750	0	0	0	0	n/a
		2(*d*) ‡											
S8	1(*c*)		0.6667	0.3333	0.6250	0.6667	0.3333	0.6250	0	0	0	0	n/a

‡ At least one set of coordinates reported for each such pair of atoms is assigned to an inappropriate 1-fold Wyckoff position with respect to the proposed supergroup, leading to the given choice of 2-fold Wyckoff positions.

† z[Zn12] assumed = 0.9169 instead of reported 0.8169; Wyckoff position corrections assumed for the three Zn4,Zn10; Zn3,Zn11 and Zn5,Zn9 pairs, also the four S1,S12; S2,S11; S6,S7 and S5,S8 pairs

Table S31

Modified atomic positions for 8H8-$In_{1.53}Zn_{4.10}S_8$ **(**Gnehm & Niggli, 1972) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [16312].
$a = 3.857(2)$, $c = 24.961(15)$ Å, $z^* = z + 0.00488$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition														
	$P3m$ 1	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	occ	u_{iso}
S1	1(a)	1(*a*)	0.0	0.0	0	0.005	0.0	0.0	0.0	0.0	0.0	0.12	0.12	1	0.12
S2	1(c)		0.6666	0.3333	0.125(1)	0.130	0.6666	0.3333	0.123	0.0	0.0	0.17	0.17	1	0.09
		2(*d*)													
S8	1(b)		0.3333	0.6666	0.879(1)	0.884	0.3333	0.6666	0.877	0.0	0.0	0.17	0.17	1	0.12
S3	1(a)		0.0	0.0	0.251(1)	0.256	0.0	0.0	0.258	0.0	0.0	-0.04	0.04	1	0.04
		2(*c*)													
S7	1(a)		0.0	0.0	0.736(1)	0.741	0.0	0.0	0.742	0.0	0.0	-0.03	0.03	1	0.04
S4	1(c)		0.6667	0.3333	0.378(1)	0.383	0.6666	0.3333	0.379	0.0	0.0	0.10	0.10	1	0.04
		2(*d*)†													
S6	1(c)		0.6666	0.3333	0.620(1)	0.625	0.6667	0.3333	0.621	0.0	0.0	0.10	0.10	1	0.04
S5	1(a)	1(*b*)	0.0	0.0	0.5042(6)	0.5091	0.0	0.0	0.50	0.0	0.0	0.23	0.23	1	0.00
Zn1	1(c)		0.6667	0.3333	0.035(2)	0.040	0.6667	0.3333	0.030	0.0	0.0	0.25	0.25	0.5	0.22
		2(*d*)													
Zn7	1(b)		0.3333	0.6666	0.975(1)	0.980	0.3333	0.6666	0.970	0.0	0.0	0.25	0.25	0.6	0.15
Zn2/In1	1(a)		0.0	0.0	0.156(1)	0.161	0.0	0.0	0.161	0.0	0.0	0.00	0.00	0.6,0.4	0.04
		2(*c*)													
Zn6/In4	1(a)		0.0	0.0	0.834(1)	0.839	0.0	0.0	0.839	0.0	0.0	0.00	0.00	0.6,0.4	0.0
Zn3	1(c)		0.6667	0.3333	0.2864(5)	0.2913	0.6667	0.3333	0.3001	0.0	0.0	-0.22	0.22	1	0.10
		2(*d*)													
In3	1(b)		0.3333	0.6666	0.6862(5)	0.6911	0.3333	0.6666	0.6999	0.0	0.0	-0.22	0.22	0.09	0.14
Zn4/In2	1(a)		0.0	0.0	0.410(2)	0.415	0.0	0.0	0.438	0.0	0.0	-0.57	0.57	0.4.0.6	0.09
		2(*c*)/2(*d*)†													
Zn5	1(c)		0.6667	0.3333	0.534(1)	0.539	0.6667	0.3333	0.562	0.0	0.0	-0.57	0.57	0.5	0.20

† At least one set of coordinates reported for the Sn4,S6 and Zn4/In2,Zn5 pairs was assigned to a 1-fold Wyckoff position that is inappropriate for the proposed supergroup..

Table S32

Modified atomic positions for K_2NaUCl_6 **(**Aurov *et al.*, 1983) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [20914].
a = 7.28(1), c = 17.79(2) Å, $z^* = z$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff	Position										
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
U1	1(*a*)	1(*a*)	0	0	0	0	0	0	0.	0.	0.	0.	n/a
U2	1(*b*)		0.3333	0.6667	0.3333	0.3333	0.6667	0.3333	0.	0.	0.	0.	n/a
		2(*d*)											
U3	1(*c*)		0.6667	0.3333	0.6667	0.6667	0.3333	0.6667	0.	0.	0.	0.	n/a
Na1	1(*a*)	1(*b*)	0	0	0.5	0	0	0.5	0.	0.	0.	0.	n/a
Na2	1(*b*)		0.3333	0.6667	0.8333	0.3333	0.6667	0.8333	0.	0.	0.	0.	n/a
		2(*d*)											
Na3	1(*c*)		0.6667	0.3333	0.1667	0.6667	0.3333	0.1667	0.	0.	0.	0.	n/a
K1	1(*c*)		0.6667	0.3333	0.9167	0.6667	0.3333	0.9167	0.	0.	0.	0.	n/a
		2(*d*)											
K2	1(*b*)		0.3333	0.6667	0.0833	0.3333	0.6667	0.0833	0.	0.	0.	0.	n/a
K3	1(*c*)		0.6667	0.3333	0.25	0.6667	0.3333	0.25	0.	0.	0.	0.	n/a
		2(*d*)†											
K6	1(*a*)		*0.3333*	*0.6667*	0.75	*0.3333*	*0.6667*	0.75	0.	0.	0.	0.	n/a
K4	1(*a*)		*0.6667*	*0.3333*	0.4167	*0.6667*	*0.3333*	0.4167	0.	0.	0.	0.	n/a
		2(*d*)†											
K5	1(*b*)		0.3333	0.6667	0.5833	0.3333	0.6667	0.5833	0.	0.	0.	0.	n/a

† The reported 1(*a*) Wyckoff locations for K6 and K4 are replaced here by the values in italic.

