Supplementary Materials

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

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Contents

2. Structures reported in space group *R*3 and predicted to be ferroelectric

[Published *x*, *y*, *z* atomic coordinates may be replaced in the tables below by a symmetry equivalent or by a rhombohedrally-centered equivalent *x*, *y*, *z* + (⅔,⅓,⅓) or + (⅓,⅔,⅔)]

Table S1(*a*)

Modified atomic positions for $RbTi_2(PO_4)_3$ at 6.2 GPa (Hazen *et al.,* 1994) and at 100 kPa with Δx, Δy, Δz and u_{iso} displacements in Å [78428]

$a = 8.239(1)$, $c = 23.563(1)$ Å. $z^* = z_{6.2\ GPa} - 0.0024^{\dagger}$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}c$	$x_{6.2\ GPa}$	$y_{6.2\ GPa}$	$z_{6.2\ GPa}$	$x_{100\ kPa}$	$y_{100\ kPa}$	$z_{100\ kPa}$	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Rb1	3(*a*)	0	0	-0.0024	0	0	0.	0	0	-0.08	0.08	0.11
	6(*b*)											
Rb2	3(*a*)	0	0	0.5033(4)	0	0	0.5	0	0	0.08	0.08	0.12
Ti1	3(*a*)	0	0	0.1505(6)	0	0	0.15143	0	0	-0.02	0.02	0.07
	6(*b*)											
Ti3	3(*a*)	0	0	0.6554(5)	0	0	0.65143	0	0	0.09	0.09	0.07
Ti2	3(*a*)	0	0	-0.1480(6)	0	0	-0.15143	0	0	0.08	0.08	0.07
	6(*b*)											
Ti4	3(*a*)	0	0	0.3490(5)	0	0	0.34857	0	0	0.01	0.01	0.07
P1	9(*b*)	0.7032(11)	-0.0083(11)	0.2528(6)	0.71968	0.	0.25	-0.14	-0.07	0.07	0.20	0.05
	18(*e*)											
P2	9(*b*)	0.2766(11)	-0.0057(11)	-0.2493(6)	0.28032	0	-0.25	-0.03	-0.05	0.02	0.07	0.05
O1	9(*b*)	0.2405(27)	0.4334(28)	0.2778(8)	0.30258	0.46650	0.26850	-0.51	-0.27	0.22	0.72	0.09
O3	9(*b*)	-0.2400(27)	-0.4585(28)	-0.2694(9)	-0.30258	-0.46650	-0.26850	0.52	0.07	-0.02	0.56	0.09
	36(*f*)‡											
O2	9(*b*)	0.4822(25)	0.3550(22)	0.2392(8)	0.46650	0.30258	0.23150	0.13	0.43	0.18	0.54	0.09
O4	9(*b*)	-0.5179(26)	-0.4013(22)	-0.2349(8)	-0.46650	-0.30258	-0.23150	-0.42	-0.81	-0.08	1.09	0.09
O5	9(*b*)	0.1855(23)	0.2035(27)	0.1964(8)	0.14697	0.21231	0.19936	0.32	-0.07	-0.07	0.30	0.10
O7	9(*b*)	-0.1525(24)	-0.2189(26)	-0.1948(8)	-0.14697	-0.21231	-0.19936	-0.05	-0.06	-0.05	0.11	0.10
	36(*f*)											
O6	9(*b*)	0.2238(28)	0.1413(28)	0.3024(8)	0.21231	0.14697	0.30064	0.09	-0.05	0.04	0.09	0.10
O8	9(*b*)	-0.2369(28)	-0.1224(27)	-0.2920(8)	-0.21231	-0.14697	-0.30064	-0.20	0.20	0.20	0.28	0.10

† Based on $\Sigma z_{100\ kPa} = 1.5$.

‡ **A**toms related over more than two positions marked by braces.

Table S1(*b*)

Modified atomic positions for $RbTi_2(PO_4)_3$ at 6.2 GPa (Hazen *et al.,* 1994) and the corresponding hypothetical $x'y'z'$ coordinates with the Δx, Δy, Δz and u_{iso} displacements in Å [78428]

$a = 7.9200(8)$, $c = 23.373(1)$ Å. $z^* = z - 0.0028^{\dagger}$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}c$											
Rb1	3(*a*)	0	0	-0.0028	0	0	-0.0015	0	0	-0.03	0.03	0.11
	6(*b*)											
Rb2	3(*a*)	0	0	0.5005(4)	0	0	0.4985	0	0	0.03	0.03	0.12
Ti1	3(*a*)	0	0	0.1477(6)	0	0	0.1499	0	0	-0.05	0.05	0.07
	12(*c*)											
Ti3	3(*a*)	0	0	0.6526(5)	0	0	0.6499	0	0	0.07	0.07	0.07
Ti2	3(*a*)	0	0	-0.1508(6)	0	0	-0.1526	0	0	0.04	0.04	0.07
	6(*b*)											
Ti4	3(*a*)	0	0	0.3462(5)	0	0	0.3474	0	0	-0.03	0.03	0.07
P1	9(*b*)	0.7032(11)	-0.0083(11)	0.2500(6)	0.7098	0.	0.2507	-0.05	-0.01	-0.02	0.06	0.05
	18(*e*)											
P2	9(*b*)	0.2766(11)	-0.0057(11)	-0.2521(6)	0.2832	0.	-0.2507	-0.05	0.01	-0.03	0.05	0.05
O1	9(*b*)	0.2405(27)	0.4334(28)	0.2750(8)	0.3092	0.4730	0.2683	-0.57	-0.33	0.16	0.80	0.09
O3	9(*b*)	-0.2400(27)	-0.4585(28)	-0.2722(9)	-0.3092	-0.4730	-0.2683	0.57	0.12	-0.09	0.64	0.09
	36(*f*)‡											
O2	9(*b*)	0.4822(25)	0.3550(22)	0.2364(8)	0.4730	0.3092	0.2317	0.08	0.38	0.11	0.44	0.09
O4	9(*b*)	-0.5179(26)	-0.4013(22)	-0.2377(8)	-0.4730	-0.3092	-0.2317	-0.37	-0.76	-0.14	1.01	0.09
O5	9(*b*)	0.1855(23)	0.2035(27)	0.1936(8)	0.1504	0.2112	0.2492	0.29	-0.06	-1.31	1.34	0.10
O7	9(*b*)	-0.1525(24)	-0.2189(26)	-0.1982(8)	-0.1504	-0.2112	-0.2492	-0.02	-0.06	1.20	1.20	0.10
	36(*f*)											
O6	9(*b*)	0.2238(28)	0.1413(28)	0.2996(8)	0.2304	0.1504	0.2508	-0.05	-0.07	1.15	1.15	0.10
O8	9(*b*)	-0.2369(28)	-0.1224(27)	-0.2948(8)	-0.2304	-0.1504	-0.2508	-0.05	0.23	-1.04	1.06	0.10

[†] Based on the 2 P and 8 O z-coordinates for which Σz is expected to be zero.

[‡] **A**toms related over more than two positions marked by braces.

Table S2(*a*)

Modified atomic positions for $LiZnPO_4$ (Bu *et al.,* 1996) with hypothetical $x'y'\ z'$ coordinates and the Δx, Δy, Δz and $u_{\rm iso}$ displacements in Å [83652]

a = 13.628(3), c = 9.096(2) Å. $z^* = z - 0.02303$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$u_{\rm iso}$
Li1	9(*b*) 18(*f*)	0.3484(15)	0.8727(17)	0.034(5)	0.3512	0.8763	-0.081	-0.04	-0.05	1.26	1.26	0.17
Li2	9(*b*)	0.6459(13)	0.1202(12)	0.196(4)	0.6488	0.1237	0.081	-0.04	-0.05	1.26	1.26	0.15
Zn1	9(*b*) 18(*f*)	0.45329(9)	0.13974(8)	0.03655	0.45578	0.13963	0.08449	-0.03	0.00	-0.22	0.22	0.12
Zn2	9(*b*)	0.54174(9)	0.86049(8)	0.86758(11)	0.54422	0.86037	0.91551	-0.03	0.00	-0.22	0.22	0.12
P1	9(*b*) 18(*f*)	0.65327(15)	0.12304(19)	-0.1314(4)	0.7278	0.0680	-0.0845	-1.02	0.75	-0.21	0.94	0.11
P2	9(*b*)	0.1976(2)	0.98708(17)	0.0375(4)	0.2722	0.9320	0.0845	-1.02	0.75	-0.21	0.94	0.11
O1	9(*b*) 18(*f*)	0.5884(5)	0.1252(5)	0.0059(7)	0.5917	0.1278	0.0810	-0.04	-0.04	-0.47	0.48	0.13
O2	9(*b*)	0.4050(4)	0.8696(5)	0.8439(7)	0.4083	0.8722	0.9190	-0.04	-0.04	-0.47	0.48	0.13
O3	9(*b*) 18(*f*)	0.3136(5)	-0.0067(5)	0.0375(7)	0.3248	-0.0112	0.0831	-0.15	0.06	-0.20	0.24	0.12
O4	9(*b*)	0.6640(5)	0.0156(5)	-0.1287(8)	0.6752	0.0112	-0.0831	-0.15	0.06	-0.20	0.24	0.12
O5	9(*b*) 18(*f*)	0.5573(5)	0.1136(5)	0.3690(7)	0.5703	0.1204	0.4016	-0.18	-0.09	-0.08	0.25	0.14
O6	9(*b*)	0.1272(4)	0.5371(5)	0.5659(7)	0.1204	0.5501	0.5984	0.09	-0.18	-0.08	0.18	0.12
O7	9(*b*) 18(*f*)	0.5925(5)	0.1278(5)	0.7296(7)	0.5783	0.1233	0.7634	0.19	0.06	-0.09	0.24	0.13
O8†	9(*b*)	0.1188(5)	0.5592(5)	0.2028	0.1233	0.5450	0.2366	-0.06	0.19	-0.09	0.19	0.12

Table S2(*b*)

Modified atomic positions for α-$LiZnAsO_4$ (Jensen *et al.,* 1998) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [86184]

a = 14.009(2), c = 9.386(2) Å. $z^* = z - 0.0814$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*$\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li1	9(*b*)	0.526(3)	0.873(3)	0.720(5)	0.528	0.877	0.750	-0.03	-0.06	-0.28	0.29	0.09
Li2	18(*f*) 9(*b*)	0.881(3)	0.354(4)	0.220(5)	0.877	0.356	0.250	0.06	-0.03	-0.28	0.28	0.09
Zn1	9(*b*)	0.2117(3)	0.0198(2)	0.8938(2)	0.2129	0.0198	0.7496	-0.02	0.0	1.35	1.35	0.10
Zn2	18(*f*)	0.1931(2)	0.2141(3)	0.3946(2)	0.1931	0.2129	0.2504	0.0	0.02	1.35	1.35	0.10
As1	9(*b*)	0.8634(2)	0.5469(2)	0.0639(2)	0.8632	0.5468	0.0833	0.0	0.0	-0.18	0.18	0.09
As2	18(*f*) 9(*b*)	0.3166(2)	0.8630(2)	0.8973(2)	0.3165	0.8632	0.9167	0.0	0.0	-0.18	0.18	0.09
O1	9(*b*)	0.2448(13)	0.7912(13)	0.0427(14)	0.2466	0.7915	0.0642	-0.02	-0.01	-0.20	0.20	0.09
O4	18(*f*) 9(*b*)	0.7917(10)	0.5431(10)	0.9144(12)	0.7915	0.5449	0.9358	0.0	-0.02	-0.20	0.20	0.08
O2	9(*b*)	0.2488(10)	0.7919(10)	0.7474(12)	0.2510	0.7917	0.7679	-0.03	0.0	-0.19	0.19	0.06
O5	18(*f*) 9(*b*)	0.7469(12)	0.2086(11)	0.2116(13)	0.7490	0.2083	0.2321	-0.01	0.0	-0.19	0.19	0.09
O3	9(*b*)	0.6685(11)	0.0083(11)	0.0532(19)	0.6680	0.0082	0.0838	0.01	0.0	-0.29	0.29	0.08
O8	18(*f*) 9(*b*)	0.3326(13)	0.9919(14)	0.8856(23)	0.3320	0.9918	0.9162	0.01	0.0	-0.29	0.29	0.14
O6	9(*b*)	0.4438(15)	0.8771(15)	0.8937(17)	0.4434	0.8814	0.9155	0.01	-0.06	-0.20	0.21	0.12
O7	18(*f*) 9(*b*)	0.8856(12)	0.4384(12)	0.0628(14)	0.8814	0.4380	0.0845	0.06	0.01	-0.20	0.21	0.08

Table S3 $RbSb_{0.33}Te_6U$

Modified atomic positions for $RbSb_{0.33}Te_6U$ (Choi & Kanatzidis, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [93834]

a = 15.741(2), c = 24.382(4) Å. $z^* = z - 0.0057$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R32$	x	y	z^*	x'	y'	z^*	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
U1	9(*b*),9(*d*)	0.3332(1)	-0.0003(1)	-0.0057(1)	0.3332	0.	0.	0.	-0.01	-0.13	0.13	0.10	1.
U2†	9(*b*),9(*e*)	0.9992(1)	0.3350(1)	0.4942(1)	0.	0.3350	0.5	-0.01	0.	-0.14	0.14	0.10	1.
Rb1	3(*a*)	0.	0.	0.662(11)	0.	0.	0.6687	0.	0.	-0.16	0.16	0.19	0.498
	6(*c*)												
Rb3	3(*a*)	0.	0.	0.3245(12)	0.	0.	0.3312	0.	0.	-0.16	0.16	0.18	0.502
Rb2	3(*a*)	0.	0.	0.6224(12)	0.	0.	0.6315	0.	0.	-0.22	0.22	0.19	0.502
	6(*c*)												
Rb4	3(*a*)	0.	0.	0.3595(12)	0.	0.	0.3685	0.	0.	-0.22	0.22	0.18	0.498
Rb5	3(*a*),3(*a*)	0.	0.	0.9937(7)	0.	0.	0.	0.	0.	-0.15	0.15	0.22	1.
Rb6	9(*b*),9(*e*)	0.9967(9)	0.6650(9)	0.4951(15)	0.	0.6650	0.5	-0.05	0.	-0.12	0.13	0.36	0.6700
Rb7	9(*b*)	0.0097(50)	0.6673(50)	0.4616(60)	0.0105	0.6781	0.4680	-0.01	-0.17	-0.16	0.24	0.36	0.179
	18(*f*)												
Rb8	9(*b*)	0.9887(50)	0.6783(50)	0.5256(60)	0.9895	0.6676	0.5320	-0.01	0.17	-0.16	0.23	0.36	0.151
Sb1	3(*a*)	0.	0.	0.7779(7)	0.	0.	0.7858	0.	0.	-0.19	0.19	0.17	0.502
	6(*c*)												
Sb2	3(*a*)	0.	0.	0.2063(6)	0.	0.	0.2142	0.	0.	-0.19	0.19	0.16	0.498
Sb3	9(*b*)	0.9946(14)	0.6637(16)	0.9459(7)	0.9906	0.6659	0.9524	0.06	-0.03	-0.16	0.17	0.13	0.179
	18(*f*)												
Sb4	9(*b*)	0.3368(18)	0.3319(14)	0.0411(8)	0.3328	0.3341	0.0476	0.06	-0.03	-0.16	0.17	0.10	0.151
Te1	9(*b*)	0.9366(3)	0.4936(3)	0.9913(3)	0.9234	0.4634	0.9555	0.21	0.48	0.87	1.06	0.21	1.
	18(*f*)												
Te12	9(*b*)	0.0899(3)	0.5097(3)	0.0804(1)	0.0767	0.4795	0.0455	0.21	0.48	0.85	1.05	0.15	1.
Te2	9(*b*)	0.0900(3)	0.5112(3)	0.9107(2)	0.1349	0.4666	0.9169	-0.71	0.70	-0.15	0.72	0.16	1.
	18(*f*)												
Te8	9(*b*)	0.4220(3)	0.1798(3)	0.0769(2)	0.4666	0.1349	0.0831	-0.70	0.71	-0.15	0.72	0.19	1.
Te3	9(*b*)	0.5066(3)	0.7346(3)	0.8227(2)	0.5359	0.7453	0.7890	-0.46	-0.17	0.96	1.11	0.19	1.
	18(*f*)												
Te6	9(*b*)	0.8199(3)	0.2440(3)	0.2447(2)	0.7906	0.2547	0.2110	0.46	0.17	0.96	1.11	0.18	1.
Te5	9(*b*))	0.6023(3)	0.8246(3)	-0.0053(2)	0.5895	0.7956	0.0432	0.20	0.46	-1.18	1.32	0.19	1.
	18(*f*)												
Te10	9(*b*)	0.4234(3)	0.1770(3)	0.9083(2)	0.4105	0.2061	0.9568	0.20	-0.46	-1.18	1.25	0.18	1.
Te4	9(*b*)	0.7536(3)	0.5751(3)	0.4109(2)	0.7899	0.5895	0.3740	-0.57	-0.23	0.90	1.15	0.16	1.
	18(*f*)												
Te9	9(*b*)	0.6039(3)	0.8261(3)	0.6629(2)	0.5895	0.7899	0.6260	0.23	0.57	0.90	1.15	0.19	1.
Te7	9(*b*)	0.5988(3)	0.4411(3)	0.166(2)	0.5235	0.5249	0.1698	1.18	-1.32	-0.09	1.26	0.16	1.
	18(*f*)												
Te11	9(*b*)	0.6088(3)	0.4482(2)	0.8264(2)	0.5249	0.5235	0.8302	1.32	-1.18	-0.09	1.26	0.15	1.

Table S4 $Ca_3Nb_{1.95}O_8V_{0.05}$

Modified atomic positions for $Ca_3Nb_{1.95}O_8V_{0.05}$ (Cranswick *et al.*, 2003) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [96423]
$a = 16.910(1)$, $c = 41.500(2)$ Å. $z^* = z - 0.0020$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
V1	3(*a*),3(*a*)	0.	0.	-0.0028(1)	0.	0.	0.	0.	0.	-0.12	0.12	0.10
Nb1	9(*b*) 18(*f*)	0.3255(1)	-0.0028(1)	0.0003(1)	0.3259	-0.0012	0.0005	-0.01	-0.02	-0.01	0.03	0.07
Nb2	9(*b*)	0.6737(1)	-0.0003(1)	-0.0008(1)	0.6741	0.0012	-0.0005	-0.01	-0.03	-0.01	0.04	0.08
Nb3	3(*a*) 6(*c*)	0.	0.	0.3341(1)	0.	0.	0.3346	0.	0.	-0.02	0.02	0.08
Nb4	3(*a*)	0.	0.	0.6650(1)	0.	0.	0.6654	0.	0.	-0.02	0.02	0.05
Ca1	9(*b*) 18(*f*)	0.0894(1)	0.1845(2)	0.0470(1)	0.0919	0.1877	0.0469	-0.04	-0.05	0.00	0.08	0.11
Ca2	9(*b*)	0.9056(2)	0.8091(2)	0.9532(1)	0.9081	0.8123	0.9531	-0.04	-0.05	0.00	0.08	0.12
Ca3	9(*b*) 18(*f*)	0.4492(2)	0.2245(2)	0.0570(1)	0.4544	0.2265	0.0561	-0.09	-0.03	0.04	0.12	0.09
Ca4	9(*b*)	0.5405(2)	0.7716(2)	0.9448(1)	0.5456	0.7735	0.9439	-0.09	-0.03	0.04	0.12	0.12
Nb5	9(*b*) 18(*f*)	0.1142(1)	0.5592(1)	0.0560(1)	0.1137	0.5579	0.0564	0.01	0.02	-0.02	0.03	0.06
Nb6	9(*b*)	0.8868(1)	0.4435(1)	0.9433(1)	0.8863	0.4421	0.9436	0.01	0.02	-0.01	0.03	0.06
Nb7	9(*b*) 18(*f*)	0.2180(1)	0.1077(1)	0.1083(1)	0.2176	0.1083	0.1092	0.01	-0.01	-0.04	0.04	0.06
Nb8	9(*b*)	0.7829(1)	0.8932(1)	0.8899(1)	0.7824	0.8927	0.8908	0.01	0.01	-0.04	0.04	0.08
Nb9	9(*b*) 18(*f*)	0.5531(1)	0.1097(1)	0.1114(1)	0.5539	0.1089	0.1115	-0.01	0.01	0.00	0.01	0.07
Nb10	9(*b*)	0.4452(1)	0.8919(1)	0.8884(1)	0.4461	0.8911	0.8885	-0.01	0.01	0.00	0.01	0.07
Nb11	9(*b*) 18(*f*)	0.2233(1)	0.4452(1)	0.1117(1)	0.2233	0.4449	0.1111	0.00	0.01	0.02	0.02	0.07
Nb12	9(*b*)	0.7767(1)	0.5554(1)	0.8894(1)	0.7767	0.5551	0.8889	0.00	0.01	0.02	0.02	0.07
Ca5	3(*a*) 6(*c*)	0.	0.	0.1667(1)	0.	0.	0.1697	0.	0.	-0.12	0.12	0.09
Ca6	3(*a*)	0.	0.	0.8274(1)	0.	0.	0.8303	0.	0.	-0.12	0.12	0.10
Nb13	9(*b*) 18(*f*)	0.3354(1)	-0.0008(1)	0.1678(1)	0.3329	-0.0034	0.1672	0.04	0.03	0.02	0.06	0.04
Nb14	9(*b*)	0.6695(1)	0.0059(1)	0.8334(1)	0.6671	0.0034	0.8328	0.04	0.04	0.02	0.07	0.07
Nb15	3(*a*),3(*b*)	0.	0.	0.5017(1)	0.	0.	0.5000	0.	0.	0.07	0.07	0.07
Ca7	9(*b*) 18(*f*)	0.2100(2)	0.4294(2)	0.0306(1)	0.2168	0.4356	0.0288	-0.11	-0.10	0.07	0.19	0.12
Ca8	9(*b*)	0.7764(2)	0.5582(2)	0.9729(1)	0.7832	0.5644	0.9712	-0.11	-0.10	0.07	0.19	0.12
Ca9	9(*b*) 18(*f*)	0.5545(2)	0.1090(2)	0.0264(1)	0.5514	0.1023	0.0257	0.05	0.11	0.03	0.14	0.11
Ca10	9(*b*)	0.4518(2)	0.9044(2)	0.9750(1)	0.4486	0.8977	0.9743	0.05	0.11	0.03	0.14	0.10

Ca11	9(*b*) 18(*f*)†	0.2621(20)	0.1357(20)	0.0296(7)	0.2637	0.1327	0.0320	-0.03	0.05	-0.10	0.11	0.10
Ca12	9(*b*)	0.7347(3)	0.8703(3)	0.9656(1)	0.7363	0.8673	0.9680	-0.03	0.05	-0.10	0.11	0.10
Ca13	9(*b*) 18(*f*)	0.3308(2)	0.0031(2)	0.0839(1)	0.3325	0.0028	0.0829	-0.03	0.01	0.04	0.05	0.12
Ca14	9(*b*)	0.6659(2)	-0.0025(2)	0.9180(1)	0.6675	-0.0028	0.9171	-0.03	0.01	0.04	0.05	0.16
Ca15	3(*a*) 6(*c*)	0.	0.	0.4152(1)	0.	0.	0.4162	0.	0.	-0.04	0.04	0.08
Ca16	3(*a*)	0.	0.	0.5829(1)	0.	0.	0.5839	0.	0.	-0.04	0.04	0.11
Ca17	9(*b*) 18(*f*)	0.6725(2)	0.0028(2)	0.0806(1)	0.6733	0.0042	0.0811	-0.01	-0.02	-0.02	0.03	0.11
Ca18	9(*b*)	0.3259(2)	-0.0057(2)	0.9185(1)	0.3267	-0.0042	0.9189	-0.01	-0.02	-0.02	0.03	0.10
Ca19	3(*a*) 6(*c*)†	0.	0.	0.0973(12)	0.	0.	0.0989	0.	0.	-0.06	0.06	0.10
Ca20	3(*a*)	0.	0.	0.8995(2)	0.	0.	0.9011	0.	0.	-0.06	0.06	0.10
Ca21	9(*b*) 18(*f*)	0.1181(2)	0.2237(2)	0.1367(1)	0.1142	0.2259	0.1349	0.07	-0.04	0.07	0.09	0.15
Ca22	9(*b*)	0.8898(2)	0.7720(2)	0.8670(1)	0.8858	0.7741	0.8652	0.07	-0.04	0.07	0.09	0.11
Ca23	9(*b*) 18(*f*)	0.4316(2)	0.2194(2)	0.1419(1)	0.4374	0.2188	0.1409	-0.10	0.01	0.04	0.10	0.10
Ca24	9(*b*)	0.5568(2)	0.7818(2)	0.8600(1)	0.5626	0.7812	0.8591	-0.10	0.01	0.04	0.10	0.11
Ca25	9(*b*) 18(*f*)	0.1063(2)	0.5506(2)	0.1356(1)	0.1052	0.5516	0.1382	0.02	-0.02	-0.11	0.11	0.08
Ca26	9(*b*)	0.8960(2)	0.4474(2)	0.8591(1)	0.8948	0.4484	0.8618	0.02	-0.02	-0.11	0.11	0.09
O1	9(*b*) 18(*f*)	0.0478(4)	0.2945(4)	0.0359(1)	0.0636	0.3016	0.0313	-0.27	-0.12	0.19	0.39	0.10
O2	9(*b*)	0.9205(4)	0.6912(4)	0.9734(2)	0.9364	0.6984	0.9687	-0.27	-0.12	0.19	0.39	0.12
O3	9(*b*) 18(*f*)	0.2139(4)	0.2860(4)	0.0185(1)	0.2266	0.2728	0.0239	-0.21	0.22	-0.22	0.31	0.11
O4	9(*b*)	0.7606(4)	0.7403(3)	0.9707(2)	0.7734	0.7272	0.9761	-0.22	0.22	-0.22	0.31	0.14
O5	9(*b*) 18(*f*)	0.0370(4)	0.4580(4)	0.0293(2)	0.0512	0.4638	0.0256	-0.24	-0.10	0.15	0.34	0.12
O6	9(*b*)	0.9345(4)	0.5304(4)	0.9781(2)	0.9488	0.5362	0.9744	-0.24	-0.10	0.15	0.34	0.13
O7	9(*b*) 18(*f*)	0.2282(4)	0.5807(4)	0.0369(1)	0.2278	0.6113	0.0357	0.01	-0.52	0.05	0.52	0.09
O8	9(*b*)	0.7726(3)	0.3582(3)	0.9654(1)	0.7722	0.3887	0.9643	0.01	-0.52	0.05	0.52	0.06
O9	9(*b*) 18(*f*)	0.0946(4)	0.6385(4)	0.0292(2)	0.0700	0.6246	0.0344	0.42	0.24	-0.22	0.62	0.12
O10	9(*b*)	0.9546(4)	0.3893(4)	0.9604(1)	0.9300	0.3754	0.9656	0.42	0.24	-0.22	0.62	0.11
O11	9(*b*) 18(*f*)	0.5592(4)	0.3100(4)	0.0198(1)	0.5630	0.2754	0.0195	-0.06	0.59	0.01	0.56	0.10
O12	9(*b*)	0.4333(4)	0.7592(4)	0.9807(2)	0.4370	0.7246	0.9805	-0.06	0.59	0.01	0.56	0.14
O13	9(*b*) 18(*f*)	0.3943(4)	0.3138(4)	0.0341(1)	0.4047	0.3030	0.0248	-0.18	0.18	0.39	0.43	0.11
O14	9(*b*)	0.5850(4)	0.7079(4)	0.9846(2)	0.5953	0.6970	0.9752	-0.17	0.18	0.39	0.43	0.12
O15	9(*b*) 18(*f*)	0.4114(4)	0.1182(4)	0.0160(1)	0.4029	0.1007	0.0255	0.14	0.30	-0.39	0.55	0.10
O16	9(*b*)	0.6056(4)	0.9168(4)	0.9651(1)	0.5971	0.8993	0.9745	0.14	0.30	-0.39	0.55	0.12

O17	9(*b*)	18(*f*)	0.1636(4)	-0.0127(4)	0.0943(2)	0.1808	-0.0032	0.0896	-0.29	-0.16	0.20	0.44	0.11
O18	9(*b*)		0.8020(4)	-0.0063(4)	0.9151(2)	0.8192	0.0032	0.9104	-0.29	-0.16	0.20	0.44	0.12
O19	9(*b*)	18(*f*)	0.1897(4)	0.1684(4)	0.0784(2)	0.1655	0.1544	0.0839	0.41	0.24	-0.23	0.61	0.13
O20	9(*b*)		0.8588(4)	0.8596(4)	0.9106(2)	0.8345	0.8456	0.9161	0.41	0.24	-0.23	0.61	0.12
O21	9(*b*)	18(*f*)	0.2013(5)	0.3485(5)	0.0861(2)	0.2004	0.3442	0.0865	0.02	0.07	-0.02	0.08	0.13
O22	9(*b*)		0.8005(5)	0.6601(5)	0.9131(2)	0.7996	0.6558	0.9135	0.02	0.07	-0.02	0.08	0.13
O23	9(*b*)	18(*f*)	0.1406(4)	0.4726(4)	0.0870(1)	0.1617	0.4833	0.0805	-0.36	-0.18	0.27	0.55	0.10
O24	9(*b*)		0.8172(4)	0.5060(4)	0.9260(1)	0.8383	0.5167	0.9195	-0.36	-0.18	0.27	0.55	0.09
O25	9(*b*)	18(*f*)	0.1978(4)	0.6667(4)	0.0876(2)	0.1821	0.6578	0.0908	0.27	0.15	-0.13	0.39	0.11
O26	9(*b*)		0.8335(4)	0.3512(4)	0.9061(2)	0.8179	0.3422	0.9092	0.26	0.15	-0.13	0.38	0.10
O27	9(*b*)	18(*f*)	0.5210(4)	-0.0195(4)	0.0878(1)	0.4914	-0.0189	0.0879	0.50	-0.01	0.00	0.49	0.08
O28	9(*b*)		0.5383(4)	0.0183(4)	0.9121(1)	0.5086	0.0189	0.9121	0.50	-0.01	0.00	0.49	0.08
O29	9(*b*)	18(*f*)	0.4846(4)	0.3274(4)	0.0984(2)	0.4943	0.3490	0.0869	-0.16	-0.37	0.47	0.67	0.12
O30	9(*b*)		0.4960(4)	0.6295(4)	0.9245(1)	0.5057	0.6510	0.9131	-0.16	-0.36	0.47	0.66	0.11
O31	9(*b*)	18(*f*)	0.4988(4)	0.1285(4)	0.0757(1)	0.4906	0.1422	0.0867	0.14	-0.23	-0.46	0.50	0.11
O32	9(*b*)		0.5177(4)	0.8441(4)	0.9023(1)	0.5094	0.8578	0.9133	0.14	-0.23	-0.46	0.50	0.11
O33	9(*b*)	18(*f*)	0.3385(4)	0.1435(4)	0.0943(2)	0.3366	0.1682	0.0927	0.03	-0.42	0.07	0.41	0.13
O34	9(*b*)		0.6653(4)	0.8070(4)	0.9089(2)	0.6634	0.8318	0.9073	0.03	-0.42	0.07	0.41	0.12
O35	9(*b*)	18(*f*)	0.1373(4)	0.0978(4)	0.1430(1)	0.1338	0.0651	0.1429	0.06	0.55	0.00	0.58	0.11
O36	9(*b*)		0.8697(4)	0.9677(4)	0.8572(2)	0.8662	0.9349	0.8571	0.06	0.55	0.00	0.58	0.12
O37	9(*b*)	18(*f*)	0.2750(4)	0.0598(4)	0.1502(2)	0.2897	0.0683	0.1462	-0.25	-0.14	0.17	0.38	0.12
O38	9(*b*)		0.6955(4)	0.9232(4)	0.8578(2)	0.7103	0.9317	0.8538	-0.25	-0.14	0.17	0.38	0.11
O39	9(*b*)	18(*f*)	0.2982(4)	0.2552(4)	0.1315(2)	0.2736	0.2406	0.1368	0.42	0.25	-0.22	0.63	0.12
O40	9(*b*)		0.7511(4)	0.7740(4)	0.8580(2)	0.7264	0.7594	0.8632	0.42	0.25	-0.22	0.63	0.12
O41	9(*b*)	18(*f*)	0.3048(4)	0.4272(4)	0.1430(2)	0.2862	0.4160	0.1454	0.31	0.19	-0.10	0.45	0.12
O42	9(*b*)		0.7324(4)	0.5952(4)	0.8523(1)	0.7138	0.5840	0.8546	0.31	0.19	-0.10	0.45	0.10
O43	9(*b*)	18(*f*)	0.2513(4)	0.5589(4)	0.1418(2)	0.2512	0.5608	0.1390	0.00	-0.03	0.12	0.12	0.12
O44	9(*b*)		0.7488(4)	0.4374(4)	0.8638(2)	0.7488	0.4392	0.8610	0.00	-0.03	0.12	0.12	0.11
O45	9(*b*)		0.2470(4)	0.8787(4)	0.1422(2)	0.2661	0.8908	0.1352	-0.32	-0.20	0.29	0.54	0.12
O46	9(*b*)		0.7147(4)	0.0970(4)	0.8719(1)	0.7339	0.1092	0.8648	-0.32	-0.21	0.29	0.55	0.09
O47	9(*b*)	18(*f*)	0.5594(4)	0.2008(4)	0.1377(2)	0.5955	0.1994	0.1387	-0.61	0.02	-0.04	0.60	0.13
O48	9(*b*)		0.3684(4)	0.8021(4)	0.8602(2)	0.4045	0.8006	0.8613	-0.61	0.03	-0.04	0.60	0.12

O49	9(*b*)	0.4166(4)	0.0231(4)	0.1308(1)	0.4364	0.0339	0.1402	-0.33	-0.18	-0.39	0.59	0.08
	18(*f*)											
O50	9(*b*)	0.5438(4)	0.9553(4)	0.8503(1)	0.5636	0.9661	0.8598	-0.33	-0.18	-0.39	0.59	0.10
O51	9(*b*)	0.5853(4)	0.0464(4)	0.1508(1)	0.5961	0.0351	0.1403	-0.18	0.19	0.44	0.48	0.09
	18(*f*)											
O52	9(*b*)	0.3931(4)	0.9762(4)	0.8702(1)	0.4039	0.9649	0.8597	-0.18	0.19	0.44	0.48	0.08
O53	9(*b*)	0.1067(10)	0.0457(10)	0.0125(4)	0.0320	0.0564	0.0141	1.26	-0.18	-0.07	1.18	0.18
	18(*f*)[†]											
O54	9(*b*)	0.0427(12)	0.9329(12)	0.9843(4)	-0.0320	0.9436	0.9859	1.26	-0.18	-0.07	1.18	0.18
O55	3(*a*)	0.	0.	0.9570(6)	0.	0.	0.9593	0.	0.	-0.10	0.10	0.18
	6(*c*)[†]											
O56	3(*a*)	0.	0.	0.0384(7)	0.	0.	0.0407	0.	0.	-0.10	0.10	0.18

[†] The occupancy of each Ca11, Ca12, Ca 19, Ca20, O53, O54, O55 and O56 site is given, respectively, as 8.7, 37.4, 1.5, 60.9, 56, 44, 56 and 44% with all other sites 100 % occupied.

Table S5

Modified atomic positions for $PbTa_3(PO_4)(P_2O_7)_{3.5}$ at ambient temperature (Murashova *et al.*, 2003) with hypothetical $x'y'\ z'$ coordinates and the$\Delta\ x$,$\Delta\ y$, Δz and u_{iso} displacements in Å [250098]

a = 11.6219(9), c = 14.3458(11) Å. $z^* = z - 0.0005$; $\Delta x = (x - x')a$,$\Delta\ y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3,R\bar{3}$	x	y	z	x'	y'	z'	$\Delta\ x$	$\Delta\ y$	$\Delta\ z$	$\Delta\xi$	u_{iso}	occ.
Pb1	3(*a*),3(*a*)	0	0	-0.0005	0	0	0	0	0	0.01	0.01	0.16	1.
Ta1	9(*b*),9(*e*)	0.4999(2)	-0.0002(1)	-0.0016(2)	0.5	0	0	-0.01	-0.01	-0.02	0.03	0.1	1.
P1	3(*a*) 6(*c*)	0	0	0.6078	0	0	0.6071	0	0	0.01	0.01	0.04	0.54
P2	3(*a*)	0	0	0.3937	0	0	0.3929	0	0	0.01	0.01	0.09	0.54
P3	9(*b*) 18(*f*)	0.6706(16)	0.0711(16)	0.1983(17)	0.6908	0.0770	0.1906	-0.23	-0.07	0.11	0.29	0.09	0.5
P4	9(*b*)	0.2890(15)	-0.0828(17)	-0.1839(16)	0.3092	-0.0770	-0.1906	-0.23	-0.07	0.10	0.29	0.11	0.5
O1	9(*b*) 18(*f*)	0.5924(18)	0.3970(18)	-0.0193(18)	0.5924	0.4012	-0.0249	0.0	-0.05	0.08	0.09	0.16	1.
O3	9(*b*)	0.4077(17)	0.5945(17)	0.0304(17)	0.4076	0.5988	0.0249	0.01	-0.05	0.08	0.09	0.14	1.
O2	3(*a*),3(*b*)	0	0	0.5054	0	0	0.5	0	0	0.08	0.08	0.24	0.54
O4	9(*b*) 18(*f*)	0.6214(19)	0.015(2)	0.0989(19)	0.6052	0.061	0.1778	0.19	-0.53	-1.13	1.22	0.15	1.
O14	9(*b*)	0.411(5)	-0.106(4)	-0.257(5)	0.3948	-0.061	-0.1778	0.19	-0.52	-1.13	1.22	0.2	0.5
O5	9(*b*) 18(*f*)	0.7008(19)	-0.0259(18)	0.2461(18)	0.6934	-0.0296	0.2443	0.09	0.04	0.02	0.12	0.14	1.
O9	9(*b*)	0.314(2)	0.0333(2)	-0.243(2)	0.307	0.0296	-0.244	0.08	0.04	0.02	0.11	0.16	1.
O6	9(*b*) 18(*f*)	0.815(3)	0.198(4)	0.194(3)	0.757	0.193	0.209	0.67	0.06	-0.21	0.73	0.12	0.5
O8	9(*b*)	0.301(3)	-0.188(3)	-0.223(3)	0.243	-0.193	-0.209	0.67	0.06	-0.20	0.73	0.12	0.5
O7	9(*b*) 18(*f*)	0.580(3)	0.098(3)	0.260(3)	0.602	0.065	0.18	-0.26	0.38	1.15	1.20	0.03	0.5
O10	9(*b*)	0.3762(19)	-0.0325(19)	-0.0990(19)	0.3981	-0.0653	-0.1802	-0.25	0.38	1.16	1.21	0.14	1.
P5	3(*a*)	0.	0.	0.679	0.	0.	0.6850	0.	0.	-0.09	0.09	0.17	0.46
P6	3(*a*)	0.	0.	0.309	0.	0.	0.3150	0.	0.	-0.09	0.09	0.15	0.46
P7	9(*b*) 18(*f*)	0.7224(16)	0.0895(16)	0.1805(16)	0.6956	0.0824	0.1920	0.31	0.08	-0.16	0.39	0.12	0.5
P8	9(*b*)	0.3312(17)	-0.0752(17)	-0.2035(19)	0.3044	-0.0824	-0.1920	0.31	0.08	-0.16	0.39	0.12	0.5
O11	3(*a*) 18(*f*)	0.	0.	0.789	0.	0.	0.787	0.	0.	0.03	0.03	0.09	0.46
O12	3(*a*)	0.	0.	0.215	0.	0.	0.213	0.	0.	0.03	0.03	0.28	0.46
O13	9(*b*) 18(*f*)	0.2090(4)	-0.188(4)	-0.206(3)	0.2385	-0.196	-0.2155	-0.34	0.09	0.14	0.34	0.14	0.5
O15	9(*b*)	0.732(5)	0.204(5)	0.225(5)	0.7615	0.196	0.2155	-0.34	0.09	0.14	0.34	0.24	0.5

Table S6(*a*)

Atomic positions for Pb_2ScTaO_6 at 4.2 K (Woodward & Baba-Kishi 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and $u_{\rm iso}$ displacements in Å for the rhombohedral setting [281087]

a_R = 8.15345(3) Å, α_R = 89.8488(3)°. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z - z')c$.

	Wyckoff position $R3$, $Fm\bar{3}$[†]	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$[†]	$u_{\rm iso}$
Pb1	1(*a*)	0.270(2)	0.270(2)	0.270(2)	0.25	0.25	0.25	0.14	0.14	0.14	0.24	0.13
Pb2	1(*a*)	0.764(2)	0.764(2)	0.764(2)	0.75	0.75	0.75	0.11	0.11	0.11	0.20	0.13
	8(*c*)[††]											
Pb3	3(*b*)	0.274(2)	0.264(3)	0.765(3)	0.25	0.25	0.75	0.20	0.11	0.12	0.26	0.13
Pb4	3(*b*)	0.255(2)	0.776(2)	0.755(3)	0.25	0.75	0.75	0.04	0.21	0.04	0.20	0.13
Ta1[‡]	1(*a*)	0	0	0	0	0	0	0	0	0	0	0.09
	4(*a*)											
Ta2	3(*b*)	0.5	0.5	0.	0.5	0.5	0.	0	0	0	0	0.09
Sc1	1(*a*)	0.5	0.5	0.5	0.5	0.5	0.5	0	0	0	0	0.09
	4(*b*)											
Sc2	3(*b*)	0.5	0	0	0.5	0	0	0	0	0	0	0.09
O1	3(*b*)	0.239(2)	-0.019(3)	0.001(3)	0.245	0	0	-0.05	-0.15	0.01	0.18	0.10
O2	3(*b*)	-0.249(2)	-0.027(3)	-0.011(3)	-0.245	0	0	-0.03	-0.22	-0.09	0.25	0.10
O3	3(*b*)	0.253(2)	0.483(3)	0.005(4)	0.255	0.5	0	-0.02	-0.14	0.04	0.16	0.10
O4	3(*b*)	0.740(2)	0.480(3)	-0.014(3)	0.745	0.5	0	-0.04	-0.16	-0.11	0.21	0.10
	24(*e*)											
O5	3(*b*)	0.493(4)	0.250(2)	-0.031(3)	0.5	0.255	0	-0.06	-0.04	-0.25	0.26	0.10
O6	3(*b*)	0.506(3)	0.742(2)	-0.016(3)	0.5	0.745	0	0.05	-0.02	-0.13	0.14	0.10
O7	3(*b*)	0.484(3)	0.474(3)	0.241(2)	0.5	0.5	0.245	-0.13	-0.21	-0.03	0.30	0.10
O8	3(*b*)	0.475(3)	0.500(4)	-0.248(2)	0.5	0.5	-0.245	-0.20	0	-0.02	0.20	0.10

[†] Origin displacement correction not applied. 'Ta' sites assigned a nominal content of 0.76 Ta and 0.24 Sc; 'Sc' sites a nominal content of 0.76 Sc and 0.24 Ta.

[‡] Space group $Fm\bar{3}m$ proposed by authors is not a supergroup either of $R3$ or $R\bar{3}$, but $Fm\bar{3}$ is a supergroup of $R\bar{3}$, see text.

[††] **A**toms related over more than two positions marked by braces.

Table S6(*b*)

Atomic positions for Pb_2ScTaO_6 at 4.2 K (Woodward & Baba-Kishi 2002) with hypothetical $x'y'\ z'$ coordinates and the Δx,Δy, Δz and $u_{\rm iso}$ displacements in Å for the rhombohedral setting.[†] [281087]

a = 8.15345(3) Å, α = 89.8488(3)°. $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$[†]	$u_{\rm iso}$
Pb1	1(*a*)	0.270(2)	0.270 (2)	0.270(2)	0.25	0.25	0.25	0.16	0.16	0.16	0.28	0.13
	2(*c*)											
Pb2	1(*a*)	0.764(2)	0.764(2)	0.764(2)	0.75	0.75	0.75	0.11	0.11	0.11	0.19	0.13
Pb3	3(*b*)	0.274(2)	0.264(3)	0.765(3)	0.25	0.25	0.75	0.20	0.11	0.12	0.26	0.13
	6(*f*)											
Pb4	3(*b*)	0.255(2)	0.776(2)	0.755(3)	0.25	0.75	0.75	0.04	0.21	0.04	0.22	0.13
Ta1	1(*a*),1(*a*)	0	0	0	0	0	0	0	0	0	0	0.09
Sc1	1(*b*),1(*b*)	0.5	0.5	0.5	0.5	0.5	0.5	0	0	0	0	0.09
Ta2	3(*b*),3(*e*)	0.5	0.5	0.	0.5	0.5	0.	0	0	0	0	0.09
Sc2	3(*b*),3(*d*)	0.5	0	0	0.5	0	0	0	0	0	0	0.09
O1	3(*b*)	0.239(2)	-0.019(3)	0.001(3)	0.244	0.004	0.005	-0.04	-0.19	-0.05	0.20	0.10
	6(*f*)											
O2	3(*b*)	-0.249(2)	-0.027(3)	-0.011(3)	-0.244	-0.004	-0.005	-0.04	-0.19	-0.05	0.20	0.10
O3	3(*b*)	0.253(2)	0.483(3)	0.005(4)	0.257	0.502	0.009	-0.03	-0.16	-0.03	0.17	0.10
	6(*f*)											
O4	3(*b*)	0.740(2)	0.480(3)	-0.014(3)	0.743	0.498	-0.009	-0.02	-0.16	-0.04	0.17	0.10
O5	3(*b*)	0.493(4)	0.250(2)	-0.031(3)	0.493	0.254	-0.008	0.00	0.03	-0.19	0.19	0.10
	6(*f*)											
O6	3(*b*)	0.506(3)	0.742(2)	-0.016(3)	0.506	0.746	0.008	0.00	-0.03	-0.20	0.20	0.10
O7	3(*b*)	0.484(3)	0.474(3)	0.241(2)	0.504	0.487	0.244	-0.11	-0.11	-0.02	0.16	0.10
	6(*f*)											
O8	3(*b*)	0.475(3)	0.500(4)	-0.248(2)	0.496	0.513	-0.244	-0.11	-0.11	-0.03	0.16	0.10

[†] Origin displacement correction not applied.

Table S6(*c*)

Atomic positions for Pb_2ScTaO_6 at 4.2 K (Woodward & Baba-Kishi 2002) with hypothetical $x'y'\,z'$ coordinates and the Δx,Δy, Δz and u_{iso} displacements in Å in a rhombohedral/cubic setting [281087]

a = 8.15345(3) Å. $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff position $R\bar{3}$,$Fm\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Pb1	1(*a*)	0.25	0.25	0.25	0.25	0.25	0.25	0	0	0	0	0.13
Pb2	1(*a*)	0.75	0.75	0.75	0.75	0.75	0.75	0	0	0	0	0.13
	8(*c*)†											
Pb3	3(*b*)	0.25	0.25	0.75	0.25	0.25	0.75	0	0	0	0	0.13
Pb4	3(*b*)	0.25	0.75	0.75	0.25	0.75	0.75	0	0	0	0	0.13
Ta1‡	1(*a*)	0	0	0	0	0	0	0	0	0	0	0.09
Ta2	3(*b*)	0.5	0.5	0.	0.5	0.5	0.	0	0	0	0	0.09
Sc1	1(*a*)	0.5	0.5	0.5	0.5	0.5	0.5	0	0	0	0	0.09
Sc2	3(*b*)	0.5	0	0	0.5	0	0	0	0	0	0	0.09
O1	3(*b*)	0.244	0.004	0.005	0.244	0	0	0	0.03	0.04	0.05	0.10
O2	3(*b*)	-0.244	-0.004	-0.005	-	0	0	0	0.03	0.04	0.05	0.10
O3	3(*b*)	0.257	0.502	0.009	0.256	0.5	0	0.01	0.02	0.08	0.08	0.10
O4	3(*b*)	0.743	0.498	-0.009	0.744	0.5	0	-0.01	-0.02	-0.07	0.07	0.10
	24(*e*)											
O5	3(*b*)	0.493	0.254	-0.008	0.5	0.256	0	-0.06	-0.02	-0.07	0.09	0.10
O6	3(*b*)	0.506	0.746	0.008	0.5	0.744	0	0.05	0.02	0.07	0.09	0.10
O7	3(*b*)	0.504	0.487	0.244	0.5	0.5	0.5	0.03	-0.11	0.11	0.11	0.10
O8	3(*b*)	0.496	0.513	-0.244	0.5	0.5	0.5	0.03	0.11	0.11	0.11	0.10

† Atoms related over more than two positions marked by braces.

‡ Origin displacement correction not applied.

Atomic coordinate relationships in the space groups $R3$, $R\bar{3}$, $R32$, $R3m$, $R3c$, $R\bar{3}c$, $R\bar{3}m$, $P31m$, $P312$, $P6_3/mcm$ and $Fm\bar{3}m$.

Atomic coordinate analysis requires the generation of coordinates in all possible supergroups that might be formed in settings corresponding to the original determination. Once generated, the distance between an atom in the supergroup and in the original location ($\Delta\xi$) is readily evaluated, see footnote 1. The coordinates used are based upon an appropriate selection from the following six paragraphs, taken the *International Tables for Crystallography* (2005).

Six further supergroups, in addition to those in footnote 2 of Part I, are used in Part II. The first is $R\bar{3}c$ with coordinates as follows for an atom in the general 36(*f*) position: (0, 0, 0)+, (⅔, ⅓, ⅓)+, and (⅓, ⅔, ⅔)+ (1) x, y, z; (2) $\bar{y}, x\text{-}y, z$; (3) $\bar{x}+y, \bar{x}, z$; (4) $y, x, \bar{z}+$ ½; (5) $x-y, \bar{y}, \bar{z}+$ ½; (6) $\bar{x}, \bar{x}+y, \bar{z}+$ ½; (7) $\bar{x}, \bar{y}, \bar{z}$; (8) $y, \bar{x}+y, \bar{z}$; (9) $x-y, x, \bar{z}$; (10) $\bar{y}, \bar{x}, z+$ ½; (11) $\bar{x}+y, y, z+$ ½; (12) $x, x - y, z+$ ½. There are also five sets of special positions: 18(*e*) at x, 0, ¼; 0, x, ¼; $\bar{x}, \bar{x}$, ¼; $\bar{x}$, 0 , ¾; 0 , $\bar{x}$, ¾; x , x, ¾; 18(*d*) at ½, 0, 0; 0, ½, 0; ½, ½, 0; 0, ½, ½; ½, 0, ½; ½, ½, ½; 12(*c*) at 0, 0, z; 0, 0, $\bar{z}+$ ½; 0, 0, $\bar{z}$; 0, 0, $z+$ ½; (6*b*) 0, 0, 0; 0, 0, ½; (6*a*) 0, 0, ¼; 0, 0, ¾.

The second supergroup, $R\bar{3}m$, has the following coordinates in the general 36(*i*) position: (0, 0, 0)+, (⅔, ⅓, ⅓)+, and (⅓, ⅔, ⅔)+ (1) x, y, z; (2) $\bar{y}, x - y, z$; (3) $\bar{x}+y, \bar{x}, z$; (4) $y, x, \bar{z}$; (5) $x - y, \bar{y}, \bar{z}$; (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) $\bar{x}+y, y, z$; (12) $x, x - y, z$ with eight sets of special positions: 18(*h*) at $x, \bar{x}, z$; $x, 2x, z$; $2\bar{x}, \bar{x}, z$; $\bar{x}, x, \bar{z}$; $2x, x, \bar{z}$; $\bar{x}, 2\bar{x}, \bar{z}$; 18(*g*) at x, 0, ½; 0, x, ½; $\bar{x}, \bar{x}$, ½;

$\bar{x}, 0, \tfrac{1}{2}$; $0, \bar{x}, \tfrac{1}{2}$; $x, x, \tfrac{1}{2}$; 18(*f*) at $x, 0, 0$; $0, x, 0$; $\bar{x}, \bar{x}, 0$; $\bar{x}, 0, 0$; $0, \bar{x}, 0$; $x, x, 0$; 9(*e*) at $\tfrac{1}{2}, 0, 0$; $0, \tfrac{1}{2}, 0$; $\tfrac{1}{2}, \tfrac{1}{2}, 0$; 9(*d*) at $\tfrac{1}{2}, 0, \tfrac{1}{2}$; $0, \tfrac{1}{2}, \tfrac{1}{2}$; $\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}$; 6(*c*) at $0, 0, z$; $0, 0, \bar{z}$; 3(*b*) at $0, 0, \tfrac{1}{2}$ and 3(*a*) at $0, 0, 0$.

The third supergroup, *P*31*m*, see §3.7, has general 6(*d*) position coordinates: (1) x, y, z; (2) $\bar{y}, x - y, z$; (3) $\bar{x} + y, \bar{x}, z$; (4) y, x, z; (5) $x - y, \bar{y}, z$; (6) $\bar{x}, \bar{x} + y, z$ and three sets of special positions in 3(*c*) at: (1) $x, 0, z$; (2) $0, x, z$; (3) $\bar{x}, \bar{x}, z$; in 2(*b*) at (1) $\tfrac{1}{3}, \tfrac{2}{3}, z$; (2) $\tfrac{2}{3}, \tfrac{1}{3}, z$ and in 1(*a*) at $0, 0, z$.

Coordinates for an atom in the general 6(*l*) position in the fourth supergroup *P*312, see §6.4, are (1) x, y, z; (2) $\bar{y}, x - y, z$; (3) $\bar{x} + y, \bar{x}, z$; (4) $\bar{y}, \bar{x}, \bar{z}$; (5) $\bar{x} + y, y, \bar{z}$; (6) $x, x - y, \bar{z}$ with 11 sets of special positions in 3(*k*) at: (1) $x, \bar{x}, \tfrac{1}{2}$; (2) $x, 2x, \tfrac{1}{2}$; (3) $2\bar{x}, \bar{x}, \tfrac{1}{2}$; in 3(*j*) at: (1) $x, \bar{x}, 0$; (2) $x, 2x, 0$; (3) $2\bar{x}, \bar{x}, 0$; in 2(*i*) at: (1) $\tfrac{2}{3}, \tfrac{1}{3}, z$; (2) $\tfrac{2}{3}, \tfrac{1}{3}, \bar{z}$; in 2(*h*) at: (1) $\tfrac{1}{3}, \tfrac{2}{3}, z$; (2) $\tfrac{1}{3}, \tfrac{2}{3}, \bar{z}$; in 2(*g*) at: (1) $0, 0, z$; (2) $0, 0, \bar{z}$; in 1(*f*) at $\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{2}$; in 1(*e*) at $\tfrac{2}{3}, \tfrac{1}{3}, 0$; in 1(*d*) at $\tfrac{1}{3}, \tfrac{2}{3}, \tfrac{1}{2}$; in 1(*c*) at $\tfrac{1}{3}, \tfrac{2}{3}, 0$; in 1(*b*) at $0, 0, \tfrac{1}{2}$ and in 1(*a*) at $0, 0, 0$.

The coordinates for an atom in the general 24(*l*) position of the fifth supergroup $P6_3/mcm$, see Appendix 2, §4.10 are: (1) x, y, z; (2) $\bar{y}, x - y, z$; (3) $\bar{x} + y, \bar{x}, z$; (4) $\bar{x}, \bar{y}, z + \tfrac{1}{2}$; (5) $y, \bar{x} + y, z + \tfrac{1}{2}$; (6) $x - y, x, z + \tfrac{1}{2}$; (7) $y, x, \bar{z} + \tfrac{1}{2}$; (8) $x - y, \bar{y}, \bar{z} + \tfrac{1}{2}$; (9) $\bar{x}, \bar{x} + y, \bar{z} + \tfrac{1}{2}$; (10) $\bar{y}, \bar{x}, \bar{z}$; (11) $\bar{x} + y, y, \bar{z}$; (12) $x, x - y, \bar{z}$; (13) $\bar{x}, \bar{y}, \bar{z}$; (14) $y, \bar{x} + y, \bar{z}$; (15) $x - y, x, \bar{z}$; (16) $x, y, \bar{z} + \tfrac{1}{2}$; (17) $\bar{y}, x - y, \bar{z} + \tfrac{1}{2}$; (18) $\bar{x} + y, \bar{x}, \bar{z} + \tfrac{1}{2}$; (19) $\bar{y}, \bar{x}, z + \tfrac{1}{2}$; (20) $\bar{x} + y, y, z + \tfrac{1}{2}$; (21) $x, x - y, z + \tfrac{1}{2}$; (22) y, x, z; (23) $x - y, \bar{y}, z$; (24) $\bar{x}, \bar{x} + y, z$ with 11 sets of special positions in12(*k*) at: (1) $x, 0, z$; (2) $0, x, z$; (3) $\bar{x}, \bar{x}, z$; (4) $\bar{x}, 0, z + \tfrac{1}{2}$; (5) $0, \bar{x}, z + \tfrac{1}{2}$; (6) $x, x, z + \tfrac{1}{2}$; (7) $0, x, \bar{z} + \tfrac{1}{2}$; (8) $x, 0, \bar{z} + \tfrac{1}{2}$; (9) $\bar{x}, \bar{x}, \bar{z} + \tfrac{1}{2}$; (10)

0, $\bar{x}$, $\bar{z}$; (11) $\bar{x}$, 0, $\bar{z}$; (12) x, x, $\bar{z}$; in 12(*j*) at: (1) x, y, ¼; (2) $\bar{y}$, $x - y$, ¼; (3) $\bar{x} + y$, $\bar{x}$, ¼; (4) $\bar{x}$, $\bar{y}$, ¾; (5) y, $\bar{x} + y$, ¾; (6) $x - y$, x, ¾; (7) y, x, ¼; (8) $x - y$, $\bar{y}$, ¼; (9) $\bar{x}$, $\bar{x} + y$, ¼; (10) $\bar{y}$, $\bar{x}$, ¾; (11) $\bar{x} + y$, y, ¾; (12) x, $x - y$, ¾; in 12(*i*) at: (1) x, $2x$, 0; (2) $2\bar{x}$, $\bar{x}$, 0; (3) x, $\bar{x}$, 0; (4) $\bar{x}$, $2\bar{x}$, ½; (5) $2x$, x, ½; (6) $\bar{x}$, x, ½; (7) $\bar{x}$, $2\bar{x}$, 0; (8) $2x$, x, 0; (9) $\bar{x}$, x, 0; (10) x, $2x$, ½; (11) $2\bar{x}$, $\bar{x}$, ½; (12) x, $\bar{x}$, ½; in 8(*h*) at: (1) ⅓, ⅔, z; (2) ⅔, ⅓, z + ½; (3) ⅔, ⅓, $\bar{z}$ + ½; (4) ⅓, ⅔, $\bar{z}$; (5) ⅔, ⅓, $\bar{z}$; (6) ⅓, ⅔, $\bar{z}$+ ½; (7) ⅓, ⅔, z + ½; (8) ⅔, ⅓, z; in 6(*g*) at: (1) x, 0, ¼; (2) 0, x, ¼; (3) $\bar{x}$, $\bar{x}$, ¼; (4) $\bar{x}$, 0, ¾; (5) 0, $\bar{x}$, ¾; (6) x, x, ¾; in 6(*f*) at: (1) ½, 0, 0; (2) 0, ½, 0; (3) ½, ½, 0; (4) ½, 0, ½; (5) 0, ½, ½; (6) ½, ½, ½; in 4(*e*) at: (1) 0, 0, z; (2) 0, 0, z + ½; (3) 0, 0, $\bar{z}$+ ½; (4) 0, 0, $\bar{z}$; in 4(*d*) at: (1) ⅓, ⅔, 0; (2) ⅔, ⅓, ½; (3) ⅔, ⅓, 0; (4) ⅓, ⅔, ½; in 4(*c*) at: (1) ⅓, ⅔, ¼; (2) ⅔, ⅓, ¾; (3) ⅔, ⅓, ¼; (4) ⅓, ⅔, ¾; in 2(*b*) at; (1) 0, 0, 0; (2) 0, 0, ½; in 2(*a*) at; (1) 0, 0, ¼; (2) 0, 0, ¾.

The sixth supergroup, $Fm\bar{3}m$, see §2.10 and Table S6(*a*), has coordinates for an atom in the highest applicable 24(*e*) symmetry position at: (0, ½, ½)+, (½, 0, ½)+, (½, ½, 0)+ (1) x, 0, 0; (2) $\bar{x}$, 0, 0; (3) 0, x, 0; (4) 0, $\bar{x}$, 0; (5) 0, 0, x; (6) 0, 0, $\bar{x}$ with the remaining four special positions in (24*d*) at: (1) 0, ¼, ¼; (2) 0, ¾, ¼; (3) ¼, 0, ¼; (4) ¼, 0,¾; (5) ¼, ¼ , 0; (6) ¾, ¼, 0; in 8(*c*) at (1) ¼, ¼, ¼; (2) ¼, ¼, ¾; in 4(*b*) at ½, ½, ½ and in 4(*a*) at 0, 0, 0.

3. Structures reported in space group *R*3 that more likely are in, or may develop into, crystal class 3*m*

3.1 $Li_{2-x}(Zr, Nb,Te)_2O_6$, $x \leq 0.5$ [71488]

Archaimbault *et al.* (1992). Cu$K\alpha$, powder diffractometer; integrated I_{obs} (I) and Rietveld profile (P) analyses, fixed temperature factor for Li, three compositions; (*a*) Li_2ZrTeO_6, $R(I) = 0.043$, $R(P) = 0.060$ and $R(P) = 0.105$; (*b*) $Li_{1.75}Zr_{0.75}Nb_{0.25}TeO_6$, $R(I) = 0.035$; and (*c*) $Li_{1.75}Nb_{1.75}Te_{0.25}O_6$, $R(I) = 0.047$. The O, Zr and Te atom locations in (*a*), under either *I* or *P* refinement, depart less than ~0.08 Å from that required for *R*3*c* symmetry although Li departs about 0.29 Å, assuming nearly identical occupation of the Zr/Te sites, see Tables S7(*a*),(*b*). The presence of $h0l$ reflections, $l = 2n + 1$, in composition (*b*) precludes a *c*-glide plane, hence Te was taken at $00z_1$ with Zr at $00z_2$ and $z_1 - z_2 \neq ½$ but the effects of annealing were not reported. Composition (*c*) is in full conformity with *R*3*c* symmetry. The results of Choisnet *et al.* (1988) for composition (*a*), given in Table S7(*e*), are identical to those in Table S7(*a*) within one estimated standard deviation. In view of the *c*-glide plane detected in composition (*c*), characteristic of the parent $LiNbO_3$ and $LiTaO_3$ structures, also $(LiTaO_3)_9{\cdot}Ta_2O_5$ in §2.10 of Part I, the development of such a glide plane above ambient temperatures is also likely in composition (*a*) assuming that annealing results in identical occupancy of glide-plane related sites. It is noted that the nominal values of $d_{Zr,Nb\text{-}O}$ and $d_{Te\text{-}O}$ do not differ significantly in compositions (*a*) and (*b*), also no coordinates in Table S7(*d*), reported as in space group *R*3*c*, differ more than ~0.80 Å from those required in $R\bar{3}c$ hence, within the uncertainty of these observations, each of the compositions above may also satisfy the conditions for ferroelectricity.

3.2 $[\mathrm{Cl\text{-}P(NPCl_3)_3}]^+\cdot\mathrm{Cl}^-$ [71913]

Belaj (1992). Mo*K*α, graphite monochromator; empirical absorption corrections; 1,981 $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$, anisotropic U^{ij}, $R = 0.031$, $wR = 0.0291$; 8 independent atoms. Two Cl, a N and a P atom have $0.19 \lesssim \Delta\xi \lesssim 0.32$ Å with respect to *R*3*m* supergroup symmetry, see Table S8. Since $u_{\mathrm{iso}} \approx 0.15$ Å at the determination temperature of 100 K, it is likely to increase at higher temperatures such that the supergroup structure will become the stable phase in a nonferroelectric phase transition to *R*3*m*. Rivard *et al.* (2004) reported the same structure but in a preparation containing 0.5 CH_2Cl_2 per molecule, resulting in monoclinic symmetry.

3.3 $\mathrm{Ba_{2.7}Ga_{5.4}Ge_{3.6}S_{18}}$ [75002]

Häuseler & Schmidt (1994). Mo*K*α, graphite monochromator; ψ-scan absorption corrections; 1,011 $I_{\mathrm{obs}} > 2\sigma(I_{\mathrm{obs}})$, anisotropic U^{ij}, $R = 0.101$, $wR = 0.133$ for $d_{\mathrm{C\text{-}H}}$ constrained at 1.08 Å; 4 independent atoms with Ga and Ge taken as occupying ¾ of the tetrahedrally-coordinated 9(*b*) sites. A pyroelectric-to-pyroelectric phase transition to space group *R*3*m* is likely at elevated temperatures in view of atomic displacements in the range $1.2 \gtrsim \Delta\xi \gtrsim 0.4$ Å, see Table S9.

3.4 $\mathrm{K_2Ca_2(CO_3)_3}$ [83431]

Winbo *et al.* (1997). Mo*K*α, graphite monochromator; decay and absorption corrections; 816 independent $I_{\mathrm{obs}} > n\sigma(I_{\mathrm{obs}})$, *n* not reported; anisotropic U^{ij}, $R = 0.018$, $wR = 0.018$; 12 independent atoms in space group *R*3. Nine of the 12 independent atoms approach *R*3*c* symmetry with all $\Delta\xi < 1.1$ Å, see Table S10, but the remaining three have $1.5 \lesssim \Delta\xi \lesssim 1.9$

Å. $K_2Ca_2(CO_3)_3$ is hence expected to remain polar above ambient T but may undergo a phase transition at $T_{P.T.}$ as a glide plane develops unless $T_{P.T.} > T_{decomposition}$ for this carbonate.