Table S33

Modified atomic positions for $KNaSO_4$ **(**Okada *et al.*, 1980) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [26014].
a = 5.607(1), c = 7.177(1) Å. z^* = z ; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	0.14
Na1	1(*a*)	1(*b*)	0	0	0.504(3)	0	0	0.5	0	0	0.03	0.03	0.16
Na2	1(*c*)		0.6667	0.3333	0.689(2)	0.6667	0.3333	0.690	0	0	-0.01	0.01	0.10
		2(*d*)											
K2	1(*b*)		0.3333	0.6667	0.309(2)	0.3333	0.6667	0.310	0	0	-0.01	0.01	0.20
S1	1(*c*)		0.6667	0.3333	0.234(1)	0.6667	0.3333	0.235	0	0	-0.01	0.01	0.15
		2(*d*)											0.13
S2	1(*b*)		0.3333	0.6667	0.764(1)	0.3333	0.6667	0.765	0	0	-0.01	0.01	0.13
O1	1(*c*)		0.6667	0.3333	0.026(2)	0.6667	0.3333	0.036	0	0	-0.07	0.07	0.10
		2(*d*)											
O2	1(*b*)		0.3333	0.6667	0.955(4)	0.3333	0.6667	0.964	0	0	-0.06	0.06	0.17
O3	3(*d*)		0.187(1)	0.813	0.710(2)	0.192	0.808	0.698	0	0	0.09	0.09	0.21
		6(*i*)											
O4	3(*d*)		0.803(1)	0.197	0.314(2)	0.808	0.192	0.302	0	0	0.09	0.09	0.28

Table S34

Modified atomic positions for I-K_2LiAlF_6 (Winkler, 1954) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [27672].
a = 5.6145(10), c = 13.754(10) Å. $z^* = z$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
K1	1(*c*)		0.6667	0.3333	-0.08(1)	0.6667	0.3333	-0.08	0	0	0	0	n/a
		2(*d*)											
K2	1(*b*)		0.3333	0.6667	0.08(1)	0.3333	0.6667	0.08	0	0	0	0	n/a
K3	1(*c*)		0.6667	0.3333	0.253(10)	0.6667	0.3333	0.333	0	0	-1.10	1.10	n/a
		2(*d*)											
K5	1(*b*)		0.3333	0.6667	0.587(10)	0.3333	0.6667	0.667	0	0	-1.10	1.10	n/a
K4	1(*a*)		0	0	0.413(10)	0	0	0.333	0	0	1.10	1.10	n/a
		2(*c*)											
K6	1(*a*)		0	0	0.747(10)	0	0	0.667	0	0	1.10	1.10	n/a
Al1	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	n/a
Al2	1(*b*)		0.3333	0.6667	0.3333	0.3333	0.6667	0.3333	0	0	0	0	n/a
		2(*d*)											
Al3	1(*c*)		0.6667	0.3333	0.6667	0.6667	0.3333	0.6667	0	0	0	0	n/a
F1	3(*d*)		0.158(20)	-0.158(20)	-0.08(1)	0.158	-0.158	-0.081	0	0	0	0	n/a
		6(*i*)											
F2	3(*d*)		-0.158(20)	0.158(20)	0.08(1)	-0.158	0.158	0.081	0	0	0	0	n/a
F5	3(*d*)		0.825(20)	0.175(20)	0.587(10)	0.825	0.175	0.667	0	0	-1.10	1.10	n/a
		6(*i*)											
F3	3(*d*)		0.175(20)	0.825	0.253(10)	0.175	0.825	0.333	0	0	-1.10	1.10	n/a
F4	3(*d*)		0.491(20)	0.509(20)	0.413(10)	0.491	0.509	0.333	0	0	1.10	1.10	n/a
		6(*i*)											
F6	3(*d*)		0.509(20)	0.491(20)	0.747(10)	0.509	0.491	0.667	0	0	1.10	1.10	n/a
Li1	1(*a*)†		*0.6667*	*0.3333*	0.1667	*0.6667*	*0.3333*	0.1667	0	0	0	0	n/a
		2(*d*)											
Li3	1(*b*)		0.3333	0.6667	0.8333	0.3333	0.6667	0.8333	0	0	0	0	n/a
Li2	1(*c*)†	1(*b*)	*0*	*0*	0.5	*0*	*0*	0.5	0	0	0	0	n/a

† Wyckoff 1(*a*) position is inconsistent with $P\bar{3}m1$ symmetry, hence replaced by coordinates in italic corresponding to the 1(*c*) position; that in 1(*c*) is also inconsistent, hence replaced in italic to correspond to the 1(*a*) position in $P3m1$ and the 1(*b*) position in $P\bar{3}m1$.

Table S35

Modified atomic positions for $LiYMo_3O_8$[‡] (de Benedittis & Katz, 1965) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [28525].
$a = 5.73$, $c = 4.94$ Å, $z^* = z - 0.243$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition													
	$P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li	1(*c*)	1(*f*)	0.6667	0.3333	0.714(87)	0.471	0.6667	0.3333	0.5	0	0	-0.14	0.14	n/a
Y	1(*b*)	1(*d*)	0.3333	0.6667	0.720(2)	0.477	0.3333	0.6667	0.5	0	0	-0.11	0.11	n/a
Mo	3(*j*)	3(*j*)	0.8534(4)	0.1466(4)	0.25	0.007	0.8534	0.1466	0.0	0	0	0.03	0.03	n/a
O1	1(*c*)[†]		*0.6667*	*0.3333*	0.495(32)	0.252	*0.6667*	*0.3333*	0.250	0	0	0.01	0.01	n/a
		2(*i*)												
O2	1(*c*)		0.6667	0.3333	-0.005(28)	-0.248	0.6667	0.3333	-0.250	0	0	0.01	0.01	n/a
O3	3(*d*)	3(*k*)	0.498(10)	0.502(10)	0.464(16)	0.221	0.498	0.502	0.5	0	0	-0.18	0.18	n/a
O4	3(*d*)	3(*j*)	0.167(9)	0.833(9)	0.062(13)	-0.181	0.167	0.833	0.0	0	0	0.30	0.30	n/a

[†] O1 in italic assumed in Wyckoff position 1(*c*) instead of 1(*a*) as reported. Li may be in error, with $d_{Li\text{-}O2} = 1.39$ Å.

[‡] The coordinates for $LiInMo_3O_8$ are closely comparable with those of $LiYMo_3O_8$ (McCarroll, 1977).

Table S36(*a*)

Atomic positions for probable γ phase CuI at 373-393 K (Kurdyumova & Baranova, 1961) [30363].

a = 4.25(1), c = 20.86(6) Å

	Wykoff $P3m1$	x	y	z		Wykoff $P3m1$	x	y	z
Cu1	1(*b*)	0.3333	0.6667	0.04167	I1	1(*a*)	0	0	0
Cu2	1(*a*)	0	0	0.125	I2	1(*b*)	0.3333	0.6667	0.1667
Cu3	1(*b*)	0.3333	0.6667	0.375	I3	1(*a*)	0	0	0.3333
Cu4	1(*a*)	0	0	0.4583	I4	1(*b*)	0.3333	0.6667	0.5
Cu5	1(*c*)	0.6667	0.3333	0.7083	I5	1(*a*)	0	0	0.6667
Cu6	1(*a*)	0	0	0.7917	I6	1(*c*)	0.6667	0.3333	0.8333

TableS36(*b*)