3.5 $Li_{0.27}Ni_{0.73}O$ [89958]

Monge *et al.* (2000). Mo$K\alpha$, graphite monochromator; extinction correction; 186 independent $F^2_{obs} > 2\sigma(F^2_{obs})$, 40 variables, U^{ij}, $R = 0.0723$, $wR(F^2) = 0.2396$; 8 independent sites, six fully occupied. Table S11 shows no atom is further than 0.02 Å from $R3m$ symmetry, with $0.03 \lesssim u_{iso} \lesssim 0.28$ Å. The polar supergroup $R3m$ is hence more likely than the assumed space group $R3$ although other space groups for $Li_xNi_{1-x}O$ with $0.01 \lesssim x \lesssim 0.49$ have been reported, including $R\bar{3}m$, $Fm\bar{3}m$ and $C2/c$.

3.6 $Cu_6Hg_3As_4S_{12}$, Aktashite [200785]

Kaplunnik *et al.,* (1980). Mo$K\alpha$, graphite monochromator; 758 independent F_{obs}, absorption corrections not reported, U_{iso} for all atoms, $R = 0.081$; 9 independent atoms. Table S12 shows that all atoms except As2 and the S1,S2 pair correspond to 9(*b*) locations, with As2 occupying the 3(*a*) and the S1,S2 pair the 18(*f*) location of supergroup $R3m$ with $0.26 \leq \Delta\xi \leq 1.11$ Å and $0.05 \leq u_{iso} \leq 0.16$ Å. A phase transition to space group $R3m$ is hence likely in mineral aktashite, probably well above ambient temperature.

3.7 $Cs_4BaTi_6Se_{27}$ and $Cs_6Ti_6S_{27}$ [280562, 280564]

3.7.1 Huang & Ibers (2001). Mo$K\alpha$, graphite monochromator, $T = 153$ K; number of independent F_{obs} not reported, numerical absorption corrections, U^{ij} varied for all atoms, R

= 0.0372, $wR(F^2)$ = 0.0926; 6 independent metal, 9 independent Se; preparation temperature 873 K. All atoms have $0.00 \lesssim \Delta\xi \lesssim 1.20$ Å with respect to the symmetry of space group *P*31*m*, see Table S13(*a*), hence a phase transition to this supergroup *via R*3*m* between measurement and preparation temperatures may be expected although it has not yet been reported. Such a transition requires the rhombohedral centering condition to be relaxed at least slightly. Each Ti has 7 independent Se as nearest neighbors with $2.51 \lesssim d_{\text{Ti-Se}} \lesssim 2.79$ Å and 8 Se atoms that form 4 bonds with $2.34 \lesssim d_{\text{Se-Se}} \lesssim 2.36$ Å, the others having $d_{\text{Se-Se}} \gtrsim 3.12$ Å.

3.7.2 Huang & Ibers (2001). Mo*K*α, graphite monochromator, T = 153 K; number of independent F_{obs} not reported, numerical absorption corrections, U^{ij} varied for all atoms, R = 0.0167, $wR(F^2)$ = 0.0452; 6 independent metal, 9 independent S atoms; preparation temperature 873 K. All atoms have $0.00 \lesssim \Delta\xi \lesssim 1.16$ Å with respect to the symmetry of space group *P*31*m*, see Table S13(*b*), assuming relaxation of the rhombohedral centering condition. Each independent Ti atom has 7 S nearest neighbors at $2.38 \lesssim d_{\text{Ti-S}} \lesssim 2.69$ Å, with two pairs of S atoms that form 4 S-S bonds of $2.06 \lesssim d_{\text{S-S}} \lesssim 2.08$ Å, the others have $d_{\text{S-S}} \gtrsim 3.02$ Å. Notably, neither the short $d_{\text{Se-Se}}$ nor the $d_{\text{S-S}}$ bonds differ significantly from those respectively in α-Se_8 (Maaninen *et al.*, 2001) or in orthorhombic S_8 [Abrahams, (1955); Carron & Donohue (1965)].

3.8 $H_2Hg_7Se_3O_{13}$ [414035]

Weil, (2004). Mo*K*α, graphite monochromator; T = 295 K; 1,395 independent $I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, numerical absorption and extinction corrections, U^{ij} varied for Hg and Se with U_{iso} varied for each O atom, site occupancies for 2 Hg atoms; R = 0.0383, wR_2 = 0.0970; 5

independent Hg, 3 Se and 7 O atoms; Flack parameter, 0.01. All atoms reported, except for Hg1 with $\Delta\xi \approx 0.55$ Å, have $0.00 \lesssim \Delta\xi \lesssim 0.08$ Å with respect to $R3m$ symmetry, see Table S14. Since $0.11 \lesssim u_{\mathrm{eq}} \lesssim 0.27$ Å, the higher symmetry is more likely to be the stable form at or above 295 K. Further refinement of the hypothetical coordinates in $R3m$, including the unequally split Hg2,Hg3 pair, proved unsuccessful (Weil, 2006) lending support to the original assignment of $R3$ symmetry at 295 K. If $\Delta\xi$(Hg1) approaches u_{eq} as T increases and the material remains stable, it is likely that a phase transition from $R3$ to $R3m$ will occur.

Tables for Appendix 1

Table S7(*a*)

Atomic positions for Li_2ZrTeO_6 at ambient temperature (Archaimbault *et al.,*1992) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å using powder pattern (*I*) intensities [71488]

$a = 5.172(2)$, $c = 13.849(6)$ Å. $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3$, $R3c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li1	3(*a*)	0	0	0.29(1)	0	0	0.275	0	0	0.21	0.21	0.11†
	6(*a*)											
Li2	3(*a*)	0	0	0.76(1)	0	0	0.775	0	0	-0.21	0.21	0.11†
Zr	3(*a*)	0	0	0.993(1)	0	0	0.996	0	0	-0.04	0.04	0.11
	6(*a*)‡											
Te	3(*a*)	0	0	0.500(1)	0	0	0.496	0	0	0.06	0.06	0.10
O1	9(*b*)	0.049(2)	0.355(3)	0.077(1)	0.0435	0.3515	0.0765	0.03	0.02	0.01	0.04	0.12
	18(*b*)											
O2	9(*b*)	0.652(2)	0.962(2)	0.576(4)	0.6485	0.9565	0.5765	0.02	0.03	-0.01	0.04	0.12

† Fixed value.

‡ Assuming comparable site occupancies.

Table S7(*b*)

Atomic positions for Li_2ZrTeO_6 at ambient temperature (Archaimbault *et al.,*1992) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å by Rietveld profile (*P*) analysis [71489]

$a = 5.1732(5)$, $c = 13.8508(7)$ Å. $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3$, $R3c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li1	3(*a*)	0	0	0.286(4)	0	0	0.2755	0	0	0.15	0.15	0.11†
	6(*a*)											
Li2	3(*a*)	0	0	0.765(3)	0	0	0.7755	0	0	-0.15	0.15	0.11†
Zr	3(*a*)	0	0	0.0002(6)	0	0	0.9972	0	0	0.04	0.04	0.11
	6(*a*)‡											
Te	3(*a*)	0	0	0.4942(5)	0	0	0.4972	0	0	-0.04	0.04	0.10
O1	9(*b*)	0.056(4)	0.360(4)	0.071(1)	0.048	0.357	0.074	0.04	0.02	-0.04	0.07	0.12
	18(*b*)											
O2	9(*b*)	0.646(3)	0.960(4)	0.577(1)	0.643	0.952	0.574	0.02	0.04	0.04	0.07	0.12

† Fixed value.

‡ Assuming comparable site occupancies.

Table S7(*c*)

Atomic positions for $Li_{1.75}Zr_{0.75}Nb_{0.25}TeO_6$ at ambient temperature (Archaimbault *et al.,*1992) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å using powder pattern (*I*) intensities [71490]

$a = 5.167(2)$, $c = 13.795(6)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*3*c*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li1	3(*a*)	0	0	0.30(1)	0	0	0.28	0	0	0.28	0.28	0.11[†]
	6(*a*)											
Li2	3(*a*)	0	0	0.76(2)	0	0	0.78	0	0	-0.28	0.28	0.11[†]
Zr,Nb[‡]	3(*a*)	0	0	0.989(1)	0	0	0.995	0	0	-0.08	0.08	0.11
	6(*a*)											
Te	3(*a*)	0	0	0.501(4)	0	0	0.495	0	0	0.08	0.08	0.11
O1	9(*b*)	0.049(2)	0.351(8)	0.084(9)	0.0435	0.348	0.0795	0.03	0.02	0.06	0.07	0.15
	18(*b*)											
O2	9(*b*)	0.655(5)	0.962(4)	0.575(8)	0.652	0.959	0.5795	0.02	0.02	-0.06	0.07	0.18

[†] Fixed value.

[‡] Occupancies: Zr, 0.75; Nb, 0.25.

Table S7(*d*)

Modified atomic positions for $Li_{1.75}Nb_{1.75}Te_{0.25}O_6$ at ambient temperature (Archaimbault *et al.,*1992) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å using powder pattern (*I*) intensities [71491]

$a = 5.148(3)$, $c = 13.763(8)$ Å. $z^* = z + 0.014$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3c$, $R\bar{3}c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Li	6(*a*),6(*a*)	0	0	0.304(1)	0	0	0.25	0	0	0.74	0.74	0.11[†]
Nb,Te[‡]	6(*a*),6(*b*)	0	0	0.998(1)	0	0	0.00	0	0	-0.03	0.03	0.11
O	18(*b*),18(*e*)	0.063(2)	0.369(1)	0.697(1)	0	0.369	0.75	0.32	0	-0.73	0.80	0.15

[†] Fixed value.

[‡] Occupancies: Nb, 0.875; Te, 0.125.

Table S7(*e*) Li_2ZrTeO_6

Atomic positions in Li_2ZrTeO_6 at ambient temperature (Choisnet *et al.*, 1988) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [202648]

$a = 5.172(2)$, $c = 13.847(6)$ Å. $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$

	Wyckoff position *R*3,*R*3*c*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Li1	3(*a*)	0	0	0.29(1)	0	0	0.275	0	0	0.21	0.21	0.11
	6(*c*)											
Li2	3(*a*)	0	0	0.76(1)	0	0	0.775	0	0	-0.21	0.21	0.11
Zr1	3(*a*)	0	0	0.993(1)	0	0	0.9965	0	0	-0.05	0.05	0.11
	6(*c*)											
Te1	3(*a*)	0	0	0.500(1)	0	0	0.4965	0	0	0.05	0.05	0.10
O1	9(*b*)	0.049(2)	0.355(3)	0.077(4)	0.0435	0.3515	0.0765	0.03	0.02	0.01	0.04	0.12
	18(*f*)											
O2	9(*b*)	0.652(2)	0.962(2)	0.576(4)	0.6485	0.9565	0.5765	0.02	0.03	-0.01	0.04	0.10

Table S8

Modified atomic positions for $[Cl\text{-}P(NPCl_3)_3]^+\cdot Cl^-$ at 100 K (Belaj, 1992) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [71913]

$a = 10.600(1)$, $c = 14.167(2)$ Å. $z^* = z - 0.17214$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*3*m*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cl1	3(*a*),3(*a*)	0	0	0.59482(10)	0	0	0.59482	0	0	0	0	0.15
Cl5	3(*a*),3(*a*)	0	0	0.827865	0	0	0.827865	0	0	0	0	0.11
P1	3(*a*),3(*a*)	0	0	0.45323(10)	0	0	0.45323	0	0	0	0	0.12
N	9(*b*),9(*b*)	0.16102(21)	0.05347(22)	0.41711(17)	0.1430	0.0715	0.41711	0.19	-0.19	0	0.19	0.12
P2	9(*b*),9(*b*)	0.31157(6)	0.18861(6)	0.43542(8)	0.3335	0.1667	0.43542	-0.23	0.23	0	0.23	0.15
Cl2	9(*b*),9(*b*)	0.44498(6)	0.21421(7)	0.33157(8)	0.43946	0.2197	0.33157	0.06	-0.06	0	0.06	0.15
Cl4	9(*b*),9(*b*)	0.40843(8)	0.17343(8)	0.55128(9)	0.3879	0.1939	0.55128	0.22	-0.22	0	0.22	0.16
Cl3	9(*b*),9(*b*)	0.31640(7)	0.37589(7)	0.44872(9)	0.3461	0.3461	0.44872	-0.31	0.32	0	0.32	0.13

Table S9

Atomic positions for $Ba_{2.7}Ga_{5.4}Ge_{3.6}S_{18}$ at 295 K (Häuseler & Schmidt, 1994) with hypothetical $x'y'\ z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [75002]

a = 9.600(1), c = 8.684(1) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z^{*} - z')c$.

	Wyckoff position $R3$, $R3m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Ba	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	0.13	0.9
Ga,Ge	9(*b*),9(*b*)	0.4799(1)	0.3779(1)	0.9119(2)	0.5719	0.2859	0.9119	-0.88	0.88	0	0.88	0.09	0.6,0.4
S1	9(*b*),9(*b*)	0.6063(4)	0.0790(3)	0.6524(3)	0.5618	0.1235	0.6524	0.43	-0.43	0	0.43	0.11	1.
S2	9(*b*),9(*b*)	0.1916(3)	-0.0460(3)	0.6803(4)	0.1188	-0.1188	0.6803	0.70	0.70	0	1.21	0.10	1.

Table S10

Atomic positions for $K_2Ca_2(CO_3)_3$ at 293 K (Winbo *et al.,* 1997) with hypothetical $x'y'\ z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [83431]

a = 13.010(4), c = 8.615(3) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z - z')c$.

	Wyckoff position $R3$,$R3c$	x	y	z^{*}	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Ca1	3(*a*)	0	0	0.4455(1)	0	0	0.4088	0	0	0.32	0.32	0.10
	6(*a*)											
K1	3(*a*)	0	0	0.8722(1)	0	0	0.9088	0	0	-0.32	0.32	0.14
Ca2	9(*b*)	0.26829(4)	0.39207(4)	0.90183(7)	0.25917	0.37759	0.92610	0.12	0.19	-0.21	0.34	0.12
	18(*b*)											
K2	9(*b*)	0.25005(6)	0.89606(6)	0.45037(9)	0.25917	0.88158	0.42610	-0.12	-0.19	0.21	0.34	0.17
O1	9(*b*)	0.0602(2)	0.6677(2)	0.3646(2)	0.0950	0.6859	0.3135	-0.45	-0.24	0.44	0.75	0.13
	18(*b*)											
O4	9(*b*)	0.2959(2)	0.8702(2)	0.7623(3)	0.3141	0.9050	0.8135	-0.24	-0.45	-0.44	0.75	0.18
O3	9(*b*)	0.2631(2)	0.4476(2)	0.1652(2)	0.3286	0.5171	0.1784	-0.85	-0.90	-0.11	1.52	0.13
	18(*f*)											
O5	9(*b*)	0.1231(2)	0.5865(2)	0.6915(2)	0.1885	0.5171	0.6784	-0.85	0.90	0.11	0.88	0.16
O2	9(*b*)	0.0828(2)	0.1628(2)	0.6367(2)	0.0895	0.1585	0.6998	-0.09	0.06	-0.54	0.55	0.13
	18(*f*)											
O6	9(*b*)	0.0962(2)	0.9354(2)	0.2628(2)	0.0895	0.9311	0.1998	0.09	0.06	0.54	0.56	0.16
C1	9(*b*)	0.1409(2)	0.5254(2)	0.7937(2)	0.1394	0.5011	0.7857	0.02	0.32	0.07	0.34	0.11
	18(*f*)											
C2	9(*b*)	0.1378(2)	0.6625(2)	0.2777(6)	0.1394	0.6383	0.2857	-0.02	0.32	-0.07	0.32	0.11

Table S11 $\mathbf{Li_{0.27}Ni_{0.73}O}$

Atomic positions for $Li_{0.27}Ni_{0.73}O$ (Monge *et al.*, 2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [89958]

a = 6.020(2), c = 14.726(5) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z - z')c$.

	Wyckoff position *R*3, *R*3*m*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occupancy %
Ni1	3(*a*)	0.	0.	0.895(9)	0.	0.	0.895	0.	0.	0.	0.	0.11	1.
Ni2	9(*b*)	0.498(3)	0.498(2)	0.399(8)	0.5	0.5	0.399	-0.01	-0.01	0.	0.01	0.11	1.
Ni3,Li1	9(*b*)	0.827(7)	1.667(7)	0.553(7)	0.831	1.663	0.553	-0.02	0.02	0.	0.02	0.20	0.52(5), 0.48(5)
Ni4,Li2	3(*a*)	0	0	0.400	0	0	0.400	0.	0.	0.	0.	0.13	0.24(8), 0.76(8)
O1	3(*a*)	0.	0.	0.142(8)	0.	0.	0.142	0.	0.	0.	0.	0.03†	1.
O2	9(*b*)	0.163(6)	0.332(5)	0.474(9)	0.165	0.330	0 .474	-0.01	0.01	0.	0.01	0.20	1.
O3	3(*a*)	0.	0.	0.981	0.	0.	0.981	0.	0.	0.	0.	0.28	1.
O4	9(*b*)	0.353(6)	0.179(5)	0.317(7)	0.355	0.177	0.317	-0.01	0.01	0	0.01	0.13	1.

† U_{eq}(O1) reported as 0.001(22) Å^2.

Table S12

Atomic positions in $Cu_6Hg_3As_4S_{12}$ (Kaplunnik *et al.,* 1980) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [200785]

a = 13.720(3), c = 9.329(1) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z - z')c$.

	Wyckoff position *R*3,*R*3*m*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Hg1	9(*b*),9(*b*)	0.310(2)	0.2263(4)	0.0273(4)	0.357	0.1788	0.0273	-0.64	0.65	0.	0.64	0.16
Cu1	9(*b*),9(*b*)	0.076(1)	0.2921(2)	0.0222(2)	0.123	0.2454	0.0222	-0.64	0.64	0.	0.64	0.11
Cu2	9(*b*),9(*b*)	0.3915(4)	0.552(3)	0.0372(6)	0.3145	0.629	0.0372	1.06	-1.06	0.	1.06	0.11
As1	9(*b*),9(*b*)	0.5610(6)	0.178(2)	0.0192(4)	0.5797	0.159	0.0192	-0.26	0.26	0.	0.26	0.10
As2	3(*a*),3(*a*)	0	0	0	0	0	0	0	0	0	0	0.05
S1	9(*b*) 18(*f*)	0.3729(8)	0.0899(5)	0.104(2)	0.4154	0.0387	0.0946	-0.58	0.70	0.09	0.65	0.08
S2	9(*b*)	0.4579(7)	0.428(3)	0.0852(5)	0.4154	0.377	0.0946	0.58	0.70	-0.09	1.11	0.07
S3	9(*b*),9(*b*)	0.1186(3)	0.1561(5)	0.1271(4)	0.0916	0.1831	0.1271	0.37	-0.376	0.	0.37	0.09
S4	9(*b*),9(*b*)	0.2036(8)	0.475(3)	0.1153(6)	0.2262	0.4524	0.1153	-0.31	0.31	0.	0.31	0.08

Table S13(*a*)

Atomic positions in $BaCs_4Ti_6Se_{27}$ at 153 K (Huang & Ibers, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [280562]

$a = 13.8039(16)$, $c = 20.8500(20)$ Å. $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, P31m$†	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Cs1	9(*b*),9(*b*)	0.36528(6)	0.37174(7)	0.20213(12)	0.36851	0.36851	0.20213	-0.04	0.04	0.0	0.04	0.16	1
Cs2	3(*a*),3(*a*)	0	0	0.76914(12)	0	0	0.76914	0.0	0.0	0.0	0.0	0.15	1
Ba1	3(*a*),3(*a*)	0	0	0.34918(15)	0	0	0.34918	0.0	0.0	0.0	0.0	0.11	0.553(3)
Ba2	3(*a*),3(*a*)	0	0	0	0	0	0	0.0	0.0	0.0	0.0	0.11	0.447(3)
Ti1	9(*b*),9(*b*)	0.68859(15)	0.67601(15)	0.14869(14)	0.68230	0.68230	0.14869	0.09	-0.09	0.0	0.09	0.14	1.
Ti2	9(*b*),9(*b*)	0.68933(15)	0.64321(16)	0.32019(13)	0.66627	0.66627	0.32019	0.32	-0.32	0.0	0.32	0.14	1.
Se1	9(*b*),9(*b*)	0.66676(9)	0.52469(8)	0.22363(12)	0.59572	0.59572	0.22363	0.98	-0.98	0.0	0.98	0.14	1.
Se2	9(*b*),9(*b*)	0.89213(9)	0.82409(9)	0.17565(12)	0.85811	0.85811	0.17565	0.47	-0.47	0.0	0.47	0.14	1.
Se3	9(*b*),9(*b*)	0.81209(9)	0.65651(9)	0.05679(12)	0.73430	0.73430	0.05679	1.07	-1.07	0.0	1.07	0.15	1.
Se4	9(*b*),9(*b*)	0.89764(9)	0.72409(11)	0.33425(12)	0.81087	0.81087	0.33425	1.20	-1.20	0.0	1.20	0.17	1.
Se5	9(*b*),9(*b*)	0.74901(9)	0.81312(9)	0.24183(12)	0.78107	0.78107	0.24183	-0.44	0.44	0.0	0.44	0.16	1.
Se6	9(*b*),9(*b*)	0.74998(10)	0.86415(9)	0.07246(12)	0.80707	0.80707	0.07246	-0.79	0.79	0.0	0.79	0.16	1.
Se7	9(*b*),9(*b*)	0.69594(10)	0.79929(9)	0.40262(12)	0.74762	0.74762	0.40262	-0.71	0.71	0.0	0.71	0.17	1.
Se8	9(*b*),9(*b*)	0.50126(10)	0.63862(10)	0.31142(12)	0.56994	0.56994	0.31142	-0.95	0.95	0.0	0.95	0.16	1.
Se9	9(*b*),9(*b*)	0.49905(9)	0.65983(10)	0.15136(12)	0.57944	0.57944	0.15136	-1.11	1.11	0.0	1.11	0.18	1.

† Assuming atoms related by rhombohedral centering below remain close to these positions above an unreported phase transition.

Table S13(*b*)

Atomic positions in $Cs_6Ti_6S_{27}$ at 153 K (Huang & Ibers, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [280564]

a = 13.5203(8), *c* = 19.7843(11) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3,P31m$†	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Cs1	9(*b*),9(*b*)	0.35947(2)	0.37347(2)	0.19929(2)	0.36647	0.36647	0.19929	-0.09	0.09	0.0	0.09	0.16
Cs2	3(*a*),3(*a*)	0	0	0.76528(2)	0	0	0.76528	0.0	0.0	0.0	0.0	0.13
Cs3	3(*a*),3(*a*)	0	0	0.33928(2)	0	0	0.33928	0.0	0.0	0.0	0.0	0.13
Cs4	3(*a*),3(*a*)	0	0	0	0	0	0	0.0	0.0	0.0	0.0	0.13
Ti1	9(*b*),9(*b*)	0.68762(5)	0.67608(4)	0.14447(3)	0.68185	0.68185	0.14447	0.08	-0.08	0.0	0.08	0.11
Ti2	9(*b*),9(*b*)†	0.69219(5)	0.64732(5)	0.31498(3)	0.66976	0.66976	0.31498	0.30	-0.30	0.0	0.30	0.11
S1	9(*b*),9(*b*)	0.66555(7)	0.52985(6)	0.21923(4)	0.59770	0.59770	0.21923	0.92	-0.92	0.0	0.92	0.12
S2	9(*b*),9(*b*)	0.88137(6)	0.81921(7)	0.17339(4)	0.85029	0.85029	0.17339	0.42	-0.42	0.0	0.42	0.12
S3	9(*b*),9(*b*)	0.79994(7)	0.65211(7)	0.04933(4)	0.72602	0.72602	0.04933	1.00	-1.00	0.0	1.00	0.13
S4	9(*b*),9(*b*)	0.89135(7)	0.71953(7)	0.33410(4)	0.80544	0.80544	0.33410	1.16	-1.16	0.0	1.16	0.13
S5	9(*b*),9(*b*)	0.75422(6)	0.81293(6)	0.23491(4)	0.78358	0.78358	0.23491	-0.40	0.40	0.0	0.40	0.12
S6	9(*b*),9(*b*)	0.74018(6)	0.85630(6)	0.06596(4)	0.79824	0.79824	0.06596	-0.78	0.78	0.0	0.78	0.12
S7	9(*b*),9(*b*)	0.70602(7)	0.80063(6)	0.40118(4)	0.75333	0.75333	0.40118	-0.64	0.64	0.0	0.64	0.13
S8	9(*b*),9(*b*)	0.50998(7)	0.64159(8)	0.31150(4)	0.57578	0.57578	0.31150	-0.89	0.89	0.0	0.89	0.14
S9	9(*b*),9(*b*)	0.50317(7)	0.65835(7)	0.14456(4)	0.58076	0.58076	0.14456	-1.05	1.05	0.0	1.05	0.13

† Assuming atoms related by rhombohedral centering below remain close to these positions above an unreported phase transition.

Table S14

Atomic positions in $H_2Hg_7Se_3O_{13}$ (Weil, 2004) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and $u_{\rm iso}$ displacements in Å [414035]

a = 5.9239(3), c = 37.096(3) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*3*m*	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$u_{\rm eq}$	occ.
Hg1	9(*b*),9(*b*)	1.07549(12)	0.39773(12)	0.07446(2)	0.98214	0.49107	0.07446	0.55	-0.55	0.	0.55	0.13	
Hg2†	9(*b*),9(*b*)	0.3837(5)	0.1843(7)	0.22504(5)	0.3787	0.1893	0.22504	0.03	-0.03	0.	0.03	0.27	0.601
Hg3	9(*b*),9(*b*)	0.545(2)	0.101(2)	0.2299(3)	0.549	0.097	0.2299	-0.02	0.02	0.	0.02	0.14	0.066
Hg4	3(*a*),3(*a*)	0.0000	0.0000	0.14916(3)	0.	0.	0.14916	0.	0.	0.	0.	0.14	
Hg5	3(*a*),3(*a*)	0.0000	0.0000	0.64822(3)	0.	0.	0.64822	0.	0.	0.	0.	0.13	
Se1	3(*a*),3(*a*)	0.0000	0.0000	-0.00003(8)	0.	0.	-0.00003	0.	0.	0.	0.	0.12	
Se2	3(*a*),3(*a*)	0.0000	0.0000	0.30117(9)	0.	0.	0.30117	0.	0.	0.	0.	0.13	
Se3	3(*a*),3(*a*)	0.0000	0.0000	0.49855(8)	0.	0.	0.49855	0.	0.	0.	0.	0.12	
O1	9(*b*),9(*b*)	1.031(3)	0.496(3)	0.1500(5)	1.018	0.509	0.1500	0.08	-0.08	0.	0.08	0.18	
O2	9(*b*),9(*b*)	0.149(3)	0.292(3)	0.2799(4)	0.147	0.294	0.2799	0.01	-0.01	0.	0.01	0.18	
O3	9(*b*),9(*b*)	0.297(3)	0.148(3)	0.0207(4)	0.297	0.148	0.0207	0.	0.	0.	0.	0.14	
O4	3(*a*),3(*a*)	0.0000	0.0000	0.0945(6)	0.	0.	0.0945	0.	0.	0.	0.	0.11	
O5	3(*a*),3(*a*)	0.0000	0.0000	0.2036(9)	0.	0.	0.2036	0.	0.	0.	0.	0.20	
O6	3(*a*),3(*a*)	0.0000	0.0000	0.5428(8)	0.	0.	0.5428	0.	0.	0.	0.	0.17	
O7	3(*a*),3(*a*)	0.0000	0.0000	0.7536(6)	0.	0.	0.7536	0.	0.	0.	0.	0.11	

† Hg2 and Hg3 may also have an 18(*c*) location relationship in *R*3*m* as shown below:

Hg2	9(*b*) 18(*c*)†	0.3837(5)	0.1843(7)	0.22504(5)	0.4643	0.1426	0.22747	-0.48	0.24	-0.09	0.42	0.27	0.601
Hg3	9(*b*)	0.545(2)	0.101(2)	0.2299(3)	0.4644	0.1426	0.22747	0.48	-0.25	0.09	0.43	0.14	0.066

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

4.1 Mg_9Sn_5 [55577]

Range *et al.* (1996). Mo*K*α, graphite monochromator; $T = 296$ K; 975 independent F_{obs}, 473 $F_{\mathrm{obs}} > 4\sigma(F_{\mathrm{obs}})$, absorption corrections, U^{ij}, $R[4\sigma(F_{\mathrm{obs}})] = 0.0297$, $wR^2[4\sigma(F_{\mathrm{obs}})]$ not given, R[all data] = 0.0773, wR^2[all data] = 0.0811; 12 independent atoms; twinning parameter, 0.437. Since $0.05 \lesssim \Delta\xi \lesssim 0.16$ Å and $0.12 \lesssim u_{\mathrm{eq}} \lesssim 0.21$ Å with respect to space group $R\bar{3}$, see Table S15, and the structural free-energy is lower in a centrosymmetric space group than in comparable symmetry without inversion centers, the space group is more likely $R\bar{3}$ at 296 K.

4.2 $Al_{4.2}Cu_{3.2}Zn_{0.7}$ [57730]

Murphy, (1975). Cu*K*α powder diffraction, one-dimensional Fourier projections; electron microscopy; $T \approx 296$ K; qualitative analysis with "centrosymmetry" assumed. All atoms were taken as unequally occupying ten equispaced locations, with every fifth position along the *c*-axis vacant, see Table S16. All atoms satisfy the Wyckoff 6(*c*) position both in space group $R\bar{3}$ and space group *R*32 in space and in occupancy equivalence. The original structural assignment of ICSD #57730 to space group *R*3 has been changed to $R\bar{3}$ (Allmann, 2006).

4.3 $Gd_{13}Ge_6O_{31}F$ [62329]

Mamin *et al.,* (1987). Mo*K*α, graphite monochromator; 1,994 independent $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$; u_{aniso}; 19 independent atoms in *R*3, $R = 0.045$, $wR = 0.052$ or 10 independent atoms in $R\bar{3}$,

R = 0.052, wR = 0.059. The former space group was proposed. However, all coordinate pairs except x(O9, O10) satisfy the Wyckoff 18(f) condition in $R\bar{3}$ with $0.02 \lesssim \Delta\xi \lesssim 0.18$ Å and $0.05 \lesssim u_{\mathrm{eq}} \lesssim 0.17$ Å, see Table S17. The reported value of $x(\mathrm{O9}) \equiv x(\mathrm{O10})$ corresponds to $d_{\mathrm{Gd1\text{-}O9}} = 1.859$ Å whereas $2.73 > d_{\mathrm{Gd\text{-}O}} > 2.20$ Å for all other $d_{\mathrm{Gd\text{-}O}}$. Reversing the sign of x(O9) leads to $d_{\mathrm{Gd1\text{-}O9}} = 2.28$ Å; the missing negative sign hence appears to be a typographic error and the centrosymmetric choice of space group thus appears to be more likely.[1]

4.4 $\mathbf{Cr_2Si_2Te_6}$ [62379, 71020]

Ouvrard *et al.,* (1988). Mo$K\alpha$, graphite monochromator; 456 independent $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$; absorption, extinction corrections; u_{eq}, R = 0.033, wR = 0.044; 6 independent atoms in $R3$. An origin shift of 0.1402 and replacing the reported x,y,z(Te1) coordinates by its rhombohedral equivalent at +⅔,⅓,⅓ reveal that all six independent atoms satisfy space group $R\bar{3}$ with $\Delta\xi_{\max} \lesssim 0.02$ Å, see Table S18(a). The erroneous choice of space group was also noted by Marsh (1988). Comparison of the final coordinate values refined by Marsh with the derived x',y',z' coordinates in Table S18(a) shows the two sets agree within 0.003 Å, see Table S18(b).

4.5 $\mathbf{(NH_4)_6NiMo_9O_{32}\cdot 6H_2O}$ [72710, 67576]

Dunne *et al.,* (1992). Mo$K\alpha$, graphite monochromator; absorption corrections; 1,741 $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$, anisotropic U^{ij} refined but not reported, R = 0.0254, wR = 0.0294; 20 independent atoms. Although Weakley (1987) had previously determined the structure of

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[1] Hypothetical atoms, or atoms with assumed sign change, here and elsewhere in the text or tables are in italic.

$(NH_4)_6NiMo_9O_{32}\cdot 6H_2O$ in space group *R*32, it was not mentioned by Dunne *et al.,* (1992) who reported their best refinement was in *R*3; the resulting coordinates, however, led to $\Delta\xi \lesssim 0.18$ Å for all atoms with respect to *R*32 symmetry except for the two water O atoms for which $\Delta\xi(O13) = \Delta\xi(O14) = 1.13$ Å, see Table S19(*a*). Stratemeier *et al.,* (1992), in an independent report, reconfirmed the space group as *R*32. A comparison of the latter's results with Dunne *et al*.s' (1992), after averaging the *R*3 coordinates in *R*32 as in Table S19(*b*), shows excellent agreement for the metal and 5 O atoms with $\Delta\xi \lesssim 0.02$ Å; the two N atoms with $0.07 \lesssim \Delta\xi \lesssim 0.18$ Å, however, clearly agree less well; only one of the two independent water O atoms, with $\Delta\xi(O) \approx 1.22$ Å, was located by Dunne *et al.,* (1992), *cf.* §4.13.

4.6 $Sr(BH)_{12}\cdot 7H_2O$ [200016]

Solntsev *et al*. (1977): Mo*K*α, graphite monochromator; 1,400 independent $I_{obs} \geq n\sigma(F_{obs})$, *n* not reported; final $R = 0.076$; 8 independent atoms in *R*3. Tiritiris & Schleid's (2001): Mo*K*α, graphite monochromator; extinction and numerical absorption corrections; 468 independent $F_{obs} \geq 4\sigma(F_{obs})$; final $R = 0.031$; 7 independent atoms in $R\bar{3}$. Solntsev *et al*.'s (1977) results placed no atom except O3 further than 0.15 Å from locations corresponding to $R\bar{3}$, see Table S20(*a*). Assuming the atom *O3A* occupies a position approximately related to that of O3 by an inversion center as in Table S20(*a*) but had not been detected,[1] then it is likely that the space group at the measurement temperature is $R\bar{3}$ since the resulting $\Delta\xi_{max} = 0.15$ Å with $0.04 \lesssim u_{iso} \lesssim 0.25$ Å. The $B_{12}H_{12}^{2-}$ and SrO_8^{2+} ions form an overall NaCl-like structure, with *O4* completing a dodecahedral arrangement of O atoms about Sr. Tiritiris & Schleid's (2001) more reliable redetermination of the structure in space group $R\bar{3}$ shows the two sets of atomic coordinates for Sr and the two independent O atoms are in close agreement, see Table S20(*b*). The centrosymmetric space group is hence confirmed but not the earlier B coordinates. Solntsev *et al.* (1977) were unable to locate the H atoms, preventing their comparison with the values in Table S20(*b*).

4.7 **MgSiO$_3$ (ilmenite type)** [31176, 75738, 89805]

Horiuchi *et al.*'s (1988). Mo*K*α, graphite monochromator; 366 unique $F_{\mathrm{obs}} > 3\sigma(F_{\mathrm{obs}})$; no absorption corrections; 3 independent atoms in $R\bar{3}$; anisotropic U^{ij}, $R = 0.049$, $wR = 0.038$, see Table S21(*a*). *Ab initio* calculations by d'Arco *et al.* (1994) of the structure under high pressure, as those by Karki *et al.* (2000) who stated ilmenite has space group *R*3*c* but used *R*3 symmetry[2] at high pressures, gave atomic coordinates in space group *R*3 that differ less than 0.03 Å from Horiuchi *et al.*'s (1988), see Tables S21(*b*) and S21(*c*).

4.8 **CdPS$_3$** [80875]

Boucher *et al.,* (1995). Mo*K*α, graphite monochromator; Gaussian absorption corrections; 914 independent I_{obs} at 133 K, 679 $I_{\mathrm{obs}} > 2.5\ \sigma(I_{\mathrm{obs}})$, anisotropic, anharmonic U^{ij}, $R = 0.019$, $wR = 0.021$; 6 independent atoms in space group *R*3, 3 in $R\bar{3}$. A phase transition from *C*2/*m* either to *R*3 or $R\bar{3}$ symmetry was found at $T_{\mathrm{P.T.}} \approx 228$ K on cooling [Boucher *et al.,* (1994); Covino & Lowe-Ma, (1986); Ouvrard *et al.,* (1985)]. Boucher *et al.,* (1995) opted for *R*3 but examination of Table S22 shows that the atomic coordinates expected at *T*

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[2] Inclusion of the symbol '*c*' in *R*3*c* was a typographic error, (private communication from Prof. Karki, 2006).

$\leqslant T_{\mathrm{P.T.}}$ differ less than 0.03 Å from those corresponding to $R\bar{3}$ symmetry. With $\Delta\xi \ll u_{iso}$, the higher symmetry is most likely the stable state.

4.9 Eudialyte-type mineral variants [90835, 91548]

4.9.1 Ekimenkova *et al.*, (2000), see also §§4.92 and 5.5, report four variants of mineral eudialyte with space group $R3$, each consisting of both 'framework' and 'non-framework' atoms in various proportions. The present study used Mo$K\alpha$, graphite monochromator; 4,920 $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$ with 3,206 independent $F_{\mathrm{obs}} > 4\sigma(F_{\mathrm{obs}})$, absorption corrections, U_{eq}, $R = 0.037$; 62 independent atoms. Table S23(*a*) reveals $0.01 \lesssim \Delta\xi \lesssim 0.17$ Å for all 34 independent framework atoms in this 62 atom eudialyte variant with $0.1 \lesssim u_{\mathrm{eq}} \lesssim 0.3$ Å, see also §2.55. The nonframework atoms, excluding one member in each of the pairs Zr2,Mn2; Zr2,Na1; Na3,Na4; Na5,Na6; Na8,Na9; Cl1,Cl2; Cl2,Cl3 and O31,O32, reportedly no further apart than ~0.8 Å, have $0.01 \lesssim \Delta\xi \lesssim 0.33$ Å. This variant strongly approaches and, thermodynamically, is hence more likely to form in space group $R32$.

4.9.2 Rastsvetaeva & Khomyakov, (2000). Mo$K\alpha$, graphite monochromator; 6,788 $I_{\mathrm{obs}} > 2\sigma(I_{\mathrm{obs}})$, 4,004 independent $F_{\mathrm{obs}} > 4\sigma(F_{\mathrm{obs}})$, absorption corrections, U_{eq}, $R = 0.036$; 69 independent atoms. A total 35 of the 36 independent framework and 22 of 33 non-framework atoms in a second eudialyte variant have $0.01 \lesssim \Delta\xi \lesssim 0.16$ Å, see Table S23(*b*) based on Rastsvetaeva & Khomyakov, (2000). The nonconforming framework atom O25 is only 0.45 Å from O24 and may be an artefact. No nonframework atom has a fully occupied site; all but six are less than half occupied and many are disordered.[3] Excluding

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[3] With $d_{\mathrm{Zr2\text{-}Fe1}}$, $d_{\mathrm{Ti1\text{-}Fe1}}$, $d_{\mathrm{Na3\text{-}Na4}}$, $d_{\mathrm{Na7\text{-}Na9}}$, $d_{\mathrm{Na11\text{-}Na12}}$, $d_{\mathrm{Sr2\text{-}Na10}}$, $d_{\mathrm{Na7\text{-}Na8}}$, $d_{\mathrm{Na7\text{-}Na9}}$, $d_{\mathrm{Na8\text{-}Na9}}$, $d_{\mathrm{Na14\text{-}Na15}} \lesssim 0.7$ Å and other pairs of atoms less than 1.1 Å.

such nonframework atoms, no $\Delta\xi \gtrsim 0.2$ Å with respect to $R32$ symmetry hence, with $0.1 \lesssim u_{\mathrm{eq}} \lesssim 0.3$ Å, this variant also is more likely to form in space group $R32$.

Johnsen & Grice (1999) investigated and reviewed a separate series of eudialyte variants in which the highest symmetry found was $R\bar{3}m$ in unsubstituted eudialyte with substitutions lowering the symmetry to $R3m$.

4.10 $\mathbf{ZrCr_2D_{3.8}}$ [90289]

Irodova & Suard (2000). Neutrons, $\lambda = 1.594$ Å; powder profile refinement of long-range order at $T = 100$ K, based on $P6_3/mmc$ model at 300 K; one B-value for each element; $R_{\mathrm{P}} = 0.064$, $R_{\mathrm{wP}} = 0.082$, $R_{\mathrm{F}} = 0.078$; 44 independent atoms; phase transition ~250 K. The metal sites were assigned full occupancy with that of the D sites ranging from 0.99 to 0.10 with average value 0.54. The four independent Zr and twelve independent Cr atom coordinates at ~300 K exactly match the symmetry of supergroup $R\bar{3}c$ but not the 28 occupied D atom site coordinates. All atoms listed, however, conform to the symmetry of space group $P6_3/mcm$ within 0.01 Å, see Table S24 whereas, notably, $P6_3/mmc$ symmetry is inapplicable. Conversion from rhombohedral to hexagonal symmetry increases the number of independent atoms in the unit cell by a factor of 3. Such an increase applies to the Zr and Cr sites in Table S24 but the D atom sites listed increase by a factor of only 1.5 to 3, possibly due to sites that were not recognized as independent. Four Cr atoms have 5 nearest neighbors (n.n.) D with $1.75 \lesssim d_{\mathrm{Cr\text{-}D}} \lesssim 1.81$ Å, 2 Cr have 6 n.n., 4 Cr have 9 n.n., and 2 Cr atoms have 10 n.n. D with 20 $d_{\mathrm{D\text{-}D}} \lesssim 1.35$ Å. Strong parameter interactions may result from refining a centrosymmetric array in $R3$, hence further investigation is appropriate.

4.11 $Cs_2SO_4Te(OH)_6$ [93016]

Dammak *et al.* (2001). Table S25 clearly shows $\Delta\xi < u_{\mathrm{eq}}$ for all atoms except H and O4 with respect to the atomic locations expected in space group *R*32. However, $\Delta\xi(\mathrm{H}) \approx 2u_{\mathrm{eq}}$ may not be significant and O4, with three $\angle$ O3-S-O3 = 119.05° in the distorted SO_4^{2-} ionic 'tetrahedron', is anomalous. If the O4 site is half- rather than fully-occupied, with a previously undetected half-occupied *O5* at the same 1.399 Å distance but of opposite sense along the *c*-axis from S, then all atoms satisfy space group *R*32. In that case, three new H1-bonds of 2.295 Å would be formed by *O5*, comparable to those formed by O4. It is expected that refinement of the modified structure in *R*32 will result in a more regular but disordered SO_4^{2-} tetrahedron.

4.12 $Ga_4Pd_7Zn_3$ [103911]

Subrahmanyam & Schubert, (1973). Cu$K\alpha,\beta$, multiple film, Al foils, Weissenberg camera, visual intensity estimates; 178 independent F_{obs}, neither absorption nor extinction corrections; *B* varied for all atoms, $R = 0.23$; 6 independent atoms. Table S26 shows that no atom is further than 0.22 Å from an inversion center in space group $R\bar{3}$ or from a like atom across such a center, assuming the two sites identified as uniquely occupied either by Zn or Ga2 are in fact half-occupied by both. With atomic numbers 30 and 31, Zn and Ga are too close to distinguish by the technique used; both sites also have 7 nearest, comparably arranged, neighbors of Pd only in the range 2.44-2.79 Å, supporting the assumed disorder. With $u_{\mathrm{iso}} \lesssim 0.15$ Å, it is hence more likely the space group is $R\bar{3}$ than *R*3.

4.13 $K_6MnMo_9O_{32}{\cdot}6H_2O$ [200048]

Weakley, (1977). Cu$K\alpha$, equi-inclination Weissenberg camera, optically-scanned multiple-film derived intensities; 636 independent F_{obs}, absorption corrections, U^{ij}, $R = 0.069$; 20 independent atoms. Space group $R3$ selected since refinement in space group $R32$, as for the corresponding ammonium salt, was found less satisfactory. All atomic coordinates in $R3$ approach $R32$ symmetry, with $0.04 \lesssim \Delta\xi \lesssim 0.15$ Å comparable in amplitude to $0.05 \lesssim u_{\mathrm{iso}} \lesssim 0.20$ Å, except for K2, O13 and O14, see Table S27(*a*). The values $\Delta\xi(\mathrm{K2}) = 0.51$ Å and $\Delta\xi(\mathrm{O13,O14}) = 3.11$ Å are most likely artefacts caused by refinement in $R3$. Dunne *et al.* (1992): Mo$K\alpha$, graphite monochromator; 1032 independent $I_{\mathrm{obs}} > 2.5\ \sigma(I_{\mathrm{obs}})$, absorption corrections, U^{ij}, $R = 0.028$, $wR = 0.031$; 13 independent atoms confirms the space group as $R32$. Comparison of Dunne *et al*'s. (1992) refined atomic coordinates with those of Weakley (1977) in Table S27(*b*) confirms the latter's location of O13 and also the choice of $R32$ as space group, *cf.* §4.5.

4.14 Pd_7P_3 [200055]

Matković & Schubert, (1977). Cu$K\alpha$, Weissenberg camera, visual intensity estimates; 289 independent F_{obs}, absorption corrections, U_{iso}, $R = 0.146$; 6 independent Pd, 2 P atoms. Table S28 shows $0.10 \lesssim \Delta\xi \lesssim 0.34$ Å, with respect to space group $R\bar{3}$, whereas $0.33 \lesssim u_{\mathrm{iso}} \lesssim 0.44$ Å. Space group $R\bar{3}$ is hence, thermodynamically, more likely than $R3$. The structure of several Pd_xP_y phases are reported in the Inorganic Crystal Structure Database, with x: y values of 3: 1, 3: 0.95, 3: 0.8, 1: 2, 4.5: 1.02, 6: 1, 7: 3 and 15: 2.

Tables for Appendix 2

Table S15

Modified atomic positions in Mg_9Sn_5 (Range *et al.*, 1996) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [55577]

a = 13.222(2), c = 13.150(2) Å. $z^* = z + 0.0083$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$

	Wyckoff position $R3, R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Sn1	9(*b*)	0.33547(9)	0.33668(9)	0.2583	0.3357	0.3353	0.24995	-0.0	0.02	0.11	0.12	0.13
	18(*f*)											
Sn2	9(*b*)	-0.3359(1)	-0.3340(1)	-0.2416(2)	-0.3357	-0.3353	-0.2499	0.0	0.02	0.11	0.12	0.12
Sn3	3(*a*)	0.	0.	0.3604(2)	0.	0.	0.3724	0.	0.	-0.16	0.16	0.19
	6(*c*)											
Sn4	3(*a*)	0.	0.	-0.3843(3)	0.	0.	-0.3724	0.	0.	-0.16	0.16	0.20
Sn5	3(*a*)	0.	0.	0.1201(3)	0.	0.	0.1312	0.	0.	-0.15	0.15	0.20
	6(*c*)											
Sn6	3(*a*)	0.	0.	-0.1422(4)	0.	0.	-0.1312	0.	0.	-0.15	0.15	0.21
Mg1	9(*b*)	0.2402(4)	0.1620(4)	0.0895(5)	0.2369	0.1592	0.0826	0.04	0.04	0.09	0.11	0.17
	18(*f*)											
Mg2	9(*b*)	-0.2337(4)	-0.1563(5)	-0.0758(6)	-0.2369	-0.1592	-0.0826	0.04	0.04	0.09	0.11	0.19
Mg3	9(*b*)	0.5161(4)	0.4134(4)	0.0878(5)	0.5163	0.4114	0.0841	-0.0	0.03	0.05	0.06	0.14
	18(*f*)											
Mg4	9(*b*)	0.4835(5)	-0.4095(4)	-0.0804(5)	0.4837	-0.4114	-0.0841	-0.0	0.03	0.05	0.06	0.14
Mg5	9(*b*)	0.4966(4)	0.5906(4)	0.2489(5)	0.4959	0.5920	0.2449	0.01	-0.02	0.05	0.05	0.13
	18(*f*)											
Mg6	9(*b*)	-0.4953(5)	0.4066(5)	-0.2409(5)	-0.4959	0.4080	-0.2449	0.01	-0.02	0.05	0.05	0.16

Table S16

Atomic positions in $Al_{4.2}Cu_{3.2}Zn_{0.7}$ (Murphy, (1975) with hypothetical $x'y'z'$ coordinates and the Δx, Δy and Δz displacements in Å [57730]

$a = 4.111$, $c = 25.036$ Å. $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^{*} - z')c$

	Wyckoff position $R3$,$R\bar{3}$	x	y	z^{*}	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	occ.
Cu1	3(a)	0	0	0.9[†]	0	0	0.9	0	0	0	0	0.9
Cu4	6(c) 3(a)	0	0	0.1	0	0	0.1	0	0	0	0	0.9
Al1,Zn1	3(a)	0	0	0.2	0	0	0.2	0	0	0.2	0	0.75,0.25
Al4,Zn4	6(c) 3(a)	0	0	0.8	0	0	0.8	0	0	0.8	0	0.75,0.25
Al2,Zn2	3(a)	0	0	0.4	0	0	0.4	0	0	0.4	0	0.9,0.1
Al3,Zn3	6(c) 3(a)	0	0	0.6	0	0	0.6	0	0	0.6	0	0.9,0.1
Cu2	3(a)	0	0	0.3	0	0	0.3	0	0	0.3	0	0.7
Cu3	6(c) 3(a)	0	0	0.7	0	0	0.7	0	0	0.7	0	0.7

[†] Murphy (1975) suggested an Al atom is located at $z = 0$ but also noted every fifth position at, *e.g.*, $z = 0$ and 0.5 is vacant. Both space groups $R\bar{3}$ and $R32$ are hence satisfied. The original ICSD listing of the space group as $R3$ is now $R\bar{3}$ (Allmann, 2006).

Table S17

Modified atomic positions for $Gd_{13}Ge_6O_{31}F$ at ~295 K (Mamin *et al.*, 1987) with hypothetical $x'y'$ z' coordinates and theΔ x,Δ y, Δz and u_{iso} displacements in Å [62329]
a = 15.922(2), c = 9.575(1) Å. $z^* = z - 0.0026$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$,$R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Gd1	3(*a*)	0	0	0.0192(1)	0	0	0	0	0	0.18	0.18	0.13
Gd2	9(*b*)	0.7460(1)	0.1566(1)	0.3146(1)	0.7456	0.1561	0.3150	0.01	0.01	-0.00	0.02	0.13
	18(*f*)											
Gd3	9(*b*)	0.2549(1)	0.8445(1)	0.6846(1)	0.2544	0.8439	0.6850	0.01	0.01	-0.00	0.02	0.12
Gd4	9(*b*)	0.8579(1)	0.0016(1)	0.3228(1)	0.8585	0.0020	0.3251	-0.01	-0.01	-0.02	0.03	0.14
	18(*f*)											
Gd5	9(*b*)	0.1409(1)	0.9976(1)	0.6727(1)	0.1415	0.9980	0.6750	-0.01	-0.01	-0.02	0.03	0.13
Ge1	9(*b*)	0.3133(2)	0.4132(1)	0.3429(3)	0.3122	0.4123	0.3443	0.02	0.01	-0.01	0.03	0.13
	18(*f*)											
Ge2	9(*b*)	0.6890(1)	0.5887(1)	0.6542(1)	0.6878	0.5877	0.6557	0.02	0.02	-0.01	0.04	0.12
O1	9(*b*)	0.0097(10)	0.7116(15)	0.3031(20)	0.0112	0.7137	0.2980	-0.02	-0.03	0.04	0.06	0.17
	18(*f*)											
O2	9(*b*)	0.9873(15)	0.2841(12)	0.7063(19)	0.9888	0.2863	0.7020	-0.02	-0.04	0.04	0.07	0.11
O3	9(*b*)	0.9458(10)	0.8035(15)	0.5511(9)	0.9496	0.8075	0.5547	-0.06	-0.06	-0.03	0.11	0.15
	18(*f*)											
O4	9(*b*)	0.0466(10)	0.1886(13)	0.4416(9)	0.0504	0.1925	0.4453	-0.06	-0.06	-0.03	0.11	0.12
O5	9(*b*)	0.7650(13)	0.1598(14)	0.0553(9)	0.7667	0.1558	0.0550	-0.03	0.06	0.00	0.05	0.11
	18(*f*)											
O6	9(*b*)	0.2315(9)	0.8482(10)	0.9452(18)	0.2333	0.8442	0.9440	-0.03	0.06	0.01	0.05	0.15
O7	9(*b*)	0.5765(10)	0.8300(11)	0.4927(16)	0.5787	0.8318	0.4913	-0.03	-0.03	0.01	0.05	0.05
	18(*f*)											
O8	9(*b*)	0.4191(9)	0.1664(18)	0.5102(10)	0.4213	0.1682	0.5087	-0.04	-0.03	0.01	0.06	0.15
O9[†]	9(*b*)	*-0.1189(9)*	0.0289(8)	0.0952(13)	*-0.1189*	0.0304	0.0961	-0.02	-0.01	-0.01	0.04	0.05
	18(*f*)											
O10	9(*b*)	0.1189(9)	0.9681(9)	0.9031(10)	0.1189	0.9696	0.9039	0.00	-0.01	-0.01	0.02	0.14
O11	3(*a*)	0	0	0.2825(12)	0	0	0.2903	0	0	-0.07	0.07	0.13
	6(*c*)											
F1	3(*a*)	0	0	0.7018(18)	0	0	0.7097	0	0	-0.07	0.07	0.16

[†] x(O9), in italic, is assumed here to have the opposite sign of that reported, see footnote 5 in the paper.

Table S18(*a*)
Modified atomic positions for $Cr_2Si_2Te_6$ at 293 K (Ouvrard *et al.*, 1988) with hypothetical $x'y'z'$ coordinates and the $\Delta x, \Delta y, \Delta z$ and u_{eq} displacements in Å [62379]
$a = 6.7578(6)$, $c = 20.6649(30)$ Å. $z^* = z - 0.1402$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
	$R3$, $R\bar{3}$											
Te1	9(*b*)	0.9738(2)	0.3064(2)	0.2511	0.9749	0.3054	0.2506	-0.01	0.01	0.01	0.01	0.12
	18(*f*)											
Te2	9(*b*)	0.6707(2)	0.9759(2)	0.7499(7)	0.6695	0.9749	0.7494	0.01	0.01	0.01	0.02	0.11
Cr1	3(*a*)	0	0	0.1652(3)	0	0	0.1662	0	0	-0.02	0.02	0.11
	6(*c*)											
Cr2	3(*a*)	0	0	0.8328(4)	0	0	0.8338	0	0	-0.02	0.02	0.11
Si1	3(*a*)	0	0	0.5559(6)	0	0	0.5548	0	0	0.02	0.02	0.12
	6(*c*)											
Si2	3(*a*)	0	0	0.4462(5)	0	0	0.4452	0	0	0.02	0.02	0.11

Table S18(*b*)
Comparison of the derived x', y', z' Ouvrard *et al.* (1988) with Marsh's (1988) refined atomic coordinates for $Cr_2Si_2Te_6$ and Δx, Δy, Δz differences in Å [71020]
$\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z - z')c$.

	Wyckoff Position	x'	y'	$z'^{\ddagger}$	Δx	Δy	Δz
	$R\bar{3}$						
$Te_{Ouvrard}$	9(*b*)	0.6695	0.9749	0.2494			
	Diff.†				0.003	0.002	0.000
Te_{Marsh}	9(*b*)	0.66902(15)	0.97459(13)	0.24939(4)			
$Cr_{Ouvrard}$	3(*a*)	0	0	0.3338			
					0	0	0.003
Cr_{Marsh}	3(*a*)	0	0	0.33394(20)			
$Si_{Ouvrard}$	3(*a*)	0	0	0.0548			
					0	0	0.002
Si_{Marsh}	3(*a*)	0	0	0.05488(31)			

‡ Ouvrard *et al.*'s (1988) origin in Table S18(*a*) displaced to 0,0,½ in Table S18(*b*).
† Ouvrard *et al.*'s (1988) x', y', z'-coordinates in the upper and Marsh's (1988) refined x, y, z-coordinates in the lower lines, respectively, of each entry with Δx, Δy, Δz values in the central lines.

Table S19(*a*)

Modified atomic positions in $(NH_4)_6NiMo_9O_{32}\cdot 6H_2O$ at ambient temperature (Dunne, *et al.,* 1992). with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [72710]

a = 15.922(1), c = 12.406(1) Å. $z^* = z + 0.0012$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*32	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	u_{iso}
Ni	3(*a*),3(*a*)	0	0	0.0012	0	0	0	0	0	0.01	0.01	n.r.†
Mo1	9(*b*),9(*d*)	0.1993(1)	-0.0010(1)	0.0024(1)	0.1993	0	0	0	-0.02	0.03	0.04	n.r.
Mo2	9(*b*)	0.1390(1)	0.0867(1)	0.2035(1)	0.1389	0.0865	0.2019	0.00	0.00	0.02	0.02	n.r.
	18(*f*)											
Mo3	9(*b*)	0.0863(1)	0.1388(1)	0.7996(1)	0.0865	0.1389	0.7981	-0.00	-0.00	0.02	0.02	n.r.
N1	9(*b*),9(*d*)	0.4379(6)	-0.0039(6)	0.0055(9)	0.4379	0	0	0	-0.06	0.07	0.09	n.r.
N2	9(*b*),9(*d*)	0.3046(6)	0.2969(5)	-0.0140(10)	0.3007	0.3007	0	0.06	-0.06	-0.17	0.18	n.r.
O1	9(*b*)	0.0453(3)	0.1086(3)	0.0925(4)	0.0434	0.1076	0.0915	0.03	0.02	0.01	0.04	n.r.
	18(*f*)											
O2	9(*b*)	0.1066(3)	0.0415(3)	-0.0905(5)	0.1076	0.0434	-0.0915	-0.02	-0.03	0.01	0.04	n.r.
O3	9(*b*)	0.2269(4)	0.1130(4)	0.0896(4)	0.2265	0.1137	0.0876	0.01	-0.01	0.02	0.02	n.r.
	18(*f*)											
O4	9(*b*)	0.1144(4)	0.2262(3)	-0.0856(4)	0.1137	0.2265	-0.0876	0.01	-0.01	0.02	0.02	n.r.
O5	9(*b*)	0.0620(4)	0.2942(4)	0.0908(5)	0.0595	0.2945	0.0878	0.04	-0.00	0.04	0.06	n.r.
	18(*f*)											
O6	9(*b*)	0.2948(4)	0.0570(4)	-0.0849(5)	0.2945	0.0595	-0.0878	0.00	-0.04	0.04	0.06	n.r.
O7	9(*b*)	0.1816(3)	0.0370(4)	0.2973(5)	0.1801	0.0367	0.2951	0.02	0.00	0.03	0.04	n.r.
	18(*f*)											
O8	9(*b*)	0.0365(4)	0.1786(4)	0.7072(5)	0.0367	0.1801	0.7049	-0.00	-0.02	0.03	0.04	n.r.
O9	9(*b*)	0.1743(4)	0.1999(4)	0.2546(5)	0.1751	0.2003	0.2513	-0.01	-0.01	0.04	0.04	n.r.
	18(*f*)											
O10	9(*b*)	0.2008(3)	0.1758(4)	0.7520(5)	0.2003	0.1751	0.7487	0.01	0.01	0.04	0.04	n.r.
O11	3(*a*)	0	0	0.2636(7)	0	0	0.2617	0	0	0.02	0.02	n.r.
	6(*c*)											
O12	3(*a*)	0	0	0.7402(7)	0	0	0.7383	0	0	0.02	0.02	n.r.
O13(w1)	9(*b*)	0.4065(6)	0.5970(7)	0.1566(9)	0.4009	0.5298	0.1690	0.09	1.07	-0.15	1.13	n.r.
	18(*f*)											
O14(w2)	9(*b*)	0.4626(13)	0.3952(13)	0.8187(9)	0.5298	0.4009	0.8310	-1.07	-0.09	-0.15	1.13	n.r.

† u_{iso} amplitudes not reported.

Table S19(*b*)

Comparison of atomic positions in $(NH_4)_6NiMo_9O_{32}\cdot 6H_2O$ at ambient temperature in Stratemeier *et al.,* (1992) with *R*32-averaged values of Dunne *et al.,* (1992); Δx, Δy, Δz and $\Delta\xi$ displacements in Å [67576, 72710].

$a_S = 15.935(6)$, $c_S = 12.407(4)$; $a_D = 15.922(1)$, $c_D = 12.406(1)$ Å.

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

		Stratemeier *et al.,* (1992) coordinates			Dunne *et al.,* (1992) coordinates							
	Wyckoff Position *R*33,⟨*R*32⟩	-*y*	- *x*	*z*		*x*′	*y*′	*z*′	Δx	Δy	Δz	$\Delta\xi$
Ni1	3(*a*)	0	0	0	Ni	0	0	0	0	0	0	0
Mo2	9(*d*)	0.19975	0	0	Mo1	0.1993	0	0	0.01	0	0	0.01
Mo1	18(*f*)	0.1389	0.0866	0.20185	Mo2	0.1389	0.0865	0.2019	0	0	0	0
O1	18(*f*)	0.0329	0.0862	0.10202	O1	0.0434	0.1076	0.0915	-0.17	0	0.13	0.21
O2	18(*f*)	0.2270	0.1136	0.08853	O3	0.2265	0.1137	0.0876	0.01	0	0.01	0.01
O3	18(*f*)	0.1800	0.0366	0.2956	O7	0.1801	0.0367	0.2951	0	0	0.01	0.01
O4	6(*c*)	0	0	0.261	O11	0	0	0.2617	0	0	-0.01	0.01
O5	18(*f*)	0.2345	-0.0602	0.08783	O5	0.2350	-0.0599	0.0878	-0.01	0.01	0	0.01
O6	18(*f*)	0.1736	0.2000	0.2517	O9	0.1751	0.2003	0.2513	-0.02	0	0.01	0.02
N1	9(*d*)	0.1083	0.3334	0.3334	N1	0.1046	0.3333	0.3333	-0.18	0	0	0.18
N2	9(*d*)	-0.33333	0.03203	0.33333	N2	-0.3333	0.0362	0.3333	0	-0.07	0	0.07
O7w[†]	18(*f*)	-0.2079	0.0609	0.4819	O14w	-0.1362	0.0676	0.4977	-1.14	-0.11	-0.20	1.22
O8w	18(*f*)	0.1383	0.0696	0.5127								

[†] Ow denotes the oxygen atom in a water molecule.

Table S20(*a*)

Atomic positions for $Sr(BH)_{12}\cdot 7H_2O$ at ambient temperature (Solntsev *et al.*, 1977) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [200016]
$a = 10.104(3)$, $c = 14.587(4)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Sr	3(*a*),3(*a*)	0.000(1)	0.000(1)	0.000(1)	0	0	0	0	0	0	0	0.24
O1	9(*b*)	0.148(2)	0.401(2)	0.734(2)	0.140	0.393	0.731	0.08	0.08	0.04	0.14	0.24
	18(*f*)											
O2	9(*b*)	-0.132(2)	-0.384(2)	0.272(2)	-0.140	-0.393	0.269	0.08	0.09	0.04	0.15	0.30
O3	3(*a*)	0.0	0.0	0.822(2)	0	0	0.822	0	0	0	0	0.24
	6(*c*)											
O3A†	3(*a*)	*0.0*	*0.0*	*0.178*	*0*	*0*	*0.178*	*0*	*0*	*0*	*0*	*n/d*†
B1	9(*b*)	0.512(2)	0.706(2)	0.561(2)	0.508	0.708	0.566	0.04	-0.02	-0.07	0.08	0.13
	18(*f*)											
B4	9(*b*)	0.497(3)	0.290(3)	0.429(3)	0.492	0.292	0.434	0.05	-0.02	-0.07	0.08	0.25
B2	9(*b*)	0.658(2)	0.429(2)	0.342(2)	0.661	0.430	0.342	-0.03	-0.01	0.0	0.04	0.15
	18(*f*)											
B3	9(*b*)	0.336(4)	0.569(4)	0.659(4)	0.339	0.570	0.658	-0.03	-0.01	0.01	0.04	0.25

† Hypothetical atom, not determined.