Modified atomic positions for β-CuI at 675 K (Sakuma, 1988) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [84217]

a = 4.279(2), c = 7.168(7) Å; $z^* = z - 0.008$.; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition $P3m1$	$P\bar{6}m2$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cu1	1(*a*)	1(*b*)	0	0	0.636(47)	0.628	0	0	0.5	0	0	0.92	0.92	0.44
Cu2	1(*b*)	1(*c*)	0.3333	0.6667	0.896(47)	0.888	0.3333	0.6667	1.0	0	0	-0.80	0.80	0.44
I1	1(*a*)	1(*a*)	0	0	0	-0.008	0	0	0	0	0	-0.06	0.06	0.23
I2	1(*b*)	1(*d*)	0.3333	0.6667	0.5	0.492	0.3333	0.6667	0.5	0	0	-0.06	0.06	0.23

Table S36(*c*)

Atomic positions for β-CuI at 655 K (Keen & Hull, 1994) [78429]

a = 4.30419(2), c = 7.18510(5) Å

	Wykoff Position $P\bar{3}m1$	x	y	z	$occ.$	u_{iso}
Cu1	2(*d*)	0.3333	0.6667	0.6214(8)	0.851(7)	0.40
Cu2	2(*d*)	0.3333	0.6667	0.8786(8)	0.149	0.40
I	2(*d*)	0.3333	0.6667	0.242(1)	1.	0.26

Table S36(*d*) β-CuI

Atomic positions for β-CuI at 647 K (Keen & Hull, 1995) [80230].

a = 4.2933(2), c = 7.1912(6) Å

	Wykoff Position $P\bar{3}m1$	x	y	z	$occ.$	u_{iso}
Cu1	2(*d*)	0.3333	0.6667	0.628(1)	0.82(1)	0.37
Cu2	2(*d*)	0.3333	0.6667	0.82(1)	0.18	0.37
I	2(*d*)	0.3333	0.6667	0.243(2)	1.	0.25

Table S37

Modified atomic positions for $BaVO_{2.5}$ (de Beaulieu & Mueller-Buschbaum, 1982) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å.[32657]
a = 5.718, c = 11.613 Å; $z^* = z + 0.0065$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$occ.$	u_{iso}
Ba1	1(*a*)	1(*a*)	0	0	0	0.0065	0	0	0	0	0	0.08	0.08	1.	0.14
Ba2	1(*b*)		0.3333	0.6667	0.7848(7)	0.7913	0.3333	0.6667	0.7829	0	0	0.10	0.1	1.	0.20
		2(*d*)													
Ba4	1(*c*)		0.6667	0.3333	0.2191(7)	0.2256	0.6667	0.3333	0.2171	0	0	0.10	0.1	1.	0.24
Ba3	1(*b*)		0.3333	0.6667	0.4085(10)	0.4150	0.3333	0.6667	0.4111	0	0	0.05	0.05	1.	0.26
		2(*d*)													
Ba5	1(*b*)		0.6667	0.3333	0.5864(8)	0.5929	0.6667	0.3333	0.5889	0	0	0.05	0.05	1.	0.22
V1	1(*a*)	1(*b*)	0	0	0.4949(12)	0.5014	0	0	0.5	0	0	0.02	0.02	1.	0.12
V2	1(*b*)		0.3333	0.6667	0.0862(8)	0.0927	0.3333	0.6667	0.1068	0	0	-0.16	0.16	1.	0.07
		2(*d*)													
V5	1(*b*)		0.6667	0.3333	0.8726(10)	0.8791	0.6667	0.3333	0.8932	0	0	-0.16	0.16	1.	0.16
V3	1(*a*)		0	0	0.6938(12)	0.7003	0	0	0.7093	0	0	-0.10	0.1	1.	0.15
		2(*c*)													
V4	1(*a*)		0	0	0.2753(9)	0.2818	0	0	0.2907	0	0	-0.10	0.1	1.	0.07
O1	3(*d*)	3(*e*)	0.5070(7)	0.0140(14)	0.0010(25)	0.0075	0.5	0	0	0.04	0.08	0.01	0.11	0.833	0.21
O2	3(*d*)		0.1620(39)	0.3240(77)	0.1890(25)	0.1955	0.1635	0.3270	0.1950	-0.01	-0.02	0.01	0.03	0.833	0.16
		6(*i*)													
O4	3(*d*)		0.8350(23)	0.6700(23)	0.7990(16)	0.8055	0.8365	0.6730	0.8050	-0.01	-0.02	0.01	0.03	0.833	0.03
O3	3(*d*)		0.1510(19)	0.3020(38)	0.5990(16)	0.6055	0.1545	0.3090	0.6030	-0.02	-0.04	0.03	0.06	0.833	0.01
		6(*i*)													
O5	3(*d*)		0.8420(57)	0.6840(28)	0.3930(24)	0.3995	0.8455	0.6910	0.3970	-0.02	-0.04	0.03	0.06	0.833	0.13

Table S38

Modified atomic positions for $Na(Cu_{0.67}Fe_{0.22}Zn_{0.11})_2S_2$ (Kaplunnik *et al.*, 1990) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [39255]
Origin translation: ⅔, ⅓, z - 0.2332.
a = 3.873(1), c = 6.848(2) Å; $z^* = z - 0.2332$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ*
Na	1(*a*)	1(*b*)	0.	0.	0.738(3)	0.5048	0.	0.	0.5	0	0	0.03	0.03	n//a	1
Cu1,Fe1,Zn1	1(*c*)		0.3333	0.6667	0.1094(3)	-0.1238	0.3333	0.6667	-0.1232	0	0	-0.01	0.01	n//a	**0.67,0.22, 0.11**
		2(*d*)													
Cu2,Fe2,Zn2	1*(b)*		0.6667	0.3333	0.3557(3)	0.1225	0.6667	0.3333	0.1232	0	0	-0.01	0.01	n//a	**0.67,0.22, 0.11**
S1	1*(b)*		0.6667	0.3333	0.	-0.2332	0.6667	0.3333	-0.2315	0	0	-0.01	0.01	n//a	1
		2(*d*)													
S2	1(*c*)		0.3333	0.6667	0.4629(5)	0.2297	0.3333	0.6667	0.2315	0	0	-0.01	0.01	n//a	1

Table S39

Atomic positions for $Cr_{0.68}Se$ (Wehmeier *et al.*, 1970) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [42703]
a = 3.873(1), c = 6.848(2) Å; $z^* = z - 0.2332$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position												
	$P3m1$	$P\bar{3}m1$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Cr1	1(*a*)	1(*b*)	0	0	0.5	0	0	0.5	0	0	0	0	1.
Cr2	1(*a*)	1(*a*)	0	0	0	0	0	0	0	0	0	0	0.36
Se1	1(*b*)		0.3333	0.6667	0.25	0.3333	0.6667	0.25	0	0	0	0	1.
		2(*d*)											
Se2	1(*c*)		0.6667	0.3333	0.75	0.6667	0.3333	0.75	0	0	0	0	1.

Table S40 .