Table S20(*b*)

Comparison of atomic positions for $Sr(BH)_{12}\cdot 7H_2O$ at 293 K determined by Tiritiris & Schleid (2001) in space group $R\bar{3}$ with those of Solntsev *et al.*, (1977) in $R3$. [94431, 200016] $a = 10.1271(6)$, $c = 14.6294(9)$ Å

T & S	Wyckoff position $R\bar{3}$	$x_{T\,\&\,S}$	$y_{T\,\&\,S}$	$z_{T\,\&\,S}$	S *et al.*	$x_{S\ et\ al.}$	$y_{S\ et\ al}$	$z_{S\ et\ al}$	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Sr	3(*a*)	0.	0.	0.	Sr	0	0	0	0	0	0	0	0.19
O1	6(*c*)	0.	0.	0.1769(2)	O3	0	0	⟨0.178⟩	0	0	-0.02	0.02	0.22
O2	18(*f*)	0.1402(2)	0.3930(2)	0.7300(1)	O1	⟨0.140⟩†	⟨0.393⟩	⟨0.731⟩	-0.0	0.01	-0.01	0.01	0.27
B1	18(*f*)	0.0295(3)	0.1126(3)	0.4080(2)	B4	⟨0.708⟩	⟨0.200⟩	⟨0.434⟩	3.26	-0.89	2.94	2.97	0.17
B2	18(*f*)	0.0474(3)	0.1826(3)	0.5217(2)	B2	⟨-0.231⟩	⟨0.339⟩	⟨0.342⟩	2.82	-1.58	2.63	3.59	0.19
H1	18(*f*)	0.048(3)	0.181(3)	0.348(3)	-	-	-	-	-	-	-	-	0.22
H2	18(*f*)	0.071(3)	0.298(3)	0.536(2)	-	-	-	-	-	-	-	-	0.23

† Solntsev *et al.*'s (1977) equivalent values averaged in $R\bar{3}$.

Table S21(*a*)

Atomic positions for $MgSiO_3$ at ~300 K (Horiuchi *et al.,* (1982) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [89805]

$a = 4.7284(4)$, $c = 13.559(2)$ Å. $z^* = z + 0.0000$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z	u_{eq}
	$R\bar{3}$				
Mg	3(*a*)	0	0	0.3597(1)	0.09
Si	3(*a*)	0	0	0.1577(1)	0.07
O	9(*b*)	0.3214(5)	0.0361(4)	0.2408(1)	0.08

Table S21(*b*)

Ab initio ambient atomic positions for $MgSiO_3$ (d'Arco *et al.,* (1994) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [75738]

$a = 4.713(1)$, $c = 13.454$ Å. $z^* = z + 0.0000$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z
	$R3$			
Mg	3(*a*)	0	0	0.3599
Si	3(*a*)	0	0	0.1556
O	9(*b*)	0.3200	0.0355	0.2396

Table S21(*c*)

Ab initio atomic positions for $MgSiO_3$ (Karki *et al.,* (2000) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [89805]

$a = 4.686$, $c = 13.291$ Å. $z^* = z + 0.0000$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z
	$R\bar{3}$			
Mg	3(*a*)	0	0	0.3586
Si	3(*a*)	0	0	0.1570
O	9(*b*)	0.3205	0.0326	0.2416

Table S22

Atomic positions for CdPS$_3$ (Boucher *et al.,* 1995) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [80875]

a = 6.224(38), *c* = 19.49(1) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Cd1	3(*a*)	0	0	0.3291(1)	0	0	0.3289	0	0	0.00	0.00	0.10
	6(*c*)											
Cd2	3(*a*)	0	0	0.67131(5)	0	0	0.67111	0	0	0.00	0.00	0.10
P1	3(*a*)	0.6667	0.3333	0.3900(1)	0.6667	0.3333	0.3905	0	0	-0.01	0.01	0.08
	6(*c*)											
P2	3(*a*)	0.3333	0.6667	0.6090(1)	0.3333	0.6667	0.6095	0	0	-0.01	0.01	0.08
S1	9(*b*)	0.3450(3)	0.3214(3)	0.4201(2)	0.3475	0.3230	0.4199	-0.02	-0.01	0.00	0.03	0.09
	18(*f*)											
S2	9(*b*)	0.6499(3)	0.6755(3)	0.5804(2)	0.6525	0.6770	0.5801	-0.02	-0.01	0.01	0.03	0.09

Table S23(*a*) Eudialyte-type Fe,Ca-silicate

Atomic positions for $Na_{15.4}K_{0.2}Al_{0.25}Ca_{3.4}Mn_{0.9}Mg_{0.2}Sr_{0.2}Fe_{2.0}RE_{0.3}Zr_{3.8}Hf_{0.1}Ti_{0.2}Nb_{0.13}$-$Si_{25}O_{73}(OH)_{0.75}Cl_{1.1}$ (Ekimenkova *et al.*, 2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [90835]

a = 14.229(7), *c* = 30.019(15) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δξ	u_{eq}	occupancy %
Zr1	9(*b*),9(*c*)	0.0001(1)	0.5000(1)	0.4999(1)	0	0.5000	0.5	0.	0.	0.	0	0.14	100
Si1	9(*b*) 18(*c*)	0.1396(1)	0.0662(1)	0.0819(1)	0.1400	0.0699	0.0816	-0.01	-0.05	0.01	0.06	0.14	100
Si2	9(*b*)	0.8595(1)	0.9264(1)	0.9187(1)	0.8600	0.9301	0.9184	-0.01	-0.05	0.01	0.06	0.14	100
Si3	9(*b*) 18(*c*)	0.4585(1)	0.5420(1)	0.2582(1)	0.4584	0.5420	0.2580	0.0	0.0	0.01	0.01	0.13	100
Si4	9(*b*)	0.5417(1)	0.0835(1)	0.7423(1)	0.5416	0.0835	0.7420	0.0	0.0	0.01	0.01	0.14	100
Si5	9(*b*) 18(*c*)	0.2712(1)	0.3258(1)	0.2371(1)	0.2705	0.3252	0.2368	0.01	0.01	0.01	0.02	0.13	100
Si7	9(*b*)	0.3247(1)	0.2697(1)	0.7635(1)	0.3252	0.2705	0.7632	-0.01	-0.01	0.01	0.02	0.12	100
Si6	9(*b*) 18(*c*)	0.0575(1)	0.3279(1)	0.2369(1)	0.0578	0.3274	0.2367	-0.01	0.01	0.01	0.01	0.12	100
Si8	9(*b*)	0.3269(1)	0.0580(1)	0.7636(1)	0.3274	0.0578	0.7633	-0.01	0.0	0.01	0.01	0.12	100
O1	9(*b*) 18(*c*)	0.0617(4)	0.1225(3)	0.0782(1)	0.0617	0.1229	0.0776	0.0	-0.01	0.02	0.02	0.17	100
O19	9(*b*)	0.9383(3)	0.8767(3)	0.9230(1)	0.9383	0.8771	0.9224	0.0	-0.01	0.02	0.02	0.16	100
O2	9(*b*) 18(*c*)	0.2236(4)	0.1048(5)	0.0412(1)	0.2262	0.1124	0.0424	-0.04	-0.11	-0.04	0.14	0.20	100
O17	9(*b*)	0.7711(4)	0.8799(5)	0.9564(1)	0.7738	0.8876	0.9576	-0.04	-0.11	-0.04	0.14	0.19	100
O3	9(*b*) 18(*c*)	0.1886(4)	0.0891(5)	0.1320(1)	0.1902	0.0944	0.1307	-0.02	-0.08	0.04	0.10	0.20	100
O18	9(*b*)	0.8083(4)	0.9004(5)	0.8706(1)	0.8098	0.9056	0.8693	-0.02	-0.07	0.04	0.09	0.18	100
O4	9(*b*) 18(*c*)	0.2635(4)	0.2305(4)	0.2074(1)	0.2607	0.2299	0.2069	0.04	0.01	0.02	0.05	0.17	100
O25	9(*b*)	0.7421(4)	0.7706(3)	0.7936(1)	0.7393	0.7701	0.7931	0.04	0.01	0.02	0.05	0.17	100
O5	9(*b*) 18(*c*)	0.2587(3)	0.2969(3)	0.2895(1)	0.2533	0.2975	0.2890	0.08	0.01	0.02	0.09	0.16	100
O21	9(*b*)	0.9589(4)	0.7019(4)	0.7116(1)	0.9643	0.7025	0.7110	-0.08	-0.01	0.02	0.09	0.16	100
O6	9(*b*) 18(*c*)	0.1789(3)	0.3519(3)	0.2195(1)	0.1796	0.3530	0.2198	-0.01	-0.02	-0.01	0.03	0.14	100
O23	9(*b*)	0.3540(4)	0.1804(3)	0.7799(1)	0.3530	0.1796	0.7802	0.01	0.02	-0.01	0.03	0.17	100
O7	9(*b*) 18(*c*)	0.3904(4)	0.4316(4)	0.2263(1)	0.3900	0.4330	0.2261	0.01	-0.02	0.01	0.02	0.17	100
O16	9(*b*)	0.6105(3)	0.0444(4)	0.7742(1)	0.6100	0.0430	0.7739	0.01	0.02	0.01	0.03	0.16	100
O8	9(*b*) 18(*c*)	0.0249(3)	0.5106(4)	0.3054(1)	0.0249	0.5105	0.3045	0.0	0.0	0.03	0.03	0.16	100
O13	9(*b*)	0.5104(4)	0.0249(4)	0.6964(1)	0.5105	0.0249	0.6955	0.0	0.0	0.03	0.03	0.18	100

O9	9(*b*)	0.2139(8)	0.6074(8)	0.2529(3)	0.2120	0.6062	0.2489	0.03	0.02	0.12	0.13	0.18	50
	18(*c*)												
O10†	9(*b*)	0.396(1)	0.611(1)	0.2725(3)	0.3955	0.608	0.2667	0.01	0.04	0.17	0.18	0.23	50
O11	9(*b*)	0.0530(5)	0.4369(4)	0.2269(1)	0.0548	0.4383	0.2268	-0.03	-0.02	0.0	0.04	0.18	100
	18(*c*)												
O15	9(*b*)	0.4397(3)	0.0566(4)	0.7733(1)	0.4383	0.0548	0.7732	0.02	0.03	0.0	0.04	0.17	100
O12	9(*b*)	0.0437(4)	0.2992(3)	0.2894(1)	0.0443	0.2990	0.2888	-0.01	0.0	0.02	0.02	0.16	100
	18(*c*)												
O24	9(*b*)	0.9551(3)	0.2552(3)	0.7118(1)	0.9557	0.2550	0.7112	-0.01	0.0	0.02	0.02	0.16	100
O20	9(*b*)	0.2600(4)	0.0277(3)	0.2067(1)	0.2606	0.0306	0.2067	-0.01	-0.04	0.0	0.05	0.17	100
	18(*c*)												
O22	9(*b*)	0.7387(4)	0.9664(4)	0.7933(1)	0.7394	0.9694	0.7933	-0.01	-0.04	0.0	0.05	0.17	100
Fe1,Ca1,Mn1	9(*b*),9(*d*)	0.0005(1)	0.2642(1)	0.0001(1)	0.0	0.2642	0.01	0.	0.0	0.01	0.01	0.15	73.3,16.7,10
Ca2, Ce1	9(*b*),9(*d*)	0.2596(1)	0.2601(1)	0.0000(1)	0.2598	0.2598	0.	0.	0.0	0.0		0.14	90,10
Zr2, Hf1	9(*b*),9(*d*)	0.5021(2)	0.0065(2)	-0.0004(1)	0.5021	0.	0.	0.0	0.09	-0.01	0.09	0.15	26.7,3.3
Na1	9(*b*),9(*d*)	0.5229(4)	0.0515(4)	-0.0042(1)	0.5229	0.	0.	0.	0.73	-0.13	0.74	0.16	50
Mn2‡	9(*b*)	0.1496(3)	0.3025(3)	0.3365(1)	-	-	-	-	-	-	-	0.12	20
Nb1,T1,Mg1	3(*a*)	0.	0.	0.6275(1)	0.	0.	0.6219	0.	0.	0.17	0.17	0.18	20,15,15
	6(*c*)												
Si11,Al2	3(*a*)	0.	0.	0.3838(2)	0.	0.	0.3781	0.	0.	0.17	0.17	0.16	40,10
Si9,Al1	3(*a*)	0.	0.	0.5810(1)	0.	0.	0.5800	0.	0.	0.03	0.03	0.17	40,10
	6(*c*)												
Si10	3(*a*)	0.	0.	0.4210(2)	0.	0.	0.4200	0.	0.	0.03	0.03	0.15	50
Na2	9(*b*)	0.2562(8)	0.5244(7)	0.1855(3)	0.2445	0.5148	0.1792	0.17	0.14	0.19	0.33	0.24	45
	18(*c*)												
Na3	9(*b*)	0.5053(1)	0.2327(1)	0.8272(4)	0.5148	0.2445	0.8208	-0.13	-0.17	0.19	0.32	0.26	35
Na4‡	9(*b*)	0.378(1)	0.552(3)	0.1629(5)	-	-	-	-	-	-	-	0.28	20
Na10	9(*b*)	0.4430(3)	0.8829(4)	0.8202(1)	0.4447	0.8851	0.8212	-0.02	-0.03	-0.03	0.05	0.23	100
	18(*c*)												
Na5,Ca3	9(*b*)	0.5536(4)	0.4425(5)	0.1777(2)	0.5553	0.4403	0.1788	-0.02	0.03	-0.03	0.04	0.18	38.3,6.7
Na6‡	9(*b*)	0.9182(4)	0.0826(4)	0.8300(2)	-	-	-	-	-	-	-	0.20	55
Na7,Ca4	9(*b*)	0.4595(5)	0.2304(3)	0.0495(1)	0.4523	0.2269	0.0504	0.10	0.05	-0.03	0.14	0.18	93.3,6.7
	18(*c*)												
Na8,Sr1,K1	9(*b*)	0.5549(3)	0.7765(3)	0.9487(1)	0.5477	0.7731	0.9496	0.10	0.05	-0.03	0.14	0.18	40,5,5
Na9,Sr2,K2‡	9(*b*)	0.5273(3)	0.7647(3)	0.9560(1)	-	-	-	-	-	-	-	0.16	46.7,1.7,1.7
O26	9(*b*)	0.197(1)	0.591(1)	0.0063(7)	0.209	0.5976	0.0044	-0.17	-0.09	0.06	0.24	0.13	20
	18(*c*)												
O28	9(*b*)	0.6234(1)	0.3959(1)	-0.0025(1)	0.6354	0.4024	-0.0044	-0.17	-0.09	0.06	0.24	0.25	50
O27‡	3(*a*)	0	0	0.333(1)	-	-	-	-	-	-	-	0.28	50
Cl1‡	3(*a*)	0	0	0.2343(2)	0	0	0.2311	0	0	0.10	0.10	0.20	50
	6(*c*)												
O32	3(*a*)	0.	0.	0.7721(8)	0.	0.	0.7689	0	0	0.10	0.10	0.26	25
O29	3(*a*)	0.	0.	0.4735(4)	0.	0.	0.4717	0	0	0.05	0.05	0.12	50
	6(*c*)												
O30	3(*a*)	0.	0.	0.5301(8)	0.	0.	0.5283	0	0	0.05	0.05	0.23	50
Cl2	3(*a*)	0	0	0.2592(4)	0	0	0.2539	0	0	0 .16	0 .16	0.20	30
	6(*c*)												
O31	3(*a*)	0.	0.	0.7515(3)	0.	0.	0.7461	0	0	0.16	0.16	0.20	75

Cl3[‡]	3(*a*)	0	0	0.2869(8)	-	-	-	-	-	-	-	0.25	20

O9	9(*b*)	0.2139(8)	0.6074(8)	0.2529(3)	0.2153	0.6057	0.2627	-0.02	0.02	-0.29	0.29	0.23	100
	18(*c*)												
O10[†]	9(*b*)	0.396(1)	0.611(1)	0.2725(3)	0.3943	0.6096	0.2627	0.02	0.02	0.29	0.29	0.23	50

O9	9(*b*)	0.2139(8)	0.6074(8)	0.2529(3)	0.2120	0.6062	0.2489	0.03	0.02	0.12	0.13	0.18	50
	18(*c*)												
O14	9(*b*)	0.6050(5)	0.2101(4)	0.7391(3)	0.6062	0.2120	0.7351	-0.02	-0.03	0.12	0.13	0.23	100
O14[†]	9(*b*)	0.6050(5)	0.2101(4)	0.7391(3)	0.6045	0.2128	0.7333	0.01	-0.04	0.17	0.17	0.23	100
	18(*c*)												
O10[†]	9(*b*)	0.396(1)	0.611(1)	0.2725(3)	0.3955	0.608	0.2667	0.01	0.04	0.17	0.18	0.23	50

[†] O10 with 50% occupancy is related to O9 both by $-y, x - y, z$ with $\Delta\xi \approx 0.29$ Å, and by $-x + y, -x, z$ with $\Delta\xi \approx 0.59$ Å. O9 and O10 are also related through O14. Further investigation of these relationships is necessary.

[‡] Mn2, with 20% occupancy and $d_{\text{Mn2-Zr2}} = 0.47$ Å; Na6 with $d_{\text{Na6-Na5}} = 0.83$ Å; O27 with $d_{\text{O27-Cl3}} = 1.38$ Å, Cl1 with $d_{\text{Cl1-O30}} = 1.10$ Å and Cl3 with $d_{\text{Cl3-Cl2}} = 0.84$ Å may each be considered as artefacts.

Table 23(*b*) Eudialyte-type Mn,Fe-silicate

Atomic positions for $Na_{16}K_{0.2}Al_{0.1}Ca_{1.77}Mn_{2.1}Sr_{0.6}Fe_{1.5}Ce_{0.63}Zr_{3.6}Ti_{0.15}Nb_{0.13}Si_{25.9}O_{77.6}$-$H_{5.75}Cl_{0.3}$ (Rastsvetaeva & Khomyakov, 2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [91548]

a = 14.205(7), *c* = 30.265(15) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	u_{eq}	occupancy %
Zr1†	9(*b*),9(*e*)	0.0001(1)	0.4915(1)	0.4999(1)	0.0	0.4915	0.5	0.	0.0	0.0	0.0	0.15	100
Mn1,Ca1,Ce1	9(*b*),9(*d*)	-0.0001(1)	0.2726(1)	-0.0002(1)	0.0	0.2726	0	0.	0.0	-0.01	0.01	0.13	70,24,6
Na1,Ca2,Ce2,Sr1	9(*b*),9(*d*)	0.2435(1)	0.2435(1)	-0.0003(1)	0.2435	0.2435	0	0.	0.	-0.01	0.01	0.14	45,35,15,5
Si1	9(*b*)	-0.0108(2)	0.6090(1)	0.0965(1)	-0.0109	0.6088	0.0963	0.	0.	0.01	0.01	0.14	100
	18(*c*)												
Si5	9(*b*)	0.6087(1)	0.9890(1)	0.9040(1)	0.6088	0.9891	0.9037	0.	0.0	0.01	0.01	0.14	100
Si2	9(*b*)	-0.0050(1)	0.3968(1)	0.0963(1)	-0.0049	0.3968	0.0961	0.	0.	0.01	0.01	0.13	100
	18(*c*)												
Si4	9(*b*)	0.3967(1)	0.9952(1)	0.9041(1)	0.3968	0.9951	0.9039	0.	0.	0.01	0.01	0.13	100
Si3	9(*b*)	0.1403(1)	0.0571(1)	0.0811(1)	0.1403	0.0570	0.0808	0.	0.	0.01	0.01	0.14	100
	18(*c*)												
Si7	9(*b*)	0.8597(1)	0.9166(1)	0.9195(1)	0.8597	0.9165	0.9192	0.	0.0	0.01	0.01	0.14	100
Si6	9(*b*)	0.2085(1)	0.4170(1)	0.0750(1)	0.2085	0.4170	0.0749	0.	0.	0.01	0.01	0.15	100
	18(*c*)												
Si8	9(*b*)	0.7914(1)	0.2086(1)	0.9253(1)	0.7915	0.2086	0.9251	0.	0.	0.01	0.01	0.15	100
O1	9(*b*)	0.8376(3)	0.6926(3)	0.3621(1)	0.8377	0.6924	0.3618	0.	0.	0.01	0.01	0.17	100
	18(*c*)												
O17	9(*b*)	0.6922(3)	0.8378(3)	0.6386(1)	0.6924	0.8377	0.6382	0.	0.	0.01	0.01	0.17	100
O2	9(*b*)	0.1840(3)	0.3537(3)	0.2210(1)	0.1841	0.3540	0.2209	0.	0.	0.	0.	0.17	100
	18(*c*)												
O22	9(*b*)	0.3543(3)	0.1842(3)	0.7792(1)	0.3540	0.1841	0.7791	0.	0.	0.	0.	0.17	100
O3	9(*b*)	0.9592(3)	0.2504(3)	0.7113(1)	0.9569	0.2571	0.7109	0.03	-0.07	0.01	0.06	0.20	100
	18(*c*)												
O20	9(*b*)	0.0454(3)	0.3002(3)	0.2895(1)	0.0431	0.3036	0.2891	0.03	-0.07	0.01	0.06	0.17	100
O4	9(*b*)	0.9700(4)	0.7074(3)	0.7119(1)	0.9700	0.7074	0.7117	0.	0.	0.	0.	0.17	100
	18(*c*)												
O21	9(*b*)	0.2625(3)	0.2926(3)	0.2885(1)	0.2625	0.2926	0.2883	0.	0.	0.	0.	0.16	100
O5	9(*b*)	0.5890(4)	0.6891(3)	0.8738(1)	0.5888	0.6887	0.8736	0.	0.01	0.01	0.01	0.18	100
	18(*c*)												
O19	9(*b*)	0.4115(4)	0.1011(4)	0.1267(1)	0.4112	0.1007	0.1264	0.	0.01	0.01	0.01	0.18	100
O6	9(*b*)	0.5963(3)	0.8936(3)	0.8727(1)	0.5958	0.8936	0.8724	0.01	0.	0.01	0.01	0.20	100
	18(*c*)												
O18	9(*b*)	0.4048(4)	0.2978(4)	0.1280(1)	0.4042	0.2978	0.1276	0.01	0.	0.01	0.01	0.20	100
O7	9(*b*)	0.8091(4)	0.8887(4)	0.8709(1)	0.8089	0.8887	0.8708	0.	0.	0.	0.	0.23	100
	18(*c*)												
O9	9(*b*)	0.1914(3)	0.0797(4)	0.1293(1)	0.1911	0.079	0.1292	0.	0.	0.	0.	0.19	100
O8	9(*b*)	0.5583(4)	0.7585(4)	0.7084(1)	0.5580	0.7582	0.7081	0.	0.	0.01	0.01	0.20	100
	18(*c*)												
O12	9(*b*)	0.4423(4)	0.1996(4)	0.2922(1)	0.4420	0.1999	0.2919	0.	0.	0.01	0.01	0.19	100

O10	9(*b*)	0.1070(4)	0.3937(5)	0.1076(1)	0.1058	0.3944	0.1074	0.06	-0.01	0.01	0.06	0.21	100
	18(*c*)												
O15	9(*b*)	0.3912(5)	0.1046(4)	0.8928(1)	0.3944	0.1058	0.8926	-0.05	-0.02	0.01	0.06	0.20	100
O11	9(*b*)	0.2726(3)	0.3708(3)	0.1058(1)	0.2723	0.3704	0.1055	0.	0.01	0.01	0.01	0.16	100
	18(*c*)												
O16	9(*b*)	0.7281(3)	0.0977(3)	0.8949(1)	0.7277	0.0973	0.8945	0.01	0.01	0.01	0.02	0.16	100
O13	9(*b*)	0.9500(3)	0.8771(3)	0.9236(1)	0.9499	0.8769	0.9232	0.	0.	0.01	0.01	0.19	100
	18(*c*)												
O14	9(*b*)	0.0729(3)	0.1233(3)	0.0772(1)	0.0728	0.1231	0.0768	0.	0.	0.01	0.01	0.20	100
O23	9(*b*)	0.2861(5)	0.5465(4)	0.0714(2)	0.2814	0.5446	0.0756	0.07	0.03	-0.13	0.16	0.27	100
	18(*c*)												
O24	9(b)	0.5428(6)	0.2767(1)	0.9201(4)	0.5446	0.2814	0.9244	-0.03	-0.07	-0.13	0.16	0.19	41(1)
O25[‡]	9(*b*)	0.550(1)	0.293(1)	0.9336(3)	0.548	0.290	0.9311	0.03	0.04	0.08	0.10	0.21	59(1)
Si9	3(*a*)	0.0	0.0	0.3768(1)	0.0	0.0	0.3769	0.0	0.0	0.	0	0.16	64(1)
	18(*c*)												
Si12,Al1	3(*a*)	0.0	0.0	0.6230(1)	0.0	0.0	0.6231	0.0	0.0	0.	0	0.16	65,10
Si10	3(*a*)	0.0	0.0	0.4215(3)	0.0	0.0	0.4212	0.0	0.0	0.01	0.01	0.18	36(1)
	18(*c*)												
Si11	3(*a*)	0.0	0.0	0.5791(3)	0.0	0.0	0.5788	0.0	0.0	0.01	0.01	0.16	25(1)
Zr2,Na2	9(*b*)	0.1842(2)	0.3526(2)	0.3315(1)	0.1836	0.3511	0.3317	0.01	0.02	-0.01	0.03	0.17	21,19
	18(*c*)												
Fe1	9(*b*)	0.3495(1)	0.1830(1)	0.6680(1)	0.3511	0.1836	0.6683	-0.02	-0.01	0.11	0.03	0.20	50
Ti1,Nb1	9(*b*),9(*d*)	0.460(1)	0.528(1)	0.0035(3)	0.494	0.494	0.	-0.48	0.48	0.11	0.49	0.18	5.6,4.4
Na3	9(*b*)	0.522(2)	0.288(2)	0.8268(7)	0.549	0.237	0.8385	-0.39	0.72	-0.35	0.72	0.32	20(1)
	18(*c*)												
Na4	9(*b*)	0.186(1)	0.577(1)	0.1499(5)	0.237	0.549	0.1615	-0.72	0.39	-0.35	0.72	0.26	25(1)
Na5	9(*b*)	0.578(1)	0.182(1)	0.8486(6)	0.576	0.205	0.8420	0.03	-0.32	0.20	0.37	0.25	25(1)
	18(*c*)												
Na6	9(*b*)	0.227(2)	0.573(2)	0.1647(7)	0.205	0.576	0.1580	0.32	-0.04	0.20	0.36	0.28	20(1)
Na7,K1	9(*b*)	0.4534(3)	0.8967(4)	0.8118(1)	0.4510	0.8943	0.8156	0.03	0.03	-0.12	0.13	0.18	40,60
	18(*c*)												
Na13	9(*b*)	0.5607(3)	0.1081(3)	0.1806(1)	0.5631	0.1057	0.1844	-0.03	0.03	-0.12	0.12	0.18	67(1)
Na8	9(*b*)	0.092(2)	0.177(2)	0.1668(5)	0.093	0.175	0.1656	-0.01	0.03	0.04	0.05	0.26	22(1)
	18(*c*)												
Na14	9(*b*)	0.9062(8)	0.0795(9)	0.8356(5)	0.907	0.082	0.8344	-0.01	-0.03	0.04	0.05	0.18	14(1)
Na9	9(*b*)	0.105(1)	0.206(1)	0.1552(4)	0.0834	0.194	0.1611	0.31	0.17	-0.18	0.36	0.25	32(1)
	18(*c*)												
Na15	9(*b*)	0.9383(2)	0.0977(2)	0.833(1)	0.9167	0.1101	0.8389	0.31	-0.18	-0.18	0.32	0.30	19(1)
Na10	9(*b*)	0.5321(3)	0.7633(2)	0.9550(1)	0.5300	0.7650	0.9565	0.03	-0.02	-0.05	0.06	0.20	90(1)
	18(*c*)												
Na12,Sr3	9(*b*)	0.4722(3)	0.2334(3)	0.0420(1)	0.4700	0.2350	0.0435	0.03	-0.02	-0.05	0.06	0.18	43,5
Sr2	9(*b*)	0.5679(7)	0.7794(7)	0.9487(3)	0.5634	0.7815	0.9489	0.06	-0.03	-0.01	0.05	0.23	10(1)
	18(*c*)												
Na11	9(*b*)	0.4411(5)	0.2165(4)	0.0510(2)	0.4366	0.2185	0.0512	0.06	-0.03	-0.01	0.05	0.20	52(1)
O26	3(*a*)	0	0	0.3304(8)	0	0	0.3282	0	0	0.07	0.07	0.27	52(3)
	6(*c*)												
O30	3(*a*)	0	0	0.674(2)	0	0	0.6718	0	0	0.07	0.07	0.30	70(1)

O27	3(*a*) 6(*c*)	0	0	0.4723(7)	0	0	0.4751	0	0	-0.08	0.08	0.20	37(3)
O28	3(*a*)	0	0	0.5222(7)	0	0	0.5249	0	0	-0.08	0.08	0.20	39(2)
O29	9(*b*) 18(*c*)	0.609(3)	0.387(3)	-0.0064(8)	0.606	0.398	-0.0047	0.04	-0.15	-0.05	0.14	0.30	40(1)
O31	9(*b*)	0.408(2)	0.603(2)	0.0029(8)	0.398	0.606	0.0047	0.15	-0.04	-0.05	0.14	0.25	30(1)
O32	3(*a*) 6(*c*)	0	0	0.2348(8)	0	0	0.2324	0	0	0.07	0.07	0.21	47(3)
O34	3(*a*)	0	0	0.7700(7)	0	0	0.7676	0	0	-0.06	0.06	0.23	50(3)
O33	3(*a*)	0	0	0.268(3)	0	0	0.261	0	0	0.22	0.22	0.34	25(4)
Cl2	3(*a*)	0	0	0.747(1)	0	0	0.739	0	0	0.23	0.23	0.22	10(2)
O35[††]	3(*a*)	0	0	0.8077(2)	0	0	-	-	-	-	-	0.32	20(2)
Cl1,O36[††]	3(*a*)	0	0	0.7104(7)	0	0	-	-	-	-	-	0.22	20,10

[†] This and most other framework atoms in the table occupy positions that do not differ significantly from space group *R*32.

[‡] $d_{\mathrm{O24\text{-}O25}}$ = 0.45 Å and $\Delta\xi$(O25) = 0.10 Å with respect toO23 in *R*32, hence O25 may be neglected.

[††] $d_{\mathrm{O34\text{-}O35}}$ = 1.14 Å; $d_{\mathrm{Cl1,O36\text{-}O34}}$ = 0.71 Å; $d_{\mathrm{Cl1,O36\text{-}Cl2}}$= 1.10 Å, hence O35 and Cl1,O36 may be neglected.