Proposed atomic positions for $H_{3.68}Fe_{1.44}O_4$ (Eggleton & Fitzpatrick, 1988) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [56287]
a = 2.96(3),† c = 9.4 Å; $z^* = z$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position												
	$P3m1$	$P\bar{3}m1$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Fe1	1(*a*)		0	0	0.025	0	0	0.025	0	0	0	0	0.18
		2(*c*)											
Fe2	1(*a*)		0	0	-0.025	0	0	-0.025	0	0	0	0	0.18
Fe3‡	1(*a*)		*0.6667*	*0.3333*	0.725	*0.6667*	*0.3333*	0.738	0	0	-0.12	0.12	0.18
		2(*d*)											
Fe7	1(*b*)		0.3333	0.6667	0.250	0.3333	0.6667	0.262	0	0	-0.11	0.11	0.1
Fe4	1(*a*)		0	0	0.775	0	0	0.795	0	0	-0.19	0.19	0.18
		2(*c*)											
Fe5	1(*a*)		0	0	0.185	0	0	0.205	0	0	-0.19	0.19	0.26
Fe6‡	1(*a*)		*0.6667*	*0.3333*	0.565	*0.6667*	*0.3333*	0.532	0	0	0.31	0.31	0.26
		2(*d*)											
Fe8	1(*b*)		0.3333	0.6667	0.5	0.3333	0.6667	0.468	0	0	0.30	0.30	0.1
O1	1(*c*)		0.6667	0.3333	0.125	0.6667	0.3333	0.125	0	0	0	0	1.
		2(*d*)											
O4	1(*b*)		0.3333	0.6667	0.875	0.3333	0.6667	0.875	0	0	0	0	1.
O2‡	1(*a*)		*0.3333*	*0.6667*	0.375	*0.3333*	*0.6667*	0.375	0	0	0	0	1.
		2(*d*)											
O3	1(*c*)		0.6667	0.3333	0.625	0.6667	0.3333	0.625	0	0	0	0	1.

† Michel *et al*., (2007) report the *a* axis is double the earlier length, in a cell with with space group $P6_3mc$, see §4.13.

‡ Fe3 and Fe6 assumed in Wyckoff position 1(*c*), O2 in 1(*b*), rather than in the positions reported, with coordinate values in italic.

Table S41(*a*)
Proposed atomic positions for $CoGaInS_4$ (Depero *et al.*, 1991) with hypothetical $x'y'z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å; the origin is shifted 1/3, 2/3, z. [86413]
a = 3.744(1), c = 12.149(3) Å, $z^* = z - 0.2009$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
In1,Co1	1(*a*)	1(*b*)	0.	0.	0.7019(4)	0.5010	0.	0.	0.5	0.	0.	0.01	0.01	**0.624,0.376**	0.14
In2,Co2,Ga1	1(*b*)		0.3333	0.6667	0.4009(1)	0.2000	0.3333	0.6667	0.2005	0.	0.	-0.01	0.01	**0.376,0.294, 0.33**	0.13
		2(*d*)													
Ga2,Co3	1(*c*)		0.6667	0.3333	0	-0.2009	0.6667	0.3333	-0.2005	0.	0.	-0.01	0.01	**0.67,0.33**	0.14
S1	1(*b*)		0.3333	0.6667	0.0742(4)	-0.1267	0.3333	0.6667	-0.1284	0.	0.	0.02	0.02	1.	0.15
		2(*d*)													
S4	1(*c*)		0.6667	0.3333	0.3309(3)	0.1300	0.6667	0.3333	0.1284	0.	0.	0.02	0.02	1.	0.14
S2	1(*c*)		0.6667	0.3333	0.8094(3)	0.6085	0.6667	0.3333	0.6102	0.	0.	-0.02	0.02	1.	0.14
		2(*d*)													
S3	1(*b*)		0.3333	0.6667	0.5890(3)	0.3881	0.3333	0.6667	0.3898	0.	0.	-0.02	0.02	1.	0.13

Table S41(*b*)
Proposed atomic positions for $CoGaInS_4$ (Depero *et al.*, 1991) with hypothetical $x'y'z'$ coordinates and Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å; the origin is shifted 1/3, 2/3, z. [86414]
a = 3.744(1), c = 12.149(3) Å, $z^* = z - 0.2009$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
In1,Co1	1(*a*)	1(*b*)	0.	0.	0.7169(15)	0.5116	0.	0.	0.5	0.	0.	0.14	0.14	**0.62,0.38**	0.06
In2,Co2,Ga1	1(*b*)		0.3333	0.6667	0.4018(10)	0.1965	0.3333	0.6667	0.1849	0.	0.	0.14	0.14	**0.38,0.29,0.33**	0.06
		2(*d*)													
Ga2,Co3	1(*c*)		0.6667	0.3333	0.	-0.1733	0.6667	0.3333	-0.1849	0.	0.	0.14	0.14	**0.67.0.33**	0.06
S1	1(*b*)		0.3333	0.6667	0.0633(12)	-0.1420	0.3333	0.6667	-0.1306	0.	0.	-0.14	0.14	1.	0.06
		2(*d*)													
S4	1(*c*)		0.6667	0.3333	0.3245(12)	0.1192	0.6667	0.3333	0.1306	0.	0.	-0.14	0.14	1.	0.06
S2	1(*c*)		0.6667	0.3333	0.8108(21)	0.6055	0.6667	0.3333	0.6116	0.	0.	-0.07	0.07	1.	0.06
		2(*d*)													
S3	1(*b*)		0.3333	0.6667	0.5876(19)	0.3823	0.3333	0.6667	0.3884	0.	0.	-0.07	0.07	1.	0.06

Table S41(*c*)
Atomic positions for $CoGaInS_4$ (Haeuseler *et al.*, 1990) with hypothetical $x'y'z'$ coordinates. [69015] a = 3.759(1), c = 12.184(2) Å.

	Wykoff Position				
	$P\bar{3}m1$	x	y	z	*occ.*
In1,Co1	1(*b*)	0	0	0.5	0.612, 0.388
Ga1,In2, Co2	2(*d*)	0.3333	0.6667	0.1995(1)	0.5, 0.194, 0.306
S1	2(*d*)	0.3333	0.6667	0.3896(1)	1.
S2	2(*d*)	0.3333	0.6667	0.8720(2)	1.