Table S24 $ZrCr_2D_{3.8}$ at 100 K

Atomic positions for $ZrCr_2D_{3.8}$ at 100 K (Irodova & Suard (2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [90289]

$a = 9.3848(3)$, $c = 26.5461(15)$ Å. $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, P6_3/mcm$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occupancy
Zr1	9(*b*)	0	0.66667	0.3115(1)	0	0.66667	0.3115	0	0	0	0	0.07	1.
Zr2	9(*b*)	0	0.66667	0.1885(1)	0	0.66667	0.1885	0.	0.	0.	0.	"	1.
	12(*k*)†												
Zr3	9(*b*)	0.33333	0.	0.8115(1)	0.33333	0.	0.8115	0	0	0	0	"	1.
Zr4	9(*b*)	0.33333	0.	0.6884(1)	0.33333	0.	0.6885	0.	0.	0.	0.	"	1.
Cr1	3(*a*)	0	0	0.33333	0	0	0.33333	0.	0	0.	0	0.10	1.
Cr7	3(*a*)	0	0	0.16667	0	0	0.16667	0.	0.	0.	0.	"	1.
	4(*e*)												
Cr9	3(*a*)	0.	0.	0.83333	0.	0.	0.83333	0	0	0	0	"	1.
Cr2	3(*a*)	0.	0.	0.66667	0.	0.	0.66667	0.	0.	0.	0.	"	1.
Cr3	3(*a*)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	"	1.
	2(*b*)												
Cr8	3(*a*)	0.	0.	0.5	0.	0.	0.5	0	0	0	0	"	1.
Cr4	9(*b*)	0	0.1603(4)	0.25	0	0.1603	0.25	0.	0.	0.	0.		1.
	6(*g*)											"	
Cr12	9(*b*)	0.8397(4)	0.	0.75	0.8397	0.	0.75	0.	0.	0.	0.	"	1.
Cr5	9(*b*)	0.66667	0.4936(4)	0.25	0.66667	0.4936	0.25	0.	0.	0.	0.	"	1.
Cr6	9(*b*)	0.4936(4)	0.66667	0.25	0.4936	0.66667	0.25	0.	0.	0.	0.	"	1.
	12(*j*)												
Cr10	9(*b*)	0.33333	0.5064(4)	0.75	0.33333	0.5064	0.75	0.	0.	0.	0.	"	1.
Cr11	9(*b*)	0.66667	0.1731(4)	0.75	0.66667	0.1731	0.75	0	0	0	0	"	1.
D1	9(*b*)	0.1223(3)	-0.0836(3)	0.3118(1)	0.1223	-0.0836	0.3118	0.	0.	0.	0.	0.13	0.882(12)
D7	9(*b*)	-0.0836(3)	0.1223(3)	0.1882(1)	-0.0836	0.1223	0.1882	0.	0.	0.	0.	"	0.882(12)
	24(*l*)												
D10	9(*b*)	0.0835(3)	0.8777(3)	0.8119(1)	0.0835	0.8777	0.8118	0.	0.	0.	0.	"	0.882(12)
D16	9(*b*)	-0.1224(3)	0.0836(3)	0.6882(1)	-0.1224	0.0836	0.6882	0.	0.	0.	0.	"	0.882(12)
D2	9(*b*)	0.7890(3)	0.2498(3)	0.3118(1)	0.7890	0.2498	0.3118	0.	0.	0.	0.	"	0.882(12)
D22	9(*b*)	0.2498(3)	0.7890(3)	0.1882(1)	0.2498	0.7890	0.1882	0.	0.	0.	0.	"	0.153(8)
	24(*l*)												
D18	9(*b*)	0.2498(3)	0.7890(3)	0.3119(1)	0.2498	0.7890	0.3119	0.	0.	0.	0.	"	0.108(7)
D9	9(*b*)	0.7502(3)	0.2110(3)	0.8119(1)	0.7502	0.2110	0.8119	0.	0.	0.	0.	"	0.882(12)
D24	9(*b*)	0.2110(3)	0.7503(3)	0.8119(1)	0.2110	0.7502	0.8119	0.	0.	0.	0.	"	0.108(7)
D3	9(*b*)	0.4571(7)	0	0.2911(2)	0.4571	0.	0.2911	0.	0.	0.	0.	"	0.850(13)
	12(*k*)												
D11	9(*b*)	0.5429(7)	0.	0.7911(2)	0.5429	0.	0.7911	0.	0.	0.	0.	"	0.850(13)
D4	9(*b*)	0.7931(12)	0.	0.5833	0.7931	0.	0.5833	0.	0.	0.	0.	"	0.570(14)
	12(*k*)											"	
D12	9(*b*)	0.2069(12)	0	0.0833	0.2069	0	0.0833	0.	0.	0.	0.	"	0.570(14)

D5	9(*b*)	0.5322(7)	0.	0.5833	0.5322	0.	0.5833	0.	0.	0.	0.	"	0.995(19)
D20	9(*b*)	0.5321(7)	0.	0.9167	0.5321	0.0	0.9167	0.	0.	0.	0.	"	0.146(10)
	12(*k*)												
D13	9(*b*)	0.4679(7)	0	0.0833	0.4679	0	0.0833	0.	0.	0.	0.	"	0.995(19)
D25	9(*b*)	0.4679(7)	0.	0.4166	0.4679	0.	0.4166	0.	0.	0.	0.	"	0.146(10)
D6	9(*b*)	0.4570(7)	0.	0.8756(2)	0.4570	0.	0.8756	0.	0.	0.	0.	"	0.850(13)
	12(*k*)												
D14	9(*b*)	0.5430(7)	0.	0.3755(2)	0.5430	0.	0.3755	0.	0.	0.	0.	"	0.850(13)
D8	9(*b*)	0.5831(3)	0.4557(3)	0.1882(1)	0.5832	0.4557	0.1882	0.	0.	0.	0.	"	0.882(12)
	24(*l*)												
D17	9(*b*)	0.4557(3)	0.5831(3)	0.3118(1)	0.4557	0.5832	0.3118	0.	0.	0.	0.	"	0.153(8)
D21	9(*b*)	0.4557(3)	0.5831(3)	0.1882(1)	0.4557	0.5832	0.1882	0.	0.	0.	0.	"	0.108(7)
D23	9(*b*)	0.4169(3)	0.5444(3)	0.8119(1)	0.4169	0.5443	0.8118	0.	0.	0.	0.	"	0.153(8)
D15	9(*b*)	0.5443(3)	0.4169(3)	0.6882(1)	0.5443	0.4169	0.6882	0.	0.	0.	0.	"	0.882(12)
D27	9(*b*)	0.0836(3)	0.8777(3)	0.0215(1)	0.0836	0.8777	0.0215	0.	0.	0.	0.	"	0.108(7)
	24(*l*)												
D28	9(*b*)	0.8777(3)	0.0836(3)	0.0215(1)	0.8777	0.0836	0.0215	0.	0.	0.	0.	"	0.153(8)
D19	9(*b*)	0.5321(7)	0	0.25	0.5321	0	0.25	0.	0.	0.	0.	"	0.146(10)
	6(*g*)												
D26	9(*b*)	0.4678(7)	0.	0.75	0.4678	0.	0.75	0.	0.	0.	0.	"	0.146(10)

[†] **A**toms related over more than two positions are marked by braces. The metal atom ratio of 3:1 is due to the change from rhombohedral to hexagonal and the resulting relaxation of the rhombohedral centering operation, see also §4.10.

Table S25 $Cs_2SO_4Te(OH)_6$

Modified atomic positions for $Cs_2SO_4Te(OH)_6$ (Dammak *et al.*, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [93016]

a = 7.4790(3), c = 16.6370(6) Å. $z^* = z - 0.01451$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Te1	3(*a*),3(*a*)	0.	0.	-0.0044(2)	0.	0.	0.	0.	0.	-0.07	0.07	0.15
Cs1	3(*a*)	0.	0.	0.24393(3)	0.	0.	0.24910	0.	0.	-0.09	0.09	0.19
	6(*c*)											
Cs2	3(*a*)	0.	0.	0.74569(8)	0.	0.	0.75090	0.	0.	-0.09	0.09	0.20
S1	3(*a*),3(*b*)	0.	0.	0.49216(6)	0.	0.	0.5000	0.	0.	-0.13	0.13	0.13
O1	9(*b*)	0.0027(11)	0.7908(10)	-0.0688(6)	0.0259	0.7915	-0.0645	-0.17	-0.01	0.07	0.19	0.22
	18(*f*)											
O2	9(*b*)	0.7921(11)	0.049(11)	0.0602(7)	0.7915	0.0259	0.0645	0.01	0.17	0.07	0.19	0.22
O3	9(*b*),9(*e*)	0.1879(13)	0.1858(13)	0.5004(15)	0.1869	0.1869	0.5000	0.01	-0.01	0.01	0.01	0.30
O4	3(*a*)	0.	0.	0.4080(9)	0.	0.	0.4231	0.	0.	-0.25	0.25	0.30
	6(*c*)											
O5[†]	*3(a)*	*0.*	*0.*	*0.5619(9)*	*0.*	*0.*	*0.5769*	*0.*	*0.*	*-0.25*	*0.25*	*n.d.*
H1	9(*b*)	0.8748(32)	0.684(10)	-0.0772(78)	0.9085	0.7312	-0.0926	-0.25	-0.35	0.26	0.58	0.24
	18(*f*)											
H2	9(*b*)	0.7783(31)	0.9422(38)	0.1080(74)	0.7312	0.9085	0.0926	0.35	0.25	0.26	0.58	0.31

[†] Undetermined atom, see §4.11.

Table S26

Atomic positions for $Ga_4Pd_7Zn_3$ (Subrahmanyam & Schubert., 1973) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [103911]

a = 11.531(20), c = 5.249(1) Å. $z^* = z - 0.014$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3, R\bar{3}$											
Ga1	3(*a*)	0	0	0.042	0	0	0.0	0	0	0.22	0.22	0.13
Ga2	9(*b*)	0.469	0.119	0.984	0.466	0.107	0.998	0.03	0.14	-0.07	0.17	0.14
	18(*f*)											
Zn1	9(*b*)	0.537	0.905	-0.012	0.534	0.893	0.002	0.03	0.14	-0.07	0.17	0.09
Pd1	3(*a*)	0	0	0.526	0	0	0.5	0	0	0.14	0.14	0.11
Pd2	9(*b*)	0.694	0.129	0.143	0.6945	0.136	0.163	-0.01	-0.08	-0.10	0.13	0.08
	18(*f*)											
Pd3	9(*b*)	0.305	0.857	0.817	0.3055	0.864	0.837	-0.01	-0.08	-0.10	0.13	0.08

Table S27(*a*)

Atomic positions for $K_6MnMo_9O_{32}\cdot 6H_2O$ (Weakley, 1977) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [200048]

a = 15.59(2), c = 12.44(2) Å. $z^* = z - 0.0033$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	x	y	z^*	x'	y'	z'	Δx	$\Delta \mathrm{y}$	Δz	$\Delta\xi$	u_{iso}	occ.
Mn1	3(*a*),3(*a*)	0	0	-0.0033	0	0	0	0	0	-0.04	0.04	0.06	1.
Mo1	9(*b*),9(*d*)	0.2022(1)	-0.0039(1)	-0.0052(5)	0.2022	0	0	0.	-0.06	-0.06	0.08	0.09	1.
Mo2	9(*b*)	0.1431(1)	0.0868(1)	0.1972(5)	0.1429	0.0886	0.2018	0.	-0.03	-0.06	0.07	0.07	1.
	18(*f*)												
Mo3	9(*b*)	0.0904(1)	0.1427(1)	-0.2064(5)	0.0886	0.1429	-0.2018	0.03	0.	-0.06	0.07	0.07	1.
K1[†]	9(*b*),9(*d*)	0.4464(4)	0.0027(4)	-0.0113(8)	0.4464	0	0	0.	0.04	-0.14	0.15	0.20	1.
K2	9(*b*),9(*d*)	0.2886(4)	0.3126(4)	0.0377(7)	0.3006	0.3006	0.	-0.19	0.19	0.47	0.51	0.16	1.
O1	9(*b*)	0.0472(9)	0.1126(9)	0.0887(11)	0.0447	0.1124	0.0935	0.04	0	-0.06	0.07	0.05	1.
	18(*f*)												
O2	9(*b*)	0.1121(10)	0.0422(10)	-0.0982(12)	0.1124	0.0447	-0.0935	0	-0.04	-0.06	0.07	0.08	1.
O3	9(*b*)	0.2306(11)	0.1144(12)	0.0844(12)	0.2310	0.1177	0.0866	-0.01	-0.05	-0.03	0.06	0.11	1.
	18(*f*)												
O4	9(*b*)	0.1209(11)	0.2314(11)	-0.0888(13)	0.1176	0.2310	-0.0866	0.05	0.01	-0.03	0.06	0.10	1.
O5	9(*b*)	0.0660(13)	0.2997(13)	0.0841(14)	0.0604	0.2989	0.0884	0.09	0.01	-0.05	0.11	0.15	1.
	18(*f*)												
O6	9(*b*)	0.2982(13)	0.0547(13)	-0.0926(16)	0.2989	0.0603	-0.0884	-0.01	-0.09	-0.05	0.11	0.15	1.
O7	9(*b*)	0.1808(12)	0.0309(11)	0.2897(13)	0.1834	0.0351	0.2913	-0.04	-0.07	-0.02	0.10	0.13	1.
	18(*f*)												
O8	9(*b*)	0.0394(11)	0.1860(11)	-0.2930(12)	0.0351	0.1834	-0.2913	0.07	0.04	-0.02	0.10	0.11	1.
O9	9(*b*)	0.1843(11)	0.2061(11)	0.2464(14)	0.1803	0.2039	0.2522	0.06	0.03	-0.07	0.11	0.11	1.
	18(*f*)												
O10	9(*b*)	0.2017(10)	0.1764(10)	-0.2580(13)	0.2039	0.1803	-0.2522	-0.03	-0.06	-0.07	0.11	0.09	1.
O11	3(*a*)	0	0	0.2547(19)	0	0	0.2608	0	0	-0.08	0.08	0.09	1.
	6(*c*)												
O12	3(*a*)	0	0	-0.2670(18)	0	0	-0.2608	0	0	-0.08	0.08	0.05	1.
O13w[‡]	9(*b*)	0.3981(19)	0.4584(19)[††]	0.1943(20)	0.2758	0.4079	0.3538	1.91	0.79	-1.98	3.11	0.23	1.
	18(*f*)												
O14w	9(*b*)	-0.1535(1)	-0.0817(22)	0.4867(25)	-0.2758	-0.1323	0.6462	1.91	0.79	-1.98	3.11	0.22	0.84

[†] Refined value of z(K1) is -0.0080(8), not -0.0880(8) as published (Weakley, 2006).

[‡] ‘w’ denotes a water oxygen atom.

Table S27(*b*)

Differences between Weakley's averaged (1977) and Dunne *et al.*'s (1992) transformed[†] atomic positions for $K_6MnMo_9O_{32}\cdot 6H_2O$ with u_{iso} displacements in Å ([200048, 71885]

a_W = 15.59(2), c_W = 12.44(2) Å; a_D = 15.569(1), c_D = 12.432(1) Å. $\Delta x = (x_W - x_D)a$,$\Delta y = (y_W - {}_D{}')a$, $\Delta z = (z_W - z_D)c$.

At_W	Wyckoff position *R*3,*R*32	x_W	y_W	z_W	u_{iso}[‡]	At_D .	x_D	y_D	z_D	u_{iso}	occ.	Δx	Δy	Δz	$\Delta\xi$
Mn1	3(*a*)	0	0	0	0.06	Mn1	0	0	0	0.10	1.	0	0	0.	0
Mo1	9(*d*)	0.2022(1)	0	0	0.09	Mo1	0.2042(1)	0	0	0.13	1.	-0.03	0	0	0.03
Mo2	18(*f*)	0.1429(1)	0.0886(1)	0.2018(5)	0.07	Mo2	0.1428(1)	0.0886(1)	0.2014(1)	0.12	1.	0.01	0	0.01	0.01
K1	9(*d*)	0.4464(4)	0	0	0.20	K1	0.4455(2)	0	0	0.22	1.	0.01	0	0	0.01
K2	9(*d*)	0.3006(4)	0.3006(4)	0	0.16	K2	0.2874(3)	0.3111(4)	0.0426(4)	0.18	0.5	0.21	-0.16	-0.52	0.55
O1	18(*f*)	0.0447(9)	0.1124(9)	0.0935(11)	0.07	O1	0.0432(5)	0.1100(5)	0.0921(4)	0.13	1.	0.02	0.04	0.02	0.06
O3	18(*f*)	0.2310(11)	0.1177(12)	0.0866(12)	0.11	O2	0.2318(5)	0.1187(5)	0.0875(4)	0.25	1.	-0.01	-0.02	-0.01	0.03
O6	18(*f*)	0.2989(13)	0.0603(13)	-0.0884(16)	0.15	O3	0.3009(5)	0.0608(5)	-0.0885(6)	0.17	1.	-0.03	-0.01	0	0.04
O7	18(*f*)	0.1834(12)	0.0351(11)	0.2913(13)	0.12	O4	0.1834(6)	0.0352(5)	0.2920(5)	0.17	1.	0.00	0.00	-0.01	0.01
O9	18(*f*)	0.1803(11)	0.2039(11)	0.2522(14)	0.10	O5	0.1795(5)	0.2034(5)	0.2553(5)	0.15	1.	0.01	0.01	-0.04	0.04
O11	6(*c*)	0	0	0.2608(19)	0.17	O6	0	0	0.2598(8)	0.11	1.	0	0	0.01	0.01
O13w[††]	18(*f*)	0.6019(19)	0.1435(19)	-0.1943(20)	0.23	O7	0.5871(22)	0.1757(25)	-0.1534(14)	0.38	0.5	0.23	-0.50	0.23	0.74
O14w	18(*f*)	0.1535(1)	0.0718(22)	0.5166(25)	0.22	O8	0.2151(18)	0.2810(17)	0.5311(16)	0.29	0.5	0.96	-3.26	-0.18	2.91

[†] Coordinates in the form -*x*, -*y*, -*z*

[‡] All Weakley occupancies are unity except for O14 at 0.84.

[††] Not averaged, transposed to –*x*,-*x*+*y*,-*z*.

Table S28

Modified atomic positions for Pd_7P_3 (Matković & Schubert., 1977) with hypothetical $x'y'z'$ coordinates and the Δx, Δy and Δz displacements in Å [200055]

a = 11.976(2), c = 7.055(2) Å. $z^* = z - 0.0341$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Pd1	9(*b*)	0.093(1)	0.260(1)	-0.034	0.096	0.261	-0.013	-0.04	-0.01	-0.15	0.16	0.41
	18(*f*)	y,y-x,-z										
Pd2	9(*b*)	0.262(1)	0.163(1)	-0.008(3)	0.261	0.166	0.013	0.01	-0.04	-0.15	0.15	0.44
Pd3	9(*b*)	0.209(2)	0.241(1)	0.3543(3)	0.2093	0.2375	0.3765	0.00	0.04	-0.16	0.16	0.41
	18(*f*)	y,y-x,-z										
Pd4	9(*b*)	0.234(1)	0.028(1)	0.6013(4)	0.2375	0.0283	0.6235	-0.04	-0.00	-0.16	0.16	0.40
Pd5	3(*a*)	0	0	0.255(4)	0	0	0.2075	0	0	0.34	0.34	0.37
	6(*c*)											
Pd6	3(*a*)	0	0	0.840(6)	0	0	0.7925	0	0	0.34	0.34	0.41
P1	9(*b*)	0.206(3)	0.011(3)	0.287(9)	0.197	0.0165	0.2905	0.11	-0.07	0.00	0.10	0.33
	18(*f*)	y,y-x,-z										
P2	9(*b*)	0.175(3)	0.188(3)	0.706(8)	0.1805	0.197	0.7095	-0.07	-0.11	0.00	0.16	0.33

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

5.1 $Sn_{4.2}Si_9P_{16}$ [68123]

Pivan *et al.*, (1988). Mo*K*α, graphite monochromator; 854 independent $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$; absorption and extinction corrections; site occupancies and U^{ij} varied, $R = 0.027$, $wR = 0.034$; 12 independent atoms; conductivity = 0.07 S m^{-1} at 150 K, 4.5 mS m^{-1} at 293 K, band gap ~0.2 eV. Table S29, in hexagonal coordinates, shows that 7 atoms with $\Delta\xi \lesssim 0.14$ Å and $u_{\mathrm{eq}} \lesssim 0.18$ Å, are very close to supergroup $R\bar{3}$ symmetry if the nominal P1 and Sn2 atoms become equivalent. The published report notes the choice between Sn and P in the 9(*b*) positions was difficult; in addition, $u_{\mathrm{eq}}(\mathrm{Sn2}) \gg u_{\mathrm{eq}}(\mathrm{P1})$. Although both observations support the possibility of equivalence above a phase transition at an undetermined T_C, the model led to excess positive and negative residual electron densities (Guerin, 2006); in addition, nearest neighbors of 'equivalent' pair members are at characteristically different distances. The remaining 5 atoms, with $u_{\mathrm{eq}}(\mathrm{max}) \approx 0.19$ Å, have $0.37 \lesssim \Delta\xi \lesssim 0.60$ Å if Si or P atoms (differing by 1 electron, each with C.N. = 4) can migrate to achieve equivalence at T_C. Thus, in the event all atomic equivalences are as in Table S29, then $Sn_{4.2}Si_9P_{16}$ satisfies the criteria for ferroelectricity but with an uncertainty too high to allow property prediction.

5.2 $Li_4Rh(SO_3)\cdot 3H_2O\cdot OH$ [67921]

Maurer *et al.*, (1993). Ag *K*α; without absorption or extinction corrections; 1,003 independent $I_{\mathrm{obs}} > 3\sigma(I_{\mathrm{obs}})$, u_{eq}; $R = 0.0286$, $wR = 0.0232$; 12 independent atoms. ICSD 67921 gives $y(\mathrm{S}) = 0.681(2)$ instead of the reported 0.0681(2). Table S30 shows that $\Delta\xi \lesssim 1.4$ Å for all atoms, with respect to supergroup *R*32, satisfying the criteria for ferroelectricity if the H3 and Li1 sites were identically occupied. However, $Li2O_6H_2$ is highly distorted, with six $d_{\mathrm{Li2\text{-}O}}$ ranging from 2.00 to 2.51 Å and two $d_{\mathrm{Li2\text{-}H}}$ at 2.24, 2.31 Å whereas $Li1O_6$ approximates a regular octahedron with 3 $d_{\mathrm{Li1\text{-}O1}}$ = 2.08 Å and 3 $d_{\mathrm{Li1\text{-}O3}}$ = 2.16 Å. Further, O5 as reported is tetrahedrally coordinated with 3 Li at $d_{\mathrm{Li2\text{-}O5}}$ = 2.00 Å and H3 at $d_{\mathrm{O5\text{-}H3}}$ = 0.60 Å whereas $d_{\mathrm{O\text{-}H}}$ in $Sr(OH)_2{\cdot}8H_2O$, for example, ranges from 0.96 to 1.01 Å (Ricci *et al.*, 2005). Hence, although it is possible that $Li_4Rh(SO_3){\cdot}3H_2O{\cdot}OH$ is ferroelectric, these structural uncertainties reduce the confidence required for property prediction.

5.3 $Cs_3[(UO_2)_{12}O_7(OH)_{13}]{\cdot}3H_2O$ [87737]

Hill & Burns (1999). Mo*K*α, graphite monochromator; empirical absorption corrections; 3,883 independent F_{obs} with 3,733 $I_{\mathrm{obs}} > 4\sigma(F_{\mathrm{obs}})$, twinning correction, U^{ij} for Cs and U, U_{iso} for O atoms, $R = 0.041$, $wR = 0.034$; 22 independent atoms. The displacement of all atoms in this material from *R*32 symmetry, except for Cs and O7, is $0.2 \lesssim \Delta\xi \lesssim 1.3$ Å. If Cs and O7 were each equally distributed over both the given and the corresponding *R*32 site at $y,x,\bar{z}$, see Table S31, then the structure would satisfy the criteria for ferroelectricity. Adding *CsA* results in 6 nearest neighbors with $d_{CsA\text{-}\mathrm{O}} \lesssim 3.3$ Å about the site compared with 7 nearest neighbors for Cs with $d_{\mathrm{Cs\text{-}O}} \lesssim 3.25$ Å, while adding *O7A* results in normal $d_{O7A\text{-}\mathrm{U1}}$ distances but gives one short $d_{O7A\text{-}\mathrm{O15}}$ at 2.0 Å; variation of the $y,x,\bar{z}$ coordinates may improve the latter. If the proposed *CsA* and *O7A* sites can be experimentally justified, the material would be a candidate for exhibiting ferroelectricity but, until then, the properties of this structure cannot be reliably predicted. A possible typographic error in the sign of *x*(Cs) that would satisfy Wyckoff position 9(*e*) in space group *R*32, hence also the criteria for ferroelectricity was eliminated by Burns (2006). Previously uninvestigated site occupancies and resulting nearest neighbor inequivalencies suggest the advisability of further study.

5.4 Li_2GeTeO_6 family [88785]

Woodward *et al.* (1999). Synchrotron, Si(111) monochromator, $\lambda = 0.50275$ Å; linear absorption corrections; 654 powder I_{obs}, 26 variables, U_{iso} gave $R_{WP} = 0.0498$, $R(F^2) = 0.0548$ by Rietveld refinement; 8 independent sites, two of which are shared by Ge and Te in space group $R3$; 4 independent sites, one shared by Ge and Te in $R\bar{3}$, final $R_{WP} = 0.0530$. Isomorphous α-Na_2GeTeO_6 and Na_2TiTeO_6 reported in $R\bar{3}$. Space group $R3$ chosen for Li_2GeTeO_6, since $R_{WP}(R3)$ was significantly smaller than $R_{WP}(R\bar{3})$. Table S32 shows $\Delta\xi = 0.01$ Å for all metal atoms and $\Delta\xi(O1, O2) \approx 0.12$ Å with $u_{iso}(O) \approx 0.07$ Å. In such cases, a centrosymmetric structure is thermodynamically more likely for materials under full thermal equilibrium. For Ge/Te sites with different composition as reported, however, the symmetry necessarily remains $R3$. The longer $d_{Ge2,Te2–O} = 1.892, 1.986$ Å at one octahedral site compared with $d_{Ge1,Te1–O} = 1.878, 1.881$ Å at the other (each site has two sets of three identical distances) fully supports their reported unequal occupancies, *cf.* Shannon's (1976) radii of $Ge^{4+}(VI) = 0.67$, $Te^{6+}(VI) = 0.70$ Å.

5.5 Eudialyte-type mineral variants [88895, 28015?, 56944]

Rastsvetaeva *et al.* (1999). Cu$K\alpha$, graphite monochromator; 3,173 $I_{obs} > 2\sigma(I_{obs})$ with 1,809 independent $F_{obs} > 4\sigma(F_{obs})$, absorption corrections, $R = 0.026$, U_{eq}; 62 independent atoms. Rastsvetaeva & Khomyakov (2001). Cu$K\alpha$, graphite monochromator; 6,206 I_{obs} >

$2\sigma(I_{\mathrm{obs}})$ with 3,503 independent $F_{\mathrm{obs}} > 4\sigma(F_{\mathrm{obs}})$, empirical absorption corrections, U_{eq}, $R = 0.054$; 110 independent atoms. Two additional variants of mineral eudialyte have been reported in space group $R3$, by Rastsvetaeva *et al.* (1999) and Rastsvetaeva & Khomyakov (2001), see §4.9.

5.5.1 All 36 framework atoms determined by Rastsvetaeva *et al.* (1999), see Table S33(*a*), have $0.01 \lesssim \Delta\xi \lesssim 0.26$ Å while 25 of the 26 nonframework atoms have $0.02 \lesssim \Delta\xi \lesssim 1.00$ Å with respect to $R32$ symmetry; all have $0.1 \lesssim u_{\mathrm{eq}} \lesssim 0.3$ Å. The one exception is the half-occupied site at Na4; if a previously undetected *Na4A* were present, related as by x-y, $\bar{y}$, $\bar{z}$, then all atoms in the structure would approach $R32$ symmetry in satisfaction of the criteria for ferroelectricity. However, the structural uncertainty due to *Na4A* is strongly increased by the 8 pairs of metal atoms reported as less than 0.95 Å apart,[4] with $d_{\mathrm{O25–O24}} = 0.50$ Å, and effectively prevents physical property prediction.

5.5.2 The c-axis length of 60.733 Å in this $R3$ variant, see Rastsvetaeva & Khomyakov (2001), is about double that in §4.9 and in §5.5.1. Notably, $\Delta\xi \lesssim 0.11$ Å for all 70 independent framework atoms with respect to $R\bar{3}m$ symmetry with $0.11 \lesssim u_{\mathrm{eq}} \lesssim 0.23$ Å, except for Ca1 and Ca2, see Table S33(*b*). Sites that are centrosymmetrically equivalent to those of Ca1 and Ca2 and that have a very nearly identical setting may be occupied by unreported *Ca1A* and *Ca2A* atoms. In that case, all but 7 of the 40 independent non-framework atoms in this variant have $\Delta\xi \lesssim 0.18$ Å. The symmetry of $R\bar{3}m$ is hence nearly satisfied, and would be fully so if, in addition to the locations proposed for *Ca1A* and *Ca2A*, six other equivalent locations containing Na, O or Cl in sites that were partially occupied but centrosymmetrically equivalent sites were also unreported. This additional

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[4] With $d_{\mathrm{Mn2\text{-}Zr2}}$, $d_{\mathrm{Na1\text{-}Na2}}$, $d_{\mathrm{Na3\text{-}Na4}}$, $d_{\mathrm{Sr1\text{-}Na5}}$, $d_{\mathrm{Zr2\text{-}Na6}}$, $d_{\mathrm{Na7\text{-}Na8}}$, $d_{\mathrm{Na9\text{-}Na10}}$, $d_{\mathrm{Na9\text{-}Na11}} \lesssim 0.95$ Å.

uncertainty, as in §5.5.1, effectively prevents physical property prediction.

The relatively small departures from centrosymmetry in both present variants may arise from a combination of experimental error and refinement in a polar space group. Johnsen & Grice (1999) noted the symmetry of unsubstituted eudialyte is $R\bar{3}m$, with its variants tending toward $R3m$ symmetry as Si and Fe are substituted by other atoms.

5.6 $\mathbf{H_3PMo_{12}O_{40}}$ [90636]

Marosi *et al.*, (2000); Cu$K\alpha$ whole-pattern powder diffraction of $H_3PMo_{12}O_{40}{\cdot}nH_2O$ at 20 K intervals from 293 to 873 K; Rietveld profile (P) analysis of 653 K data, $R_{WP} = 0.162$, $R_{exp} = 0.131$; 10 independent P and Mo atom position coordinates only refined, all U^{ij}, H and O atoms omitted.[5] Analysis of the P and Mo atomic coordinates shows that all 8 independent Mo atoms have $0.18 \lesssim \Delta\xi \lesssim 0.46$ Å with respect to space group $R\bar{3}$, see Table S34. The two independent P(00*z*) coordinates, however, have $\Delta\xi \approx 1.24$ Å. If these two P atom coordinates are neglected, then the remaining Mo atoms are characterized by $0.10 \lesssim \Delta\xi \lesssim 0.13$ Å; an error in at least one *z*(P) coordinate is hence indicated. The space group of $H_3PMo_{12}O_{40}$ thus appears more likely to be $R\bar{3}$ than $R3$ and a complete reinvestigation of the structure would be appropriate.

5.7 $\mathbf{Ca_4(Ca_{0.7}Na_{0.3})_3Na_{0.7}Li_5(B_{22}O_{39}(OH)_3)(CO_3)(OH)(OH)_{0.8}(H_2O)_{0.2}}$ [97107]

Yamnova *et al.,* (2002). Mo$K\alpha$, graphite monochromator; 3,281 independent $I_{obs} \geq 1.96\sigma(I_{obs})$, absorption and extinction corrections not stated, B_{iso}, $R = 0.0716$, $wR = 0.1018$. This basic hydrate has 33 independent atoms of which all but two have coordinate

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[5] The full analysis, noted in the report as planned for later publication, is not in ICSD release 2006/1.

displacements $0.2 \lesssim \Delta\xi \lesssim 1.2$ Å with respect to the symmetry of space group *R*32, see Table S35. The Li1 and Li3 atomic coordinates would cease being exceptions, with $\Delta\xi \approx 1.3$ Å, if z(Li1) ≈ 0.035 instead of the reported 0.085 and if an unreported *Li3A* atom were present at ~$0,0,\bar{z}$ (Li3), a site with a coordination sphere comparable to that of Li2 and Li3. The structure in Table 35 would then fully satisfy the criteria for ferroelectricity, provided both modified Li locations could be confirmed. Until then, the resulting structural uncertainty effectively prevents physical property prediction.

5.8 $Ga_2Cr_{1.33}Se_5$ [99119]

Okońska-Kozlowska *et al.,* (2004). Mo*K*α, graphite monochromator; 899 independent $I_{obs} > 2\sigma(I_{obs})$, numerical absorption and extinction corrections, U^{ij}, $R = 0.0612$, $wR = 0.135$; 10 independent atoms; semiconductor, $\sigma_{300K} = 1.14\times10^{-3}\ \Omega^{-1}m^{-1}$. All independent atoms in this structure are located on the *c*-axis and form two $CrSe_6$ and two $SeCr_3Ga_3$ octahedra, three $GaSe_4$, one $SeGa_4$ and two $SeCr_3Ga$ tetrahedra. If such atom pairs as octahedral Se and tetrahedral Ga, also octahedral Cr and tetrahedral Ga could exchange sites as in Table S36(*a*), then all atoms present would have $0.42 \lesssim \Delta\xi \lesssim 1.56$ Å with respect to *R*32 and hence would satisfy the structural criteria for ferroelectricity, although barely. Such exchanges are possible even if not likely as, consequently, would be the resulting phase transition. It is noted that, should the origin for Se1, Se2, Ga2 and Ga3 on the polar axis differ from that for Se2, Se3, Se4, Cr1 and Cr2 by $\Delta z \approx 0.05$, then $0.04 \lesssim \Delta\xi \lesssim 0.63$ Å, see Table S36(*b*). The origin sensitivity together with the high *R*, *wR* values suggest the advisability of further structural investigation before property predictions can be made.

5.9 $[Zn(H_2O)_4]_2\cdot[H_2As_6V_{15}O_{42}H_2O]\cdot 2H_2O$ [99351]

Cui Xiao-Bing *et al.,* (2003). Mo$K\alpha$, graphite monochromator; 1,650 independent $F_{\rm obs}$, absorption corrections, $U_{\rm eq}$, R = 0.0569, $wR(F^2)$ = 0.1203; 9 independent metal, 22 O atoms; third-order harmonic generation. The coordinates of all but two atoms, see Table S37(*a*), are approximately related in pairs or singly by the symmetry of supergroup $R\bar{3}$ with 21 atoms having $0.03 \lesssim \Delta\xi \lesssim 0.2$ Å and 8 with $0.44 \lesssim \Delta\xi \lesssim 1.55$ Å; however, $\Delta\xi$(O22) ≈ 2.07 Å and $\Delta\xi$(V5) ≈ 2.65 Å. But for the two latter atoms, the structure would satisfy the criteria for ferroelectricity. However, these large $\Delta\xi$ together with the major angular distortions in both AsO_4 tetrahedra and the smaller but still substantial distortions in the five 'square' pyramidal VO_5 ions result in major structural uncertainty. It may be noted that $\Delta\xi$(V5) would be reduced to 0.76 Å, with no $\Delta\xi \gtrsim 1.55$ Å, if the transition were to supergroup $R\bar{3}m$ through $R3m$ or $R32$, see Table S37(*b*). Such a transition is clearly unlikely since the occupancy of each site would thereby be reduced by the factor 2. Further structural refinement and calorimetric measurement is thus necessary before any prediction of physical properties may be made with confidence.