Table S42

Proposed atomic positions for $LaNdO_{1.75}S$ (Kuz'micheva *et al.*, 1980) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [86550]
$a = 4.052$. $c = 6.958$ Å; $z^* = z + 0.01074$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*	u_{iso}
La	1(*b*)		0.3333	0.6667	0.7209	0.7316	0.3333	0.6667	0.7198	0	0	0.08	0.08	1.	0.05
		2(*d*)													
Nd	1(*c*)		0.6667	0.3333	0.2813	0.2920	0.6667	0.3333	0.2802	0	0	0.08	0.08	1.	0.04
O1	1(*b*)		0.3333	0.6667	0.3497	0.3604	0.3333	0.6667	0.3776	0	0	-0.12	0.12	1.	0.08
		2(*d*)													
O2	1(*c*)		0.6667	0.3333	0.5944	0.6051	0.6667	0.3333	0.6224	0	0	-0.12	0.12	0.75	0.09
S	1(*a*)	1(*a*)	0	0	0	0.0107	0	0	0	0	0	0.07	0.07	1.	0.02

Table S43

Proposed atomic positions for $Cs_3Sb_2I_9$ (Arakcheeva *et al.*, 1999) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [89694]
a = 8.435(7), c = 10.390(7) Å; z = z – 0.0032 ; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition													
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cs1	1(*a*)	1(*a*)	0	0	0.0201(8)	0.0169	0	0	0.	0	0	0.18	0.18	0.27
Cs2	1(*b*)		0.3333	0.6667	0.6715(9)	0.6683	0.3333	0.6667	0.6718	0	0	-0.04	0.04	0.27
		2(*d*)												
Cs3	1(*c*)		0.6667	0.3333	0.3280(9)	0.3248	0.6667	0.3333	0.3282	0	0	-0.04	0.04	0.27
Sb1	1(*b*)		0.3333	0.6667	0.1932(8)	0.1900	0.3333	0.6667	0.1903	0	0	-0.00	0.0	0.18
		2(*d*)												
Sb2	1(*c*)		0.6667	0.3333	0.8126(8)	0.8094	0.6667	0.3333	0.8097	0	0	-0.00	0.0	0.18
I1	3(*d*)		0.8327(4)	0.6654(6)	0.6615(4)	0.6583	0.8324	0.6647	0.6616	0.0	0.01	-0.03	0.03	0.27
		6(*i*)												
I2	3(*d*)		0.664(1)	0.8320(7)	0.3383(5)	0.3351	0.6647	0.8324	0.3384	-0.01	0.0	-0.03	0.03	0.27
I3	3(*d*)	3(*e*)	0.002(9)	0.5009(9)	0	-0.0032	0	0.5	0	0.02	0.01	-0.03	0.03	0.28

Table S44

Proposed atomic positions for $Ba((Fe_{0.5}Ta_{0.5})O_3)$ (Li *et al.*, 2004) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [99484]

$a = 5.7414(1)$, $c = 14.0634(1)$ Å; $z^* = z - 0.0065$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition													
	$P3c1$†	$P\bar{3}c1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Ba1	1(*a*)		0.	0.	0.	-0.0065	0.	0.	0.	0.	0.	-0.09	0.09	1.
		2(*b*)												
Ba2	1(*a*)		0.	0.	0.4999(1)	0.4934	0.	0.	0.5	0.	0.	-0.09	0.09	1.
Ba4	1(*a*)		0.3333	0.6667	0.3331(1)	0.3266	0.3333	0.6667	0.3333	0.	0.	-0.09	0.09	1.
Ba3	1(*a*)		0.3333	0.6667	0.8331(1)	0.8266	0.3333	0.6667	0.8333	0.	0.	-0.09	0.10	1.0
		4(*d*)												
Ba6	1(*c*)		0.6667	0.3333	0.1663(1)	0.1598	0.6667	0.3333	0.1667	0.	0.	-0.10	0.10	1.
Ba5	1(*c*)		0.6667	0.3333	0.6663(1)	0.6598	0.6667	0.3333	0.6667	0.	0.	-0.10	0.10	1.
Ta1,Fe1	1(*a*)		0.	0.	0.7594(1)	0.7529	0.	0.	0.75	0.	0.	0.04	0.04	0.5,0.5
		2(*a*)												
Ta2,Fe2	1(*a*)		0.	0.	0.2595(1)	0.2530	0.	0.	0.25	0.	0.	0.04	0.04	0.5,0.5
Ta4,Fe4	1(*b*)		0.3333	0.6667	0.0930(1)	0.0865	0.3333	0.6667	0.0832	0.	0.	0.05	0.05	0.5,0.5
Ta3,Fe3	1(*b*)		0.3333	0.6667	0.5929(1)	0.5864	0.3333	0.6667	0.5832	0.	0.	0.05	0.05	0.5,0.5
		4(*d*)												
Ta6,Fe6	1(*c*)		0.6667	0.3333	0.4267(1)	0.4202	0.6667	0.3333	0.4168	0.	0.	0.05	0.05	0.5,0.5
Ta5,Fe5	1(*c*)		0.6667	0.3333	0.9265(1)	0.9200	0.6667	0.3333	0.9167	0.	0.	0.05	0.05	0.5,0.5
O1	3(*d*)		0.1633(1)	0.8367(1)	0.6767(1)	0.6702	0.1667	0.8333	0.6667	-0.02	0.02	0.05	0.05	1.
O6	3(*d*)		0.8300(1)	0.1700(1)	0.3434(1)	0.3369	0.8333	0.1667	0.3333	-0.02	0.02	0.05	0.05	1.
		12(*g*)												
O2	3(*d*)		0.1633(1)	0.8367(1)	0.1767(1)	0.1702	0.1667	0.8333	0.1667	-0.02	0.02	0.05	0.05	1.
O5	3(*d*)		0.8300(1)	0.1700(1)	0.8434(1)	0.8369	0.8333	0.1667	0.8333	-0.02	0.02	0.05	0.05	1.
O3	3(*d*)		0.4967(1)	0.5033(1)	0.0101(1)	0.0036	0.5	0.5	0.	-0.02	0.02	0.05	0.05	1.
		6(*e*)												
O4	3(*d*)		0.4967(1)	0.5033(1)	0.5101(1)	0.5036	0.5	0.5	0.5	-0.02	0.02	0.05	0.05	1.

† Assigned to space group $P3m1$ with Wyckoff positions as in Table S44, an overlooked *c*-glide plane is clearly present and hence appropriate space group is $P3c1$.