5.10 $Bi_{11.23}IrCl_{12.23}$ family [412014]

Ruck & Hampel, (2002). $Bi_{11.23}IrCl_{12.23}$. Ag$K\alpha$, graphite monochromator; T = 293 K; 2,443 independent $F_{\rm obs} > 4\sigma(F_{\rm obs})$, numerical absorption and extinction corrections, U^{ij} varied for all atoms, 4 site-occupancies varied, R = 0.030, wR_2 = 0.030; 5 independent metal, 6 Cl atoms; underlying symmetry claimed as triclinic with multiple twinning; semiconductor, band gap ~0.4 eV at 293 K. Except for $\Delta\xi$(Cl6) = 3.70 Å, the atomic displacements are $0.09 \lesssim \Delta\xi \lesssim 0.32$ Å with respect to supergroup $R\bar{3}$. With Cl6 located at

0, 0, 0.2335, if *Cl6A* were assumed to be located at 0, 0, ~0.2335 then $\Delta\xi$(Cl6) would be reduced to zero. If both sites were ~0.112 occupied, see Table S38(*a*), then the crystal symmetry in such a case would more likely be centrosymmetric. The environments of Cl6 and *Cl6A* are closely comparable, both having 6 closest Bi atoms. All five Bi atoms are differently coordinated and Ir is octahedrally coordinated by Bi. However, the Cl4 and Cl5 atoms are reported on sites ~0.66 Å apart, with occupancies of 0.77 and 0.23 respectively. The largest $\Delta\xi$ after Cl6 is that for the related Cl3,Cl5 pair at ~0.32 Å, with $\Delta\xi$(Cl3,Cl4) much smaller; The uncertainty associated with *Cl6A* and the Cl4,Cl5 disorder indicates the need for additional investigation before any predictions of physical properties can be made.

Isomorphous $Bi_{11.7}RhCl_{12.7}$, with $R = 0.037$ and $wR_2 = 0.048$, has $0.09 \lesssim \Delta\xi \lesssim 0.36$ Å for all atoms, see Table S38(*b*), and is very similar to $Bi_{11.23}IrCl_{12.23}$ as is $Bi_{11.28}RhBr_{12.28}$ with $R = 0.038$, $wR_2 = 0.050$ and $0.04 \le \Delta\xi \le 0.35$ Å for all atoms, see Table S38(*c*).

Tables for Appendix 3

Table S29

Modified atomic positions for $Sn_{4.2}Si_9P_{16}$ at room temperature (Pivan *et al.*, 1988) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [68123]

a = 15.665(3), c = 8.761(4) Å. $z^* = z - 0.0157$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3, R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Sn1	3(*a*), 3(*a*)	0	0	-0.0157	0	0	0	0	0	-0.14	0.14	0.18	1.
Sn2	9(*b*)	-0.0298(1)	-0.2239(1)	0.4941(1)	-0.0338	-0.2445	0.5199	0.06	0.32	-0.23	0.42	0.13	1.
	18(*f*)												
P1	9(*b*)	0.2312(2)	-0.0379(2)	0.4543(2)	0.2107	-0.0338	0.4801	0.32	-0.06	-0.23	0.37	0.09	1.
Sn3	3(*a*), 3(*b*)	0	0	0.5607(8)	0	0	0.5	0	0	0.53	0.53	0.19	0.20
Si1	9(*b*)	0.3805(3)	0.0823(3)	0.5313(3)	0.3844	0.0861	0.5406	-0.06	-0.06	-0.08	0.13	0.09	1.
	18(*f*)												
P3	9(*b*)	-0.3885(2)	-0.0899(2)	0.4501(2)	-0.3844	-0.0861	0.4594	-0.06	-0.06	-0.08	0.13	0.09	1.
Si2	9(*b*)	0.2337(3)	-0.1739(3)	0.5385(3)	0.2324	-0.1746	0.5378	0.02	0.01	0.01	0.03	0.09	1.
	18(*f*)												
P2	9(*b*)	0.4076(3)	0.2312(2)	0.4629(2)	0.4069	0.2324	0.4622	0.01	-0.02	0.01	0.02	0.10	1.
Si3	9(*b*)†	0.0719(3)	0.5567(3)	0.5413(3)	0.0756	0.5592	0.5394	-0.06	-0.04	0.02	0.09	0.09	1.
	18(*f*)												
P5	9(*b*)	-0.0793(2)	0.4384(2)	0.4624(2)	-0.0756	0.4408	0.4606	-0.06	-0.04	0.02	0.09	0.09	1.
P4	9(*b*)	-0.1336(3)	-0.1165(3)	0.7772(3)	-0.1095	-0.0976	0.7631	-0.38	-0.30	0.12	0.60	0.12	1.
	18(*f*)												
P6	9(*b*)	0.0853(1)	0.0787(1)	0.2510(1)	0.1094	0.0976	0.2369	-0.38	-0.30	0.12	0.60	0.17	0.33

Table S30

Modified atomic positions for $Li_4Rh(SO_3)$ •$3H_2O$•OH at 293 K (Mäurer *et al*., 1993) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [67921]

a = 8.077(2), c = 13.381(6) Å. $z^* = z + 0.0201$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3, *R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
Rh1	3(*a*)	0	0	0.0201	0	0	0	0	0	0.27	0.27	0.09
S1	9(*b*),9(*d*)	0.2588(2)	0.0681(2)	-0.0696(1)	0.2588	0	0	0	0.55	-0.93	1.08	0.12
O1	9(*b*)	0.2384(4)	0.0943(4)	0.8221(2)	0.2157	0.1346	0.8502	0.18	-0.33	-0.38	0.48	0.15
	18(*f*)											
O4	9(*b*)	0.0583(5)	-0.1749(5)	0.1217(2)	0.0811	-0.1346	0.1498	-0.18	-0.33	-0.38	0.59	0.14
O2	9(*b*)	0.2969(4)	-0.0923(4)	-0.0570(2)	0.2727	-0.1692	-0.0144	0.20	0.62	-0.57	0.93	0.17
	18(*f*)											
O3	9(*b*)	0.4177(4)	0.2462(4)	-0.0283(2)	0.4419	0.1692	0.0144	-0.20	0.62	-0.57	0.79	0.15
H1	9(*b*)†	0.1308(21)	-0.1033(21)	0.1678(19)	0.1979	0.0184	0.1523	-0.54	-0.98	0.21	1.35	0.20
	18(*f*)											
H2	9(*b*)†	-0.0577(21)	-0.2649(21)	0.1367(21)	-0.1794	-0.1979	0.1523	0.98	-0.54	-0.21	0.88	0.29
O5	3(*a*),3(*b*)	0	0	0.4367(4)	0	0	0.5000	0	0	-0.84	0.84	0.16
H3	3(*a*)	0	0	0.4813(20)	0	0	0.3753	0	0	1.42	1.42	0.18
	6(*c*)††											
Li1	3(*a*)	0	0	0.7307(9)	0	0	0.6247	0	0	1.42	1.42	0.16
Li2	9(*b*),9(*d*)	0.0856(14)	0.6135(14)	0.0426(9)	0	0.6135	0	0.69	0	0.57	0.89	0.27

† For H1, H2 related as in *R*3, at the x, y, z and the $-x+y$, $-x$, z positions.

†† Assuming equal occupation of the H3 and Li1 sites.

Table S31

Modified atomic positions for $Cs_3[(UO_2)_{12}O_7(OH)_{13}]\cdot 3H_2O$ (Hill & Burns 1999) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [87737]

a = 14.124(6), c = 22.4073(14) Å. $z^* = z - 0.00568$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R32$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
U1	9(*b*)	0.47576(8)	0.33444(8)	0.96513(5)	0.49964	0.34548	0.98203	-0.34	-0.16	-0.38	0.58	0.11
	18(*f*)											
U3	9(*b*)	0.35652(9)	0.52352(8)	0.00107(4)	0.34548	0.49964	0.01797	0.16	0.34	-0.38	0.58	0.11
U2	9(*b*),9(*d*)	0.35595(9)	0.0247(1)	0.98573(5)	0.35595	0.0	0.0	0.0	0.35	-0.32	0.47	0.12
U4	9(*b*),9(*d*)	0.17139(9)	0.15090(8)	0.00641(4)	0.16115	0.16115	0.0	0.14	-0.14	0.14	0.20	0.11
Cs	9(*b*)	0.19698(2)	0.79232(2)	0.49115(9)	0.53031	0.45899	0.15782	0.0	0.0	0.0	0.0	0.12
	18(*f*)†											
CsA	*9(b)*	*0.79232*	*0.19698*	*0.50885*	0.45899	0.53031	*0.84218*	*0.0*	*0.0*	*0.0*	*0.0*	*n.d.*
O1	9(*b*)	0.361(2)	0.493(2)	0.0765(9)	0.350	0.474	0.0954	0.16	0.27	-0.42	0.56	0.15
	18(*f*)											
O5	9(*b*)	0.455(2)	0.339(2)	0.8858(9)	0.474	0.350	0.9046	-0.27	-0.16	-0.42	0.56	0.15
O2	9(*b*)	0.348(2)	0.547(2)	-0.0749(9)	0.339	0.527	-0.0576	0.13	0.28	-0.39	0.53	0.15
	18(*f*)											
O10	9(*b*)	0.507(2)	0.331(2)	0.040(1)	0.527	0.339	0.058	-0.28	-0.11	-0.40	0.53	0.20
O3	9(*b*)	0.220(2)	0.188(2)	0.080(1)	0.169	0.154	0.073	0.72	0.48	0.16	1.06	0.16
	18(*f*)											
O4	9(*b*)	0.119(2)	0.118(2)	-0.0657(9)	0.154	0.169	-0.0730	-0.49	-0.72	0.16	1.07	0.15
O6	9(*b*)	0.311(2)	-0.020(1)	-0.0901(8)	0.258	0.006	-0.0557	0.75	-0.37	-0.77	1.01	0.14
	18(*f*)											
O14	9(*b*)	0.032(1)	0.206(1)	0.0213(8)	0.006	0.258	0.0559	0.37	-0.73	-0.77	1.00	0.11
O7	3(*a*)	0	0	0.358(1)	0	0	0	0	0	0	0	0.12
	18(*f*)‡											
O7A	*3(a)*	*0*	*0*	*0.642*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*n.d.*
O12	3(*a*),3(*a*)	0	0	0.040(1)	0	0	0.	0	0	0.90	0.90	0.07
O8	9(*b*)	0.395(1)	0.068(1)	0.0613(9)	0.427	0.116	0.0214	-0.45	-0.68	0.89	1.33	0.13
	18(*f*)											
O13	9(*b*)	0.164(1)	0.460(1)	0.0185(7)	0.116	0.427	-0.0214	0.68	0.47	0.89	1.34	0.10
O9	9(*b*)	0.498(2)	0.504(2)	-0.024(1)	0.486	0.517	0.017	0.17	-0.19	-0.92	0.94	0.16
	18(*f*)											
O15	9(*b*)	0.527(1)	0.198(1)	-0.0580(9)	0.514	0.186	-0.017	0.18	0.17	-0.92	0.97	0.12
O11	9(*b*)	0.324(1)	0.159(1)	-0.0270(8)	0.328	0.223	0.0002	-0.06	-0.90	-0.61	1.11	0.12
	18(*f*)											
O16	9(*b*)	0.287(2)	0.331(2)	-0.0276(9)	0.223	0.328	-0.0002	0.90	0.04	-0.61	1.10	0.15
O17	9(*b*),9(*e*)	0.013(2)	0.554(2)	0.5194(9)	0.0	0.554	0.50	0.18	0.0	0.43	0.47	0.17

† Assuming *CsA*, at Cs(y, x, $\bar{z}$), with site occupancy of 50% for Cs and Cs*A*.

‡ Assuming *O7A* at O7(0, 0, $\bar{z}$).

Table S32

Modified atomic positions for Li_2GeTeO_6 (Woodward *et al.* 1999) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [88785]

a = 5.00795(5), c = 14.3422(2) Å. $z^* = z + 0.00045$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta \xi$	occ.	u_{iso}
Li1	3(a) 6(c)	0	0	0.132(5)	0	0	0.133	0	0	-0.01	0.01	1.	0.20
Li2	3(a)	0	0	0.866(5)	0	0	0.867	0	0	-0.01	0.01	1.	0.20
Ge1,Te1	3(a) 6(c)	0	0	0.66014(4)	0	0	0.65969	0	0	0.01	0.01	0.82,0.18	0.07
Te2,Ge2	3(a)	0	0	0.34075(4)	0	0	0.34031	0	0	0.01	0.01	0.82,0.18	0.07
O1	9(b) 18(f)	0.309(2)	-0.024(2)	0.2598(8)	0.292	-0.032	0.2596	0.09	0.04	0.0	0.12	1.	0.07
O2	9(b)	0.725(2)	0.040(2)	0.7405(9)	0.708	0.032	0.7404	0.09	0.04	0.0	0.12	1.	0.07

Table S33(*a*) Eudialyte-type Mn,Ce-silicate

Atomic positions for $Na_{16}K_{0.1}Ca_{2.10}Mn_{3.6}Sr_{0.45}Fe_{0.15}Ce_{1.15}Zr_{3.30}Hf_{0.05}Ti_{0.10}Nb_{0.40}Si_{25.6}$-$O_{74.54}(OH)_{0.82}F_{0.28}Cl_{0.17}(H_2O)_{1.75}$ (Rastsvetaeva *et al.* 1999) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [88895]

$a = 14.182(7)$, $c = 30.37(1)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')$

	Wyckoff position *R*3, *R*32	*x*	*y*	*z*	*x*′	*y*′	*z*′	Δ*x*	Δ*y*	Δ*z*	Δ*ξ*	u_{eq}	occ. %
Zr1,Ti11	9(*b*),9(*e*)	0.0002(1)	0.4922(1)	0.4999(1)	0	0.4922	0.5	0.0	0.0	0.0	0.0	0.15	96.7,3.3
Mn1	9(*b*),9(*d*)	-0.0006(1)	0.2718(1)	0.0001(1)	0	0.2718	0	0.01	0	0	0.01	0.15	100
Ca1,Ce1	9(*b*),9(*d*)	0.2448(1)	0.2447(1)	0.0001(1)	0.2448	0.24475	0	0	0	0	0.0	0.15	70,30
Si	9(*b*)	-0.0107(2)	0.6076(2)	0.0975(1)	-0.0107	0.6081	0.0971	0	-0.01	0.01	0.01	0.14	100
	18(*c*)												
Si5	9(*b*)	0.6086(2)	0.9892(2)	0.9033(1)	0.6081	0.9892	0.9029	0.01	0	0.01	0.01	0.15	100
Si2	9(*b*)	-0.0065(2)	0.3953(2)	0.0966(1)	-0.0067	0.3949	0.0964	0.0	0.01	0.01	0.01	0.14	100
	18(*c*)												
Si4	9(*b*)	0.3945(2)	0 .9939(2)	0.9039(1)	0.3949	0 .9937	0.9036	-0.01	0.01	0.01	0.01	0.14	100
Si3	9(*b*)	0.1397(2)	0.0588(2)	0.0809(1)	0.1404	0.0588	0.0805	-0.01	0.0	0.01	0.01	0.15	100
	18(*c*)												
Si7	9(*b*)	0.8590(2)	0.9185(2)	0.9199(1)	0.8596	0.9185	0.9195	-0.01	0.0	0.01	0.01	0.15	100
Si6	9(*b*)	0.2083(2)	0.4156(2)	0.0767(1)	0.2088	0.4154	0.0763	-0.01	0.0	0.01	0.01	0.13	100
	18(*c*)												
Si8	9(*b*)	0.7907(2)	0.2072(2)	0.9241(1)	0.7912	0.2074	0.9237	-0.01	0.0	0.01	0.01	0.15	100
O1	9(*b*)	0.8430(5)	0.6930(6)	0.3635(2)	0.8437	0.6945	0.3627	-0.01	-0.02	0.02	0.03	0.17	100
	18(*c*)												
O17	9(*b*)	0.6959(6)	0.8444(6)	0.6382(2)	0.6945	0.8437	0.6373	0.02	0.01	0.03	0.04	0.20	100
O2	9(*b*)	0.1828(5)	0.3533(6)	0.2210(2)	0.1832	0.3533	0.2212	-0.01	0.00	-0.01	0.01	0.17	100
	18(*c*)												
O22	9(*b*)	0.3533(6)	0.1837(5)	0.7786(2)	0.3533	0.1832	0.7788	0.00	0.01	-0.01	0.01	0.17	100
O3	9(*b*)	0.9594(7)	0.2576(5)	0.7122(2)	0.9576	0.2563	0.7120	0.03	0.02	0.01	0.04	0.20	100
	18(*c*)												
O20	9(*b*)	0.0441(6)	0.2991(6)	0.2883(2)	0.0424	0.2987	0.2881	0.02	0.01	0.01	0.03	0.17	100
O4	9(*b*)	0.9736(6)	0.7068(5)	0.7128(2)	0.9860	0.7072	0.7122	-0.18	-0.01	0.02	0.19	0.17	100
	18(*c*)												
O21	9(*b*)	0.2642(5)	0.2924(5)	0.2885(2)	0.2518	0.2928	0.2878	0.18	-0.01	0.02	0.18	0.16	100
O5	9(*b*)	0.5888(6)	0.6898(6)	0.8722(2)	0.5884	0.6906	0.8718	0.01	-0.01	0.01	0.01	0.18	100
	18(*c*)												
O19	9(*b*)	0.4120(6)	0.1029(6)	0.1285(2)	0.4116	0.1022	0.1282	0.01	-0.01	0.01	0.01	0.18	100
O6	9(*b*)	0.5927(7)	0.8923(6)	0.8727(2)	0.5926	0.8931	0.8719	0.0	-0.01	0.02	0.02	0.20	100
	18(*c*)												
O18	9(*b*)	0.4075(7)	0.2981(7)	0.1289(3)	0.4074	0.2973	0.1281	0.0	0.01	0.02	0.02	0.20	100

O7	9(*b*)	0.8085(8)	0.8947(9)	0.8709(2)	0.8075	0.8942	0.8708	0.01	0.01	0.01	0.02	0.23	100
	18(*c*)												
O9	9(*b*)	0.1935(5)	0.0863(6)	0.1293(2)	0.1925	0.0868	0.1292	0.01	-0.01	0.01	0.01	0.19	100
O8	9(*b*)	0.5578(7)	0.7631(6)	0.7090(2)	0.5583	0.7629	0.7083	-0.01	0.0	0.02	0.02	0.20	100
	18(*c*)												
O12	9(*b*)	0.4412(6)	0.2044(7)	0.2924(2)	0.4417	0.2042	0.2917	-0.01	0.0	0.02	0.02	0.19	100
O10	9(*b*)	0.1072(7)	0.3909(8)	0.1079(2)	0.1054	0.3898	0.1069	0.03	0.02	0.03	0.05	0.21	100
	18(*c*)												
O15	9(*b*)	0.3887(7)	0.1037(6)	0.8940(2)	0.3898	0.1054	0.8931	-0.02	-0.02	0.03	0.05	0.20	100
O11	9(*b*)	0.2721(5)	0.3706(5)	0.1085(2)	0.2739	0.3698	0.1075	-0.03	-0.01	0.03	0.05	0.16	100
	18(*c*)												
O16	9(*b*)	0.7243(5)	0.0951(5)	0.8936(2)	0.7261	0.0959	0.8925	-0.03	-0.01	0.03	0.02	0.17	100
O13	9(*b*)	0.9480(6)	0.8793(5)	0.9229(2)	0.9484	0.8778	0.9229	-0.01	0.02	0.0	0.02	0.19	100
	18(*c*)												
O14	9(*b*)	0.0709(6)	0.1237(6)	0.0771(2)	0.0706	0.1222	0.0771	0.01	0.02	0.0	0.03	0.20	100
O23	9(*b*)	0.2833(9)	0.5474(8)	0.0708(5)	0.2786	0.5429	0.0785	0.07	0.06	-0.23	0.26	0.27	100
	18(*c*)												
O24	9(*b*)	0.5383(2)	0.274(2)	0.9138(7)	0.5429	0.2786	0.9215	-0.06	-0.07	-0.23	0.26	0.23	45
O23[†]	9(*b*)	0.6166(9)	0.2141(8)	0.7375(5)	0.6198	0.2134	0.7375	-0.05	0.01	0.0	0.05	0.27	100
	18(*c*)												
O25	9(*b*)	0.377(1)	0.593(1)	0.2622(4)	0.3802	0.5937	0.2622	-0.04	-0.01	0.0	0.05	0.21	55
Si9	3(*a*)	0.0	0.0	0.3777(2)	0.0	0.0	0.3770	0.0	0.0	0.02	0.02	0.10	51
	6(*c*)												
Nb1	3(*a*)	0.0	0.0	0.6237(1)	0.0	0.0	0.6230	0.0	0.0	0.02	0.02	0.17	40
Si10	3(*a*)	0.0	0.0	0.4235(2)	0.0	0.0	0.4205	0.0	0.0	0.09	0.09	0.17	49
	6(*c*)												
Si11	3(*a*)	0.0	0.0	0.5825(8)	0.0	0.0	0.5795	0.0	0.0	0.09	0.09	0.26	60
Mn2,Fe1	9(*b*)	0.1833(4)	0.3551(5)	0.3314(1)	0.1880	0.3632	0.3309	-0.07	-0.11	0.02	0.16	0.15	20, 5
	18(*c*)												
Zr2,Hf1	9(*b*)	0.3712(4)	0.1926(5)	0.6696(2)	0.3632	0.1880	0.6691	0.11	0.07	0.02	0.16	0.17	13.3,1.7
Na1	9(*b*)	0.190(1)	0.615(2)	0.1527(6)	0.213	0.565	0.1655	-0.33	0.71	-0.39	0.73	0.31	50
	18(*c*)												
Na2	9(*b*)	0.515(1)	0.236(1)	0.8217(4)	0.565	0.213	0.8345	-0.71	0.33	-0.39	0.73	0.27	50
Na9	9(*b*)	0.5612(4)	0.1117(4)	0.1804(1)	0.5552	0.1115	0.1802	0.09	0.0	0.01	0.09	0.22	96.7,3.3
	18(*f*)												
Na3,Ce2	9(*b*)	0.4508(4)	0.8901(5)	0.8201(1)	0.4448	0.8899	0.8198	0.09	0.01	0.01	0.09	0.21	39.7,8.3
Sr1	9(*b*)	0.5729(9)	0.7792(9)	0.9443(4)	0.5485	0.7938	0.9510	0.35	-0.20	-0.20	0.36	0.22	10
	18(*f*)												
Na8,Sr2	9(*b*)	0.4760(5)	0.2355(5)	0.0423(2)	0.4515	0.2209	0.0490	0.35	0.20	-0.20	0.52	0.18	45,5
Na5	9(*b*)	0.5299(4)	0.7617(4)	0.9557(1)	0.5455	0.7727	0.9512	-0.22	-0.17	0.14	0.37	0.19	90
	18(*f*)												
Na7	9(*b*)	0.4388(7)	0.2142(6)	0.0534(3)	0.4545	0.2273	0.0488	-0.22	-0.17	0.14	0.37	0.19	50

Na4[‡]	9(*b*)	0.077(2)	0.162(2)	0.1700(4)	0.077	0.162	0.1700	0	0	0	0	0.30	52
	18(*c*)												
Na4A	*9(b)*	*0.915*	*0.838*	*0.8300*	*0.923*	*0.838*	*0*	*0*	*0*	*0*	*0*	*n.d.*	*n.d.*
Na6	9(*b*),9(*d*)	0.446(1)	0.550(1)	0.0036(3)	0.498	0.498	0	-0.74	0.74	0.11	0.75	0.28	60
O26	9(*b*)	0	0	0.330(1)	0	0	0.350	0	0	-0.61	-0.61	0.23	51
	18(*c*)												
F1,Cl1	3(*a*)	0	0	0.7091(4)	0	0	0.729	0	0	-0.61	-0.61	0.18	4.24,4.24
O27	9(*b*)	0	0	0.4773(8)	0	0	0.4742	0	0	0.09	0.09	0.19	55
	18(*c*)												
O28	9(*b*)	0	0	0.529(1)	0	0	0.5258	0	0	0.10	0.10	0.31	53
O29	9(*b*)	0.605(1)	0.400(2)	0.0058(6)	0.6055	0.397	-0.0039	-0.01	0.04	-0.06	0.07	0.23	44
	18(*c*)												
O30	9(*b*)	0.411(8)	0.606(6)	0.002(3)	0.4055	0.603	0.0039	0.01	0.04	-0.06	0.07	0.24	15
O31	3(*a*)	0	0	0.248(2)	0	0	0.216	0	0	0.98	0.98	0.32	43
	18(*c*)												
O34	3(*a*)	0	0	0.817(2)	0	0	0.784	0	0	0.98	0.98	0.32	42
O32	3(*a*)	0	0	0.289(2)	0	0	0.256	0	0	1.00	1.00	0.22	32
	18(*c*)												
O33	3(*a*)	0	0	0.777(1)	0	0	0.744	0	0	1.00	1.00	0.28	58

[†] The fully-occupied O23 site as reported is related both to the half-occupied O24 and O25 sites as shown.

[‡] Hypothetical *Na4A* is only 0.90 Å from Na9 (*cf.* $d_{\mathrm{Na7\text{-}Na8}}$ = 0.57 Å) and has comparable nearest neighbors.

Table S33(*b*) Eudialyte-type Ca,Fe-silicate

Atomic positions for (Na,Sr,K)$_{35}$Ca$_{12}$Fe$_3$Zr$_6$TiSi$_{51}$O$_{144}$(O,OH,H$_2$O)$_9$Cl$_3$ (Rastsvetaeva & Khomyakov, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [93950]

a = 14.239(1), c = 60.733(7) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occupancy
Zr1	9(*b*)	0.1659(1)	0.3321(1)	0.0829(1)	0.1660	0.3320	0.0841	0	0	-0.07	0.07	0.13	1
	18(*h*)												
Zr2	9(*b*)	0.3321(1)	0.1659(1)	0.9148(1)	0.3320	0.1660	0.9159	0	0	-0.07	0.07	0.13	1
Ca1	9(*b*)	0.0727(1)	0.6678(1)	0.1658(1)	0.0725	0.6666	0.1667	0.0	0.02	-0.05	0.06	0.12	0.5
Ca1A	*9(b)*	*0.0727*	*0.4049*	*0.1658*	*0.0725*	*0.4049*	*0.1667*	*0*	*0*	*-0.05*	*0.05*	*n.d.*	*n.d.*[‡]
	36(*i*) *[†]												
Ca2A	*9(b)*	*0.9278*	*0.5951*	*0.8325*	*0.9275*	*0.5951*	*0.8333*	*0*	*0*	*-0.05*	*0.05*	*n.d.*	*n.d.*
Ca2	9(*b*)	0.9278(1)	0.3346(1)	0.8325(1)	0.9275	0.3334	0.8333	0.0	0.02	-0.05	0.05	0.11	0.5
Ca3	9(*b*)	-0.0004(1)	0.2620(1)	-0.0009(1)	0.0000	0.2620	-0.00085	-0.01	0.0	-0.05	0.05	0.11	1
	18(*f*)												
Ca4,Sr1	9(*b*)	0.2615(1)	0.2620(1)	-0.0008(1)	0.2620	0.2620	-0.00085	0.01	0.0	-0.05	0.05	0.11	0.95,0.05
Si1	9(*b*)	0.3248(2)	0.0551(1)	0.1182(1)	0.3266	0.0576	0.1185	-0.01	-0.04	-0.04	0.05	0.13	1
Si16	9(*b*)	0.6717(1)	0.9403(1)	0.8812(1)	0.6734	0.9424	0.8815	-0.02	-0.03	-0.02	0.05	0.12	1
	36(*i*)												
Si2	9(*b*)	0.3263(1)	0.2685(1)	0.1178(1)	0.3266	0.2690	0.1185	-0.01	-0.01	-0.04	0.04	0.12	1
Si15	9(*b*)	0.6731(1)	0.7303(1)	0.8808(1)	0.6734	0.7310	0.8815	-0.01	-0.01	-0.04	0.04	0.13	1
Si3	9(*b*)	0.2496(1)	0.1253(1)	0.2948(1)	0.2495	0.1248	0.2956	0.0	0.01	-0.05	0.05	0.12	1
	18(*h*)												
Si14	9(*b*)	0.7506(1)	0.8758(1)	0.7036(1)	0.7505	0.8752	0.7044	0.0	0.01	-0.05	0.05	0.12	1
Si6	9(*b*)	0.5979(1)	0.4037(1)	0.2910(1)	0.5968	0.4050	0.2918	0.02	-0.02	-0.05	0.05	0.11	1
	18(*h*)												
Si7	9(*b*)	0.4043(1)	0.8095(1)	0.7075(1)	0.4032	0.8082	0.7082	0.02	0.02	-0.04	0.05	0.11	1
Si 4	9(*b*)	0.0641(1)	0.3419(1)	0.2841(1)	0.0639	0.3403	0.2838	0.0	0.02	0.02	0.05	0.11	1
Si12	9(*b*)	0.3403(1)	0.0637(1)	0.7175(1)	0.3403	0.0639	0.7162	0.0	0.0	0.08	0.05	0.13	1
	36(*i*)												
Si5	9(*b*)	0.2766(1)	0.3401(1)	0.2839(1)	0.2764	0.3403	0.2838	0.0	0.0	0.01	0.02	0.16	1
Si11	9(*b*)	0.3387(1)	0.2755(1)	0.7153(1)	0.3403	0.2761	0.7162	-0.01	-0.01	-0.05	0.03	0.12	1
Si8	9(*b*)	0.4044(1)	0.5962(1)	0.2068(1)	0.4041	0.5960	0.2075	0.0	0.0	-0.04	0.04	0.11	1
	18(*h*)												
Si10	9(*b*)	0.5958(1)	0.1928(1)	0.7919(1)	0.5959	0.1919	0.7925	-0.0	0.01	-0.04	0.04	0.12	1
Si9	9(*b*)	0.5418(2)	0.4589(2)	0.1281(1)	0.5419	0.4581	0.1288	-0.0	0.01	-0.04	0.04	0.15	1
	18(*h*)												
Si13	9(*b*)	0.4576(2)	0.9152(2)	0.8705(1)	0.4581	0.9162	0.8712	-0.01	-0.01	-0.04	0.04	0.14	1
O1	9(*b*)	0.3551(6)	0.1766(5)	0.1089(1)	0.3552	0.1776	0.1096	-0.0	0.0	-0.04	0.04	0.16	1
	18(*h*)												
O10	9(*b*)	0.6444(6)	0.8216(5)	0.8898(1)	0.6448	0.8224	0.8904	-0.00	0.0	-0.04	0.04	0.17	1