Table S45

Proposed atomic positions for AlCuMg[†] (Komura, 1962) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [109103]
a = 5.14, c = 21.05 Å.; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position											
	$P3m1$	$P\bar{6}m2$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	*occ.*
Al1,Cu1	3(*d*)	3(*j*)	0.5	0	0	0.5	0	0	0	0	0	0	0.5,0.5
Al2,Cu2	1(*b*)		0.3333	0.6667	0.1	0.3333	0.6667	0.1	0	0	0	0	0.5,0.5
		2(*h*)											
Al10,Cu10	1(*b*)		0.3333	0.6667	0.9	0.3333	0.6667	0.9	0	0	0	0	0.5,0.5
Al3,Cu3	3(*d*)		0.1667	0.3334	0.2	0.1667	0.3334	0.2	0	0	0	0	0.5,0.5
		6(*n*)											
Al9,Cu9	3(*d*)		0.1667	0.3334	0.8	0.1667	0.3334	0.8	0	0	0	0	0.5,0.5
Al4,Cu4	1(*a*)		0.0	0.0	0.3	0	0	0.3	0	0	0	0	0.5,0.5
		2(*g*)[‡]											
Al8,Cu8	1(*b*)		0.0	0.0	0.7	0	0	0.7	0	0	0	0	0.5,0.5
Al5,Cu5	3(*d*)		0.8333	0.1667	0.4	0.8333	0.1667	0.4	0	0	0	0	0.5,0.5
		6(*n*)[‡]											
Al7,Cu7	3(*d*)		0.8333	0.1667	0.6	0.8333	0.1667	0.6	0	0	0	0	0.5,0.5
Al6,Cu6	1(*c*)	1(*f*)	0.6667	0.3333	0.5	0.6667	0.3333	0.5	0	0	0	0	0.5,0.5
Mg1	1(*a*)		0	0	-0.075	0	0	-0.075	0	0	0	0	1.
		2(*g*)											
Mg2	1(*a*)		0	0	0.075	0	0	0.075	0	0	0	0	1.
Mg3	1(*c*)		0.6667	0.3333	0.125	0.6667	0.3333	0.125	0	0	0	0	1.
		2(*i*)											
Mg10	1(*c*)		0.6667	0.3333	0.875	0.6667	0.3333	0.875	0	0	0	0	1.
Mg4	1(*c*)		0.6667	0.3333	0.275	0.6667	0.3333	0.275	0	0	0	0	1.
		2(*i*)											
Mg9	1(*c*)		0.6667	0.3333	0.725	0.6667	0.3333	0.725	0	0	0	0	1.
Mg5	1(*b*)		0.3333	0.6667	0.325	0.3333	0.6667	0.325	0	0	0	0	1.
		2(*h*)[‡]											
Mg8	1(*a*)		0.3333	0.6667	0.675	0.3333	0.6667	0.675	0	0	0	0	1.
Mg6	1(*b*)		0.3333	0.6667	0.475	0.3333	0.6667	0.475	0	0	0	0	1.
		2(*h*)[‡]											
Mg7	1(*a*)		0.3333	0.6667	0.525	0.3333	0.6667	0.525	0	0	0	0	1.

[‡] All coordinates in Table S46 as given by ICSD except for the Wyckoff locations assigned Al7/Cu7, Al8/Cu8, Mg7 and Mg8. The resulting location changes have little effect on interatomic distances. The primary interest in this study was the nature of the structural stacking faults and related disorder.

Table S46(*a*)

Proposed atomic positions for $CeCuSnD_{0.33}$ (Maehlen *et al.*, 2005) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [152855]
$a = 4.53244(5)$, $c = 4.0660(1)$ Å; $z^* = z - 0.0131$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	Wykoff Position														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
Ce	1(*a*)	1(*a*)	0.	0.	0.	-0.013	0.	0.	0.0	0.	0.	-0.05	0.03	0.10	1.
Cu1	1(*b*)		0.3333	0.6667	0.517(4)	0.504	0.3333	0.6667	0.446	0.	0.	0.24	0.26	0.10	0.57(1)
		2(*d*)													
Cu2	1(*c*)		0.6667	0.3333	0.626(5)	0.613	0.6667	0.3333	0.555	0.	0.	0.24	0.26	0.10	0.43(1)
Sn1	1(*b*)		0.3333	0.6667	0.474(4)	0.461	0.3333	0.6667	0.499	0.	0.	-0.15	0.14	0.10	0.43(1)
		2(*d*)													
Sn2	1(*c*)		0.6667	0.3333	0.475(5)	0.462	0.6667	0.3333	0.501	0.	0.	-0.16	0.14	0.10	0.57(1)
D1	1(*c*)		0.6667	0.3333	0.959(8)	0.946	0.6667	0.3333	0.959	0.	0.	0.	0.	0.07	0.33(2)
		2(*d*)													
D2	1(*b*)†		*0.3333*	*0.6667*	*0.041(8)*	*0.028*	*0.3333*	*0.6667*	*0.041*	*0.*	*0.*	*0.*	*0.*	n/a	n/a

† The atom D2, with coordinates in italic, is assumed present with same site occupancy as reported for D1.

Table S46(*b*)

Proposed atomic positions for $CuLaSnD_{0.47}$ (Maehlen *et al.*, 2005) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [152857]
$a = 4.54106(6)$, $c = 4.19101(9)$ Å; $z^* = z + 0.002$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]

	WykoffPosition														
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	*occ.*
La	1(*a*)	1(*a*)	0.	0.	0.	0.002	0.	0.	0	0.	0.	0.01	0.01	0.10	1.
Cu1	1(*b*)		0.3333	0.6667	0.441(1)	0.443	0.3333	0.6667	0.429	0.	0.	0.06	0.06	0.08	0.5
		2(*d*)													
Cu2	1(*c*)		0.6667	0.3333	0.583(1)	0.585	0.6667	0.3333	0.5712	0.	0.	0.06	0.06	0.08	0.5
Sn1	1(*b*)		0.3333	0.6667	0.523(1)	0.525	0.3333	0.6667	0.523	0.	0.	0.01	0.01	0.08	0.5
		2(*d*)													
Sn2	1(*c*)		0.6667	0.3333	0.477(1)	0.479	0.6667	0.3333	0.476	0.	0.	0.01	0.01	0.08	0.5
D1	1(*c*)		0.6667	0.3333	0.96(3)	0.962	0.6667	0.3333	0.962	0.	0.	0.0	0.0	0.04	0.47(5)
		2(*d*)													
D2	1(*b*) †		*0.3333*	*0.6667*	*0.036*	*0.038*	*0.3333*	*0.6667*	*0.038*	*0.*	*0.*	*0.0*	*0.0*	n/a	n/a

† The atom D2, as in Table S46(*a*), is assumed present with same site occupancy as reported for D1..

Table S47

Proposed atomic positions for Ni_2H **(**Khodyrev *et al.*, 1978) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [201088]
$a = 2.66$, $c = 4.33$ Å; $z^* = z - 0.028$ Å; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.[2]
.

	Wykoff Position													
	$P3m1$	$P\bar{3}m1$	x	y	z	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ni1	1(*b*)		0.3333	0.6667	0.254	0.226	0.3333	0.6667	0.2255	0	0	0.0	0.0	0.09
		2(*d*)												
Ni2	1(*c*)		0.6667	0.3333	0.803	0.775	0.6667	0.3333	0.7745	0	0	0.0	0.0	0.09
H	1(*a*)	1(*a*)	0	0	0.027	-0.001	0	0	0	0	0	-0.01	0.01	0.09

9. Entries for structures reported in space group *P*3*m*1 that are as likely without a change in phase

5.1 5*H*-Si_5C_5 [107204][5]

Gevorkyan *et al.* (1976), paper inaccessible; five independent Si, five C atoms forming perfect interlocking SiC_4 and Si_4C tetrahedra with $d_{Si\text{-}C}$ = 1.855 Å and all Si-C-Si, C-Si-C angles = 109.47° in a unit cell with a = 3.03, c = 12.37 Å. All five Si and 4 of 5 C atoms satisfy $P\bar{3}m1$ symmetry within $\Delta\xi_{max} \lesssim 0.31$ Å if Si4 were in Wyckoff location 1(*b*) rather than 1(*a*) as reported, see Table S48. However, such a Wyckoff location change would result in higher coordination for Si3, Si and C3. Further, atom C5 prevents such an approach to supergroup symmetry unless disordered. A comparable study of the related 6*H*-SiC polytype, with a = 3.0807 and c = 15.1174 Å, reports space group $P6_3mc$ rather than $P3m1$ (Gomes de Mesquita, 1967). Reexamination of the 5*H* polytype is hence appropriate.

5.2(*a*) $(CoI(NP(CH_3)_3))_4(CH_2Cl_2)_3$ [404305]

Prepared at 455 K; Mo*K*α diffractometry, sample at 225 K, 2376 independent $I_{obs} \geqslant 2\sigma(I_{obs})$, absorption corrections, U^{ij}, R = 0.033, wR^2 = 0.0982 (Abram *et al.,* 1996). The structural complexity of this compound, in which many pairs of independent atoms such as N1 and P1 with $d_{N1\text{-}P1}$ = 1.58 Å are strongly bonded, see Table S49(*a*), prevents any approach to potential supergroup symmetry, hence a phase transition above ambient temperature is not expected.

[5] A report of the 21*H*-$Si_{21}C_{21}$ polytype, with a = 3.07, c = 52.87 Å (Singh, 1984), is more recent but the 5*H*-Si_5C_5 polytype with a smaller unit cell is likely to be more reliable, hence was selected as representative.

5.2(*b*) $ZnI(NP(CH_3)_3))_4(CH_2Cl_2)_3$ [404306]

Similarly prepared at 455 K, see §5.4; Mo$K\alpha$ diffractometry, crystal at 215 K, 2197 independent $I_{obs} \geqslant 2\sigma(I_{obs})$, absorption corrections, U^{ij}, $R = 0.043$, $wR^2 = 0.1141$ (Abram *et al.,* 1996). Strong bonds exist between many pairs of atoms in this Zn member of the family represented in §5.4, among the 48 atoms listed in Table S49(*b*), such as N1-P1 with $d_{N1\text{-}P1} =$ 1.61 Å. Such bonds prevent either member yfrom satisfying the symmetry of a potential supergroup, since one atom only in any pair can occupy a location of higher symmetry, as is also the case in §5.4. A phase transition above ambient temperature is hence not expected.

10. Tabular data for structures reported in space group *P*3*m*1 that are as likely without a change in phase

Table S48

Modified atomic positions for 5*H*-Si_5C_5 **(**Gevorkyan *et al.*, 1976) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [107204].
$a = 3.03$, $c = 12.37$ Å., $z^* = z + 0.025$; $\Delta x = (x - x')\,a$, $\Delta y = (y - y')\,a$, $\Delta z = (z^* - z')\,c$.[2]

	WykoffPosition												
	*P*3*m*1	$P\bar{3}m1$	*x*	*y*	*z*	*z**	*x′*	*y′*	*z′*	Δ*x*	Δ*y*	Δ*z*	Δξ
Si1	1(*a*)	1(*a*)	0	0	0	0.025	0	0	0	0	0	0.31	0.31
Si2	1(*b*)		0.3333	0.6667	0.2	0.225	0.3333	0.6667	0.2	0	0	0.31	0.31
		2(*d*)											
Si5	1(*c*)		0.6667	0.3333	0.8	0.825	0.6667	0.3333	0.8	0	0	0.31	0.31
Si3	1(*c*)		0.6667	0.3333	0.4	0.425	0.6667	0.3333	0.4	0	0	0.31	0.31
		2(*d*)											
Si4	1(*a*)[†]		*0.3333*	*0.6667*	0.6	0.625	*0.3333*	*0.6667*	0.6	0	0	0.31	0.31
C1	1(*a*)		0	0	0.15	0.175	0	0	0.2	0	0	-0.31	0.31
		2(*c*)											
C4	1(*a*)		0	0	0.75	0.775	0	0	0.8	0	0	-0.31	0.31
C2	1(*b*)		0.3333	0.6667	0.35	0.375	0.3333	0.6667	0.4	0	0	-0.31	0.31
		2(*d*)											
C3	1(*c*)		0.6667	0.3333	0.55	0.575	0.6667	0.3333	0.6	0	0	-0.31	0.31
C5	1(*c*)		0.6667	0.3333	0.95	0.975	0.6667	0.3333	0	0	0	-0.31	0.31

[†] Placing Si4 in 1(*b*), instead of 1(*a*) as reported, jointly satisfies location 2(*d*) in supergroup $P\bar{3}m1$ together with Si3 but results in distorted octahedra about Si4 and C4. Similarly, if Si3 is placed in 1(*a*), then 2(*c*) in this supergroup would be satisfied, but Si3 becomes 7-, Si4 becomes 5- and C becomes 6-coordinated. Simultaneously, C5 cannot satisfy this supergroup unless becoming disordered.

Table S49(*a*)

Atomic positions for $(CoI(NP(CH_3)_3))_4(CH_2Cl_2)_3$ (Abram *et al.,* 1996) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [404305]
a = 14.558(1), c = 12.705(2) Å

	Wykoff Position					Wykoff Position			
	*P*3*m*1	*x*	*y*	*z*		*P*3*m*1	*x*	*y*	*z*
I1	1(*c*)	0.6667	0.3333	0.46045(9)	N3	1(*a*)	0.0000	0.0000	0.3735(9)
I2	3(*d*)	0.50574(3)	1.01148(5)	0.90188(6)	N4	3(*d*)	0.0676(3)	-0.0676(3)	0.1854(6)
Co1	1(*c*)	0.6667	0.3333	0.66270(15	P3	1(*a*)	0.0000	0.0000	0.4996(3)
Co2	3(*d*)	0.60293(4)	1.20585(9)	0.84319(9)	P4	3(*d*)	0.12733(9)	-0.12733(9)	0.1471(2)
N1	1(*c*)	0.6667	0.3333	0.9412(9)	C4	3(*d*)	0.0664(6)	0.1328(12)	0.5491(10)
P1	1(*c*)	0.6667	0.3333	1.0657(3)	H10	6(*e*)	0.0317(6)	0.1697(12)	0.5232(10)
N2	3(*d*)	0.7340(3)	0.2660(3)	0.7512(6)	H11	6(*e*)	0.1389(6)	0.1686(12)	0.5259(10)
P2	3(*d*)	0.79323(9)	0.20677(9)	0.7102(2)	H12	6(*e*)	0.0642(6)	0.1313(12)	0.6246(10)
C1	3(*d*)	0.7331(5)	0.4662(10)	1.1176(11)	C5	6(*e*)	0.2418(7)	-0.0457(9)	0.0702(7)
H1	6(*e*)	0.6995(5)	0.5039(10)	1.0913(11)	H13	6(*e*)	0.2883(7)	0.0173(9)	0.1090(7)
H2	6(*e*)	0.8061(5)	0.5020(10)	1.0962(11)	H14	6(*e*)	0.2209(7)	-0.0265(9)	0.0060(7)
H3	6(*e*)	0.7291(5)	0.4635(10)	1.1931(11)	H15	6(*e*)	0.2781(7)	-0.0838(9)	0.0541(7)
C2	6(*e*)	0.7064(9)	0.0925(7)	0.6304(8)	C6	3(*d*)	0.1724(4)	-0.1724(4)	0.2577(12)
H4	6(*e*)	0.6798(9)	0.1147(7)	0.5725(8)	H16	6(*e*)	0.2172(4)	-0.1131(4)	0.3019(12)
H5	6(*e*)	0.6481(9)	0.0422(7)	0.6726(8)	H17	6(*e*)	0.2118(4)	-0.2048(4)	0.2326(12)
H6	6(*e*)	0.7453(9)	0.0601(7)	0.6040(8)	H18	6(*e*)	0.1123(4)	-0.2234(4)	0.2975(12)
C3	3(*d*)	0.8401(5)	0.1599(5)	0.8163(13)	C7	3(*d*)	-0.0282(15)	0.4859(8)	0.3532(16)
H7	6(*e*)	0.8865(5)	0.2185(5)	0.8604(13)	H19	6(*e*)	-0.0707(15)	0.5185(8)	0.3686(16)
H8	6(*e*)	0.8780(5)	0.1271(5)	0.7884(13)	Cl1	3(*d*)	0.0054(4)	0.5027(2)	0.2163(4)
H9	6(*e*)	0.7809(5)	0.1090(5)	0.8571(13)	Cl2	3(*d*)	0.0778(8)	0.5389(4)	0.4301(6)
I3	1(*a*)	0.0000	0.0000	-0.10605(8)	C8	3(*d*)	0.5488(17)	0.7744(9)	0.7471(26)
I4	3(*d*)	0.31788(5)	0.15894(3)	0.34392(5)	H20	6(*e*)	0.5136(17)	0.7029(9)	0.7754(26)
Co3	1(*a*)	0.0000	0.0000	0.0968(2)	Cl3	3(*d*)	0.6848(5)	0.8424(2)	0.7889(5)
Co4	3(*d*)	0.12731(9)	0.06366(4)	0.27665(9)	Cl4	3(*d*)	0.5375(13)	0.7687(6)	0.6232(11)

Table S49(*b*)

Atomic positions for $(ZnI(NP(CH_3)_3))_4(CH_2Cl_2)_3$ (Abram *et al.,* 1996) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz, $\Delta\xi$ and u_{iso} displacements in Å. [404306]
a = 14.549(1), c = 12.705(2) Å

	Wykoff Position						Wykoff Position				
	*P*3*m*1	*x*	*y*	*z*	*occ.*		*P*3*m*1	*x*	*y*	*z*	*occ.*
I1	1(*b*)	0.3333	0.6667	-0.14711(11)	1	N3	1(*c*)	0.6667	0.3333	0.8981(15)	1
I2	3(*d*)	0.01330(8	0.50665(4	0.30250(7)	1	N4	3(*d*)	0.5995(4)	0.4005(4)	0.7085(8)	1
Zn1	1(*b*)	0.3333	0.6667	0.0521(2)	1	P3	1(*c*)	0.6667	0.3333	1.0207(4)	1
Zn2	3(*d*)	0.20101(1	0.60051(6	0.23456(10	1	P4	3(*d*)	0.54030(1)	0.45970(14	0.6685(3)	1
N1	1(*b*)	0.3333	0.6667	0.3297(12)	1	C4	3(*d*)	0.6004(7)	0.3996(7)	1.0743(12)	1
N2	3(*d*)	0.2663(4)	0.7337(4)	0.1444(8)	1	H10	6(*e*)	0.6333(7)	0.4708(7)	1.0477(12)	0.50
P1	1(*b*)	0.3333	0.6667	0.4561(4)	1	H11	6(*e*)	0.6058(7)	0.4013(7)	1.1497(12)	0.50
P2	3(*d*)	0.20649(1	0.79351(1	0.1063(3)	1	H12	6(*e*)	0.5270(7)	0.3619(7)	1.0542(12)	0.50
C1	3(*d*)	0.2664(7)	0.7336(7)	0.5046(14)	1	C5	3(*d*)	0.4926(7)	0.5074(7)	0.7731(17)	1
H1	6(*e*)	0.3017(7)	0.8053(7)	0.4790(14)	0.50	H13	6(*e*)	0.5508(7)	0.5539(7)	0.8176(17)	0.50
H2	6(*e*)	0.2676(7)	0.7340(7)	0.5801(14)	1	H14	6(*e*)	0.4410(7)	0.4484(7)	0.8137(17)	0.50
H3	6(*e*)	0.1942(7)	0.6972(7)	0.4805(14)	0.50	H15	6(*e*)	0.4604(7)	0.5454(7)	0.7440(17)	0.50
C2	6(*e*)	0.0902(9)	0.7105(11	0.0287(9)	1	C6	6(*e*)	0.6281(12)	0.5750(10)	0.5879(10)	1
H4	6(*e*)	0.1100(9)	0.6838(11	-0.0310(9)	1	H16	6(*e*)	0.6555(12)	0.5528(10)	0.5306(10)	1
H5	6(*e*)	0.0589(9)	0.7514(11	0.0051(9)	1	H17	6(*e*)	0.6859(12)	0.6258(10)	0.6303(10)	1
H6	6(*e*)	0.0399(9)	0.6522(11	0.0709(9)	1	H18	6(*e*)	0.5889(12)	0.6068(10)	0.5606(10)	1
C3	3(*d*)	0.1610(6)	0.8390(6)	0.2150(16)	1	C7	3(*d*)	0.1074(14)	0.8926(14)	0.7081(31)	1
H7	6(*e*)	0.2201(6)	0.8839(6)	0.2593(16)	0.50	H19	6(*e*)	0.0361(14)	0.8561(14)	0.7369(31)	0.50
H8	6(*e*)	0.1098(6)	0.7791(6)	0.2548(16)	0.50	H20	6(*e*)	0.1439(14)	0.9639(14)	0.7369(31)	0.50
H9	6(*e*)	0.1289(6)	0.8782(6)	0.1890(16)	0.50	Cl1	3(*d*)	0.1752(3)	0.8248(3)	0.7476(6)	1
I3	1(*c*)	0.6667	0.3333	0.41852(12	1	Cl2	3(*d*)	0.1007(8)	0.8993(8)	0.5862(16)	1
I4	3(*d*)	0.34385(8	0.17193(4	0.86238(9)	1	C8	3(*d*)	0.3573(19)	0.1786(9)	1.3135(22)	1
Zn3	1(*c*)	0.6667	0.3333	0.6172(2)	1	H21	6(*e*)	0.3994(19)	0.1458(9)	1.3301(22)	0.50
Zn4	3(*d*)	0.53527(1	0.26763(6	0.80179(10	1	Cl3	3(*d*)	0.3279(6)	0.1639(3)	1.1768(5)	1
N3	1(*c*)	0.6667	0.3333	0.8981(15)	1	Cl4	3(*d*)	0.2500(11)	0.1250(5)	1.3871(8)	1