O2	9(*b*)	18(*h*)	0.3083(5)	0.1521(5)	0.3182(1)	0.3079	0.1540	0.3185	0.01	-0.03	-0.02	0.04	0.15	1
O48	9(*b*)		0.6934(5)	0.8432(4)	0.6811(1)	0.6921	0.8460	0.6815	0.01	-0.03	-0.02	0.04	0.14	1
O3	9(*b*)	18(*h*)	0.5157(4)	0.0326(5)	0.1518(1)	0.5158	0.0316	0.1523	-0.0	0.01	-0.03	0.03	0.12	1
O46	9(*b*)		0.4837(5)	0.9698(5)	0.8471(1)	0.4842	0.9684	0.8477	-0.0	0.02	-0.04	0.04	0.17	1
O4	9(*b*)	36(*i*)	0.3856(4)	0.2808(3)	0.0534(1)	0.3877	0.2820	0.0539	-0.03	-0.02	-0.03	0.05	0.10	1
O41	9(*b*)		0.6099(8)	0.7165(6)	0.9455(1)	0.6123	0.7180	0.9460	-0.03	-0.02	-0.03	0.06	0.22	1
O5	9(*b*)		0.3875(6)	0.1063(6)	0.0534(1)	0.3877	0.1057	0.0539	-0.	0.01	-0.03	0.03	0.20	1
O40	9(*b*)		0.6125(4)	0.8945(4)	0.9455(1)	0.6123	0.8943	0.9460	0.	0.0	-0.03	0.04	0.10	1
O6	9(*b*)	36(*i*)	0.0729(5)	0.3691(5)	0.3089(1)	0.0717	0.3688	0.3096	0.02	0.0	-0.04	0.04	0.15	1
O21	9(*b*)		0.3684(6)	0.0704(5)	0.6896(1)	0.3688	0.0717	0.6904	-0.01	-0.01	-0.05	0.05	0.17	1
O7	9(*b*)		0.2917(5)	0.3688(5)	0.3092(1)	0.2926	0.3687	0.3101	-0.01	0.0	-0.05	0.06	0.10	1
O20	9(*b*)		0.3686(4)	0.2935(4)	0.6891(1)	0.3687	0.2926	0.6899	-0.0	0.01	-0.05	0.05	0.13	1
O8	9(*b*)	36(*i*)	0.0300(5)	0.2585(6)	0.1038(1)	0.0303	0.2583	0.1042	-0.0	-0.0	-0.02	0.02	0.17	1
O34	9(*b*)		0.7714(6)	0.0307(6)	0.8955(1)	0.7716	0.0303	0.8958	-0.0	0.01	-0.02	0.02	0.19	1
O9	9(*b*)		0.2257(5)	0.2542(6)	0.1039(1)	0.2284	0.2583	0.1042	-0.04	-0.06	-0.02	0.08	0.18	1
O35	9(*b*)		0.7691(5)	0.7379(5)	0.8954(1)	0.7716	0.7417	0.8958	-0.04	-0.06	-0.02	0.08	0.17	1
O11	9(*b*)	36(*i*)	0.1008(5)	0.4032(5)	0.0632(1)	0.1031	0.4040	0.0642	-0.03	-0.01	-0.06	0.07	0.16	1
O32	9(*b*)		0.9010(5)	0.2991(6)	0.9349(1)	0.8969	0.3030	0.9358	0.06	-0.06	-0.05	0.08	0.13	1
O12	9(*b*)		0.3028(5)	0.4070(5)	0.0636(1)	0.3030	0.4040	0.0642	0.0	0.04	-0.04	0.06	0.16	1
O31	9(*b*)		0.4017(5)	0.3008(4)	0.9350(1)	0.4040	0.3030	0.9357	-0.03	-0.03	-0.04	0.07	0.14	1
O13	9(*b*)	18(*h*)	0.0566(7)	0.1175(6)	0.2051(1)	0.0598	0.1195	0.2066	-0.05	-0.03	-0.09	0.11	0.23	1
O42	9(*b*)		0.9370(7)	0.8785(7)	0.7920(1)	0.9402	0.8805	0.7934	-0.05	-0.03	-0.09	0.11	0.21	1
O14	9(*b*)	18(*h*)	0.5687(5)	0.1407(5)	0.2664(1)	0.5715	0.1432	0.2672	-0.04	-0.04	-0.05	0.08	0.16	1
O30	9(*b*)		0.4257(1)	0.8542(5)	0.7321(1)	0.4285	0.8568	0.7328	-0.04	-0.04	-0.04	0.08	0.14	1
O15	9(*b*)	18(*h*)	0.2344(5)	0.4731(6)	0.1013(1)	0.2368	0.4736	0.1016	-0.03	-0.01	-0.02	0.03	0.18	1
O47	9(*b*)		0.7636(5)	0.2399(5)	0.8980(1)	0.7632	0.2368	0.8984	0.01	0.04	-0.02	0.03	0.17	1
O16	9(*b*)	36(*i*)	0.2986(4)	0.2515(3)	0.1438(1)	0.3007	0.2542	0.1444	-0.03	-0.04	-0.04	0.07	0.09	1
O23	9(*b*)		0.6967(6)	0.7432(5)	0.8551(1)	0.6993	0.7458	0.8556	-0.03	-0.04	-0.03	0.07	0.17	1
O17	9(*b*)		0.3007(5)	0.0467(5)	0.1437(1)	0.3007	0.0465	0.1444	0.0	0.0	-0.04	0.04	0.15	1
O22	9(*b*)		0.6999(4)	0.9538(4)	0.8550(1)	0.6993	0.9535	0.8556	0.0	0.0	-0.04	0.04	0.12	1
O18	9(*b*)	18(*h*)	0.5523(4)	0.4493(4)	0.3103(1)	0.5518	0.4481	0.3109	0.01	0.02	-0.04	0.04	0.12	1
O37	9(*b*)		0.4468(5)	0.8967(5)	0.6885(1)	0.4481	0.8962	0.6891	-0.02	0.01	-0.04	0.04	0.16	1
O19	9(*b*)	18(*h*)	0.2715(5)	0.5439(5)	0.2054(1)	0.2717	0.5434	0.2057	0.0	0.01	-0.02	0.02	0.16	1
O29	9(*b*)		0.7298(4)	0.2728(4)	0.7940(1)	0.7283	0.2717	0.7943	0.02	0.02	-0.02	0.03	0.14	1

O24	9(*b*)	0.1232(4)	0.0606(4)	0.0395(1)	0.1238	0.0624	0.0396	-0.01	-0.03	-0.01	0.03	0.12	1
	18(*h*)												
O25	9(*b*)	0.8756(5)	0.9359(5)	0.9602(1)	0.8762	0.9376	0.9604	-0.01	-0.02	-0.01	0.03	0.16	1
O26	9(*b*)	0.0572(5)	0.2937(6)	0.2189(1)	0.0547	0.2904	0.2198	0.04	0.05	-0.05	0.09	0.17	1
O44	9(*b*)	0.9455(8)	0.2351(8)	0.7793(1)	0.9442	0.2335	0.7802	0.02	0.02	-0.05	0.06	0.26	1
	36(*i*)												
O27	9(*b*)	0.2332(4)	0.2871(4)	0.2188(1)	0.2323	0.2904	0.2197	0.01	-0.05	-0.05	0.07	0.10	1
O43	9(*b*)	0.7687(5)	0.0516(5)	0.7794(1)	0.7665	0.0547	0.7803	0.03	-0.04	-0.05	0.06	0.18	1
O28	9(*b*)	0.5067(4)	0.0190(5)	0.0564(1)	0.5088	0.0173	0.0679	-0.03	0.02	-0.09	0.10	0.14	1
	18(*h*)												
O33	9(*b*)	0.4891(4)	0.9845(5)	0.9406(1)	0.4912	0.9827	0.9421	-0.03	0.03	-0.09	0.10	0.15	1
O36	9(*b*)	0.5468(5)	0.2715(7)	0.0333(1)	0.5468	0.2736	0.0335	0.0	-0.03	-0.01	0.03	0.22	1
	18(*h*)												
O45	9(*b*)	0.4532(5)	0.7243(8)	0.9663(1)	0.4532	0.7264	0.9665	0.0	-0.03	-0.01	0.03	0.23	1
O38	9(*b*)	0.2201(4)	0.4411(5)	0.1445(1)	0.2189	0.4388	0.1452	0.02	0.03	-0.04	0.06	0.14	1
	18(*h*)												
O39	9(*b*)	0.4364(6)	0.2178(5)	0.8541(1)	0.4388	0.2189	0.8548	-0.03	-0.02	-0.04	0.06	0.17	1
Si20	3(*a*)	0.	0.	0.1938(1)	0.	0.	0.1962	0.0	0.0	-0.15	0.15	0.16	0.5
Si20	3(*a*)	0.	0.	0.1938(1)	0.	0.	0.1925	0.0	0.0	0.08	0.08	0.16	0.5
	6(*c*)												
Si23	3(*a*)	0.	0.	0.8013(8)	0.	0.	0.8038	0.0	0.0	-0.15	0.15	0.29	0.20[‡‡]
Ti1[††]	3(*a*)	0.	0.	0.8088(1)	0.	0.	0.8075	0.0	0.0	0.08	0.08	0.20	0.52
Si21	3(*a*)	0.	0.	0.2888(1)	0.	0.	0.2890	0.0	0.0	-0.01	0.01	0.13	1
	6(*c*)												
Si22	3(*a*)	0.	0.	0.7108(1)	0.	0.	0.7110	0.0	0.0	-0.01	0.01	0.14	1
Fe1	9(*b*)	0.3253(2)	0.1613(2)	0.1663(1)	0.3034	0.1517	0.1676	0.30	0.14	-0.08	0.40	0.17	0.73
	18(*h*)												
Mn1	9(*b*)	0.7172(4)	0.8585(4)	0.8311(1)	0.6966	0.8483	0.8324	0.30	0.14	-0.08	0.40	0.16	0.27
Na1	9(*b*)	0.0971(3)	0.5479(3)	0.3033(1)	0.0969	0.5478	0.3043	0.0	0.0	-0.06	0.06	0.18	1.0
	18(*h*)												
Na3	9(*b*)	0.5476(3)	0.0967(3)	0.6948(1)	0.5478	0.0969	0.6957	-0.0	-0.0	-0.05	0.05	0.18	1.0
Na2	9(*b*)	0.2205(3)	0.1110(3)	0.0760(1)	0.1981	0.0996	0.0798	0.31	0.16	-0.23	0.48	0.17	1.0
	18(*h*)												
Na8	9(*b*)	0.8244(4)	0.9118(4)	0.9164(1)	0.8019	0.9004	0.9202	0.31	0.16	-0.23	0.48	0.22	1.0
Na4,Sr2	9(*b*)	0.4391(5)	0.5604(5)	0.0889(1)	0.4428	0.5572	0.0899	-0.05	0.05	-0.06	0.08	0.19	0.261,0.089
	18(*h*)												
Na7	9(*b*)	0.5535(3)	0.1080(3)	0.9092(1)	0.5572	0.1144	0.9101	-0.05	-0.09	-0.05	0.13	0.19	1.
Na5[††]	9(*b*)	0.1687(9)	0.5859(8)	0.0817(1)	0.1697	0.5849	0.0817	-0.01	0.01	0.0	0.01	0.28	0.65
	18(*h*)												
Na5A		*0.5859*	*0.1687*	*0.9183*	*0.5849*	*0.1697*	*0.9183*	*0.01*	*-0.01*	*0.0*	*0.01*	*n.d.*	*n.d.*
Na6,K1	9(*b*)	0.5659(2)	0.4352(2)	0.1903(1)	0.5609	0.4369	0.1916	0.07	-0.02	-0.08	0.10	0.18	0.789,0.211
	18(*h*)												
Na15,Sr3	9(*b*)	0.4387(4)	0.8810(5)	0.8072(1)	0.4369	0.8760	0.8084	0.03	0.07	-0.07	0.11	0.20	0.303,0.067

Na10	9(*b*)	0.156(1)	0.127(1)	0.2470(2)	0.1548	0.1196	0.2473	0.02	-0.39	-0.02	0.40	0.30	0.49
Na12[††]	9(*b*)	0.8365(5)	0.9230(6)	0.7528(1)	0.8452	0.8804	0.7527	-0.12	0.61	0.01	0.56	0.26	0.80
	36(*i*)[‡‡]												
Na11	9(*b*)	0.154(2)	0.035(3)	0.2449(6)	0.1548	0.0352	0.2473	-0.01	0.0	-0.15	0.15	0.30	0.22
Na13[††]	9(*b*)	0.8543(2)	0.9977(3)	0.7498(4)	0.8452	0.9648	0.7527	0.13	0.46	-0.18	0.57	0.25	0.20
Na9[††]	9(*b*)	0.4293(2)	0.8327(1)	0.9153(3)	0.4207	0.8413	0.9153	0.	0.	0.	0.	0.31	0.29
	18(*h*)												
Na9A	*9(b)*	*0.8327*	*0.4293*	*0.0847*	*0.8327*	*0.4293*	*0.0847*	*0.*	*0.*	*0.*	*0.*	*n.d.*	*n.d.*
Na14,K2[††]	9(*b*)	0.0926(4)	0.1835(4)	0.1439(1)	0.0920	0.1841	0.1439	0.01	-0.01	0.	0.01	0.17	0.356,0.273
	18(*h*)												
Na21	*9(b)*	0.1835	0.0926	*0.8561*	0.1841	0.0920	*0.8561*	*-0.01*	*0.01*	*0.*	*0.01*	*n.d.*	*n.d.*
Na16	9(*b*), 9(*e*)	0.993(1)	0.494(1)	0.0025(2)	0	0.5	0	0.10	-0.09	0.15	0.18	0.18	0.41
Na18,Sr5, Ce2	9(*b*)	0.1147(4)	0.5585(3)	-0.0031(1)	0.1176	0.5595	-0.0025	-0.04	-0.01	-0.04	0.06	0.16	0.491,0.022,0.017
	18(*h*)												
Na17,Sr4, Ce1	9(*b*)	0.5604(3)	0.4390(3)	0.0018(1)	0.5595	0.4419	0.0025	0.01	-0.04	-0.04	0.05	0.16	0.537,0.017,0.017
O49	3(*a*)	0.	0.	0.2631(1)	0.	0.	0.2626	0.	0.	0.03	0.03	0.16	1
	6(*c*												
O50	3(*a*)	0.	0.	0.7378(2)	0.	0.	0.7374	0	0	0.03	0.03	0.18	1
O57	3(*a*)	0.	0.	0.1198(2)	0.	0.	0.1221	0	0	-0.14	0.14	0.20	0.86
	6(*c*)												
O56	3(*a*)	0.	0.	0.8757(6)	0.	0.	0.8779	0	0	-0.14	0.14	0.23	0.32
O53	3(*a*)	0.	0.	0.1681(2)	0.	0.	0.1711	0	0	-0.18	0.18	0.26	1
	6(*c*)												
O52	3(*a*)	0.	0.	0.826(2)	0.	0.	0.8289	0	0	-0.18	0.18	0.31	0.20
O51[††]	9(*b*)	0.556(2)	0.281(2)	0.1639(3)	0.556	0.281	0.1639	0.	0.	0.	0.	0.24	0.50
	36(*i*)												
O51A	*9(b)*	*0.444*	*0.719*	*0.8361*	*0.444*	*0.719*	*0.8361*	*0.*	*0.*	*0.*	*0.*	*n.d.*	*n.d.*
O54	3(*a*)	0.	0.	0.5961(3)	0.	0.	0.5935	0	0	0.15	0.15	0.30	1
	6(*c*)												
O55	3(*a*)	0.	0.	0.409(1)	0.	0.	0.4065	0	0	0.16	0.16	0.34	0.66
Cl1	3(*a*)	0.	0.	0.6451(1)	0.	0.	0.6459	0.0	0.0	-0.05	0.05	0.22	1
	6(*c*)												
Cl2	3(*a*)	0.	0.	0.3533(1)	0.	0.	0.3541	0.0	0.0	-0.05	0.05	0.21	0.90
Cl3[††]	3(*a*)	0.	0.	0.379(1)	0.	0.	0.379	0.	0.	0.	0.	0.19	0.10
	6(*c*)												
Cl3A	*3(a)*	*0.*	*0.*	*0.621*	*0.*	*0.*	*0.621*	*0.*	*0.*	*0.*	*0.*	*n.d.*	*n.d.*
Cl4,F1[††]	3(*a*)	0.	0.	0.8831(1)	0.	0.	0.8831	0.	0.	0.	0.05	0.17	0.34.0.34
	6(*c*)												
Cl4A,F1A	*3(a)*	*0.*	*0.*	*0.1169(1)*	*0.*	*0.*	*0.1169*	*0.*	*0.*	*0.*	*0.*	*n.d.*	*n.d.*

[*] **A**toms related over more than two positions are marked by braces.

[†] With Ca5 and Ca6 assumed omitted from the original analysis but at *x*,*x*-*y*,*z* and –*x*,*y*-*x*, -*z* with respect to Ca1.

[‡] Not determined.

[††] Note $d_{\mathrm{Ti1\text{-}Si23}}$ = 0.46Å, $d_{\mathrm{Na4\text{-}Na5}}$ = 0.73Å, $d_{\mathrm{Na12\text{-}Na13}}$ = 0.98 Å, $d_{\mathrm{Na9\text{-}Na11}}$ = 1.65 Å, $d_{\mathrm{Na14\text{-}Na15}}$ = 0.43 Å, $d_{\mathrm{O51\text{-}O52}}$ = 1.40 (×3) Å, $d_{\mathrm{Cl3\text{-}Cl2}}$ = 1.58, $d_{\mathrm{Cl4\text{-}O56}}$ = 0.45Å.

[‡‡] With appropriate occupancies. *Cl4A,F1A*

Table S34 $H_3PMo_{12}O_{40}$

Modified atomic positions for $H_3PMo_{12}O_{40}$ (Marosi *et al.*, 2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz displacements in Å; u_{eq} not reported. [90636]

$a = 15.875(6)$, $c = 20.752(10)$ Å. $z^* = z - 0.1684$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$
	$R3$, $R\bar{3}$										
P1	3(*a*)	0	0	-0.1224(39)	0	0	-0.1820	0	0	1.24	1.24
	6(*c*)										
P2	3(*a*)	0	0	0.2416(41)	0	0	0.1820	0	0	1.24	1.24
Mo1	9(*b*)	0.8801(13)	0.8507(11)	0.3776(7)	0.8856	0.8462	0.3947	-0.09	0.07	-0.35	0.36
	18(*f*)										
Mo8	9(*b*)	0.0440(14)	0.8910(4)	0.5882(7)	0.0395	0.8856	0.6053	0.07	0.09	-0.35	0.38
Mo2	9(*b*)	0.1962(12)	-0.0500(12)	0.7301(13)	0.1954	-0.0448	0.7442	0.01	-0.08	-0.29	0.30
	18(*f*)										
Mo7	9(*b*)	0.2349(12)	0.1945(12)	0.2416(12)	0.2296	0.1954	0.2558	0.08	-0.01	-0.29	0.30
Mo3	9(*b*)	0.2436(11)	0.2096(11)	0.7287(8)	0.2520	0.2018	0.7484	-0.13	0.12	-0.41	0.43
	18(*f*)										
Mo6	9(*b*)	0.1940(11)	-0.0586(10)	0.2319(10)	0.2018	-0.0502	0.2516	-0.12	-0.13	-0.41	0.46
Mo4	9(*b*)	0.0298(14)	0.8960(14)	0.1112(7)	0.0318	0.8954	0.1198	-0.03	0.01	-0.18	0.18
	18(*f*)										
Mo5	9(*b*)	0.8948(14)	0.8617(13)	-0.1284(7)	0.8954	0.8598	-0.1198	-0.01	0.03	-0.18	0.18

Table S35

Modified atomic positions for $Ca_4(Ca_{0.7}Na_{0.3})_3Na_{0.7}Li_5(B_{22}O_{39}(OH)_3)(CO_3)(OH)$-$((OH)_{0.8}(H_2O)_{0.2})$ (Yamnova *et al.,* 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [97107]

a = 8.99(2), *c* = 35.91(2) Å. $z^* = z + 0.0093$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occ.
Ca1	9(*b*)	0.7630(1)	0.7353(1)	0.9193(1)	0.7474	0.7419	0.9379	0.14	-0.06	-0.67	0.68	0.10	1.
Ca2,Na1	9(*b*)	0.9898(1)	0.2515(1)	0.0435(1)	0.0055	0.2581	0.0621	-0.14	-0.06	-0.67	0.69	0.10	0.7,0.3
Ca3	3(*a*)	0.	0.	0.4160(6)	0.	0.	0.4010	0.	0.	0.54	0.54	0.10	1.
	6(*c*)												
B7	3(*a*)	0.	0.	0.6141(8)	0.	0.	0.5990	0.	0.	0.54	0.54	0.10	1.
Na2	3(*a*)	0.	0.	0.2766(6)	0.	0.	0.2699	0.	0.	0.24	0.24	0.17	0.7
	6(*c*)												
C1	3(*a*)	0.	0.	0.7368(3)	0.	0.	0.7301	0.	0.	0.24	0.24	0.12	1.
B1	9(*b*),9(*d*)	0.0225(5)	0.8432(5)	0.9804(1)	0.	0.8432	0.	0.20	0.	-0.70	0.73	0.09	1.
B2	9(*b*)	0.4211(5)	0.3938(5)	0.9478(1)	0.4355	0.3868	0.9674	-0.13	0.06	-0.70	0.71	0.08	1.
	18(*f*)												
B8	9(*b*)	0.5501(7)	0.9444(6)	0.0131(1)	0.5645	0.9514	0.0327	-0.13	-0.06	-0.70	0.72	0.10	1.
B3	9(*b*)	0.5907(6)	0.5791(6)	0.7923(1)	0.5403	0.5619	0.8178	0.45	0.15	-0.91	1.06	0.09	1.
	18(*f*)												
B5	9(*b*)	0.5101(6)	0.0063(6)	0.1568(1)	0.4597	0.0226	0.1822	0.45	-0.15	-0.91	0.99	0.09	1.
B4	9(*b*)	0.5877(6)	0.9862(6)	0.8801(1)	0.6269	0.8878	0.8559	-0.35	0.88	0.87	1.16	0.09	1.
	18(*f*)												
B6	9(*b*)	0.3339(6)	0.1626(6)	0.1683(1)	0.3731	0.2609	0.1441	-0.35	-0.88	0.87	1.40	0.10	1.
Li1[†]	9(*b*),9(*d*)	0.9617(2)	0.5883(2)	*0.035* (5)	0.	0.5883	0.	-0.34	0.	1.25	1.30	0.16	1.
Li2	3(*a*),3(*b*)	0.	0.	0.5102(9)	0.	0.	0.5	0.	0.	0.37	0.37	0.12	1.
Li3	3(*a*)	0.	0.	0.8470(4)	0.	0.	0.847	0.	0.	0.	0.	0.15	1.
	6(*c*)												
Li3A	3(*a*)	*0.*	*0.*	*0.153*	*0.*	*0.*	*0.153*	*0.*	*0.*	*0.*	*0.*	*n.d.*	*1.*
O1	9(*b*)	0.4981(4)	0.9748(4)	0.9124(1)	0.4992	0.0919	0.9197	-0.01	-1.05	-0.26	1.09	0.10	1.
	18(*f*)												
O16	9(*b*)	0.5002(6)	0.2414(6)	0.0730(2)	0.5008	0.1243	0.0803	-0.01	-1.05	-0.26	1.09	0.16	1.
O2	9(*b*)	0.4867(4)	0.9591(5)	0.9784(1)	0.4833	0.0244	0.9675	0.03	-0.59	0.39	0.69	0.12	1.
	18(*f*)												
O9	9(*b*)	0.4555(3)	0.9103(5)	0.0435(1)	0.4589	0.9756	0.0325	-0.03	-0.59	0.39	0.72	0.12	1.
O3	9(*b*)	0.5827(4)	0.9504(4)	0.6807(1)	0.5966	0.9261	0.7055	-0.12	0.22	-0.89	0.91	0.10	1.
	18(*f*)												
O13	9(*b*)	0.9018(4)	0.6104(4)	0.2792(1)	0.9261	0.5966	0.2945	-0.22	0.12	-0.89	0.91	0.09	1.
O5	9(*b*),9(*d*)	0.8553(3)	0.8342(3)	0.9823(1)	0.8448	0.8448	0.0	0.09	-0.09	-0.98	0.98	0.08	1.
O4	9(*b*)	0.8567(4)	0.5646(4)	0.8660(1)	0.7366	0.5937	0.8626	1.08	-0.26	0.12	0.98	0.11	1.
	18(*f*)												
O6	9(*b*)	0.3834(4)	0.8862(4)	0.1407(1)	0.2634	0.8571	0.1374	1.08	0.26	0.12	1.24	0.11	1.
O7	9(*b*)	0.5059(4)	0.4892(4)	0.7617(1)	0.5270	0.4267	0.7401	-0.19	0.56	0.77	0.91	0.10	1.
	18(*f*)												
O12	9(*b*)	0.4520(4)	0.8372(4)	0.2815(1)	0.4730	0.8997	0.2599	-0.19	-0.56	0.77	1.02	0.11	1.

O8	9(*b*)	0.4419(5)	0.1034(5)	0.1867(1)	0.4440	0.1239	0.1899	-0.02	-0.18	-0.11	0.22	0.11	1.
	18(*f*)												
O15	9(*b*)	0.5539(5)	0.7005(5)	0.8070(1)	0.5560	0.7211	0.8101	-0.02	-0.19	-0.11	0.23	0.11	1.
O10	9(*b*)	0.5573(5)	0.8359(4)	0.8644(1)	0.5586	0.8612	0.8569	-0.01	-0.23	0.27	0.36	0.12	1.
	18(*f*)												
O11	9(*b*)	0.4400 (5)	0.3278(4)	0.1506(1)	0.4414	0.3026	0.1431	-0.01	0.23	0.27	0.35	0.12	1.
O14	3(*a*)	0.	0.	0.9058(1)	0.	0.	0.9223	0.	0.	-0.59	0.59	0.10	1.
	6(*c*)												
O17	3(*a*)	0.	0.	0.0612(2)	0.	0.	0.0777	0.	0.	-0.59	0.59	0.09	1.

Table S36(*a*)

Modified atomic positions for $Ga_2Cr_{1.33}Se_5$ (Okońska-Kozlowska *et al.,* 2004) with hypothetical $x'y'z'$ coordinates as in Table 36(*a*) and Δx, Δy, Δz and u_{eq} displacements in Å [99119]

$a = 3.7810(10)$, $c = 46.807(9)$ Å. $z^* = z + 0.0420$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Se1	3(*a*)	0.	0.	0.0149(1)	0.	0.	0.0441	0.	0.	-1.37	1.37	0.10	1.
	6(*a*)												
Ga3	3(*a*)	0.	0.	0.9267(1)	0.	0.	0.9559	0.	0.	-1.37	1.37	0.15	0.667
Se2	3(*a*)	0.	0.	0.7549(1)	0.	0.	0.7792	0.	0.	-1.14	1.14	0.08	1.
	6(*a*)												
Ga2	3(*a*)	0.	0.	0.1964(1)	0.	0.	0.2208	0.	0.	-1.14	1.14	0.21	0.667
Se3	3(*a*)	0.	0.	0.1447(1)	0.	0.	0.1337	0.	0.	0.51	0.51	0.08	1.
	6(*a*)												
Se4	3(*a*)	0.	0.	0.8773(1)	0.	0.	0.8663	0.	0.	0.51	0.51	0.16	1.
Se5	3(*a*)	0.	0.	0.6171(1)	0.	0.	0.5838	0.	0.	1.56	1.56	0.10	1.
	6(*a*)												
Cr1	3(*a*)	0.	0.	0.4496(1)	0.	0.	0.4162	0.	0.	1.56	1.56	0.10	0.667
Cr2	3(*a*)	0.	0.	0.3138(3)	0.	0.	0.3048	0.	0.	0.42	0.42	0.29	0.667
	6(*a*)												
Ga1	3(*a*)	0.	0.	0.7042(1)	0.	0.	0.6952	0.	0.	0.42	0.42	0.13	0.667

Table S36(*b*)

Modified atomic positions for $Ga_2Cr_{1.33}Se_5$ (Okońska-Kozlowska *et al.,* 2004) as in Table 36(*a*) but with z^* replaced by $z + 0.0300$ for Se1,Ga3,Se2,Ga2, by $z - 0.0200$ for Se3-Se5, Cr1-2,Ga1, with hypothetical $x'y'z'$ coordinates as in Table 36(*a*) and Δx, Δy, Δz and u_{eq} displacements in Å [99119]

$a = 3.7810(10)$, $c = 46.807(9)$ Å. $z^* = z + 0.0420$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3, *R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Se1	3(*a*)	0.	0.	0.0449(1)	0.	0.	0.0441	0.	0.	0.04	0.04	0.10	1.
	6(*a*)												
Ga3	3(*a*)	0.	0.	0.9567(1)	0.	0.	0.9559	0.	0.	0.05	0.05	0.15	0.667
Se2	3(*a*)	0.	0.	0.7849(1)	0.	0.	0.7792	0.	0.	0.27	0.27	0.08	1.
	6(*a*)												
Ga2	3(*a*)	0.	0.	0.2264(1)	0.	0.	0.2208	0.	0.	0.26	0.26	0.21	0.667
Se3	3(*a*)	0.	0.	0.1247(1)	0.	0.	0.1337	0.	0.	-0.42	0.42	0.08	1.
	6(*a*)												
Se4	3(*a*)	0.	0.	0.8573(1)	0.	0.	0.8663	0.	0.	-0.42	0.42	0.16	1.
Se5	3(*a*)	0.	0.	0.5971(1)	0.	0.	0.5838	0.	0.	0.62	0.62	0.10	1.
	6(*a*)												
Cr1	3(*a*)	0.	0.	0.4296(1)	0.	0.	0.4162	0.	0.	0.63	0.63	0.10	0.667
Cr2	3(*a*)	0.	0.	0.2938(3)	0.	0.	0.3048	0.	0.	-0.51	0.51	0.29	0.667
	6(*a*)												
Ga1	3(*a*)	0.	0.	0.6842(1)	0.	0.	0.6952	0.	0.	-0.51	0.51	0.13	0.667

Table S37(*a*)

Modified atomic positions for $2Zn(H_2O)_4{\bullet}H_2As_6V_{15}O_{42}H_2O{\bullet}2H_2O$ (Cui Xiao-Bing *et al.*, 2003) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [99351] $a = 12.0601(10)$, $c = 33.970(7)$ Å. $z^* = z + 0.0438$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3,R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occ.
As1	9(*b*)	0.6524(1)	-0.0544(1)	0.3606(1)	0.6605	-0.1029	0.3611	-0.10	0.58	-0.02	0.54	0.19	1
	18(*f*)												
As2	9(*b*)	0.7714(1)	0.8485(1)	0.6385(1)	0.7634	0.8971	0.6389	0.10	-0.59	-0.01	0.55	0.19	1
V1	9(*b*)	0.7174(2)	0.0927(2)	0.2686(1)	0.7254	0.0947	0.2688	-0.10	-0.02	-0.01	0.11	0.17	1
	18(*f*)												
V2	9(*b*)	0.6287(2)	0.7333(2)	0.7310(1)	0.6306	0.7254	0.7312	-0.02	0.10	-0.01	0.09	0.17	1
V3	9(*b*)	0.8564(2)	0.3603(2)	0.2443(1)	0.8603	0.3705	0.2445	-0.05	-0.12	-0.01	0.15	0.17	1
	18(*j*)												
V4	9(*b*)	0.4797(2)	0.8643(2)	0.7553(1)	0.4899	0.8603	0.7555	-0.12	0.05	-0.01	0.10	0.18	1
V5	9(*b*),9(*e*)	0.2464(2)	0.8796(2)	0.9993(1)	0.5	0.	1.0	-3.06	1.45	-0.02	2.65	0.18	1
Zn1	3(*a*)	0.	0.	0.7961(1)	0.	0.	0.7948	0.	0.	0.04	0.04	0.28	1
	6(*c*)												
Zn2	3(*a*)	0.	0.	0.2064(1)	0.	0.	0.2052	0.	0.	0.04	0.04	0.22	1
O1	9(*b*)	0.7362(10)	-0.0051(10)	0.2400(3)	0.7473	-0.0011	0.2402	-0.13	-0.05	-0.01	0.16	0.21	1
	18(*j*)												
O4	9(*b*)	0.7444(9)	0.7584(10)	0.7596(3)	0.7484	0.7473	0.7598	-0.05	0.13	-0.01	0.11	0.20	1
O2	9(*b*)	0.0114(9)	0.1635(9)	0.3319(3)	0.0023	0.1743	0.3325	0.11	-0.13	-0.02	0.12	0.21	1
	18(*j*)												
O8	9(*b*)	0.8172(11)	0.9932(11)	0.6669(4)	0.8280	0.0023	0.6675	-0.13	-0.11	-0.02	0.21	0.16	0.64
O3	9(*b*)	0.8750(10)	0.6112(10)	0.4614(3)	0.8879	0.6049	0.4625	0.16	0.08	-0.04	0.22	0.21	1
	18(*j*)												
O5	9(*b*)	0.5987(10)	0.7042(11)	0.5364(3)	0.6049	0.7171	0.5375	-0.07	-0.16	-0.04	0.21	0.22	1
O6	9(*b*)	0.9713(9)	0.5050(8)	0.2796(3)	0.9669	0.5143	0.2804	0.05	-0.11	-0.03	0.10	0.19	1
	18(*j*)												
O11	9(*b*)	0.5236(8)	0.5517(8)	0.7189(3)	0.5143	0.5473	0.7196	0.11	0.05	-0.02	0.14	0.19	1
O7	9(*b*)	0.6292(8)	0.4430(9)	0.4281(3)	0.5869	0.3991	0.4276	0.53	0.53	0.02	0.92	0.19	1
	18(*f*)												
O12	9(*b*)	0.3551(9)	0.5447(8)	0.5728(3)	0.3991	0.5869	0.5724	-0.53	-0.51	0.01	0.90	0.19	1
O9	9(*b*)	0.0324(17)	0.5703(18)	0.3328(6)	0.0652	0.4882	0.3385	-0.40	0.99	-0.18	0.88	0.13	0.36
	18(*f*)												
O14	9(*b*)	0.4060(8)	0.3902(8)	0.6568(3)	0.4882	0.4230	0.6615	-0.99	-0.40	-0.18	1.08	0.18	1
O10	9(*b*)	0.5998(9)	0.0352(9)	0.3877(3)	0.5886	0.0403	0.3874	0.14	-0.06	0.01	0.12	0.19	1
	18(*f*)												
O13	9(*b*)	0.5432(9)	0.5774(9)	0.6130(2)	0.5483	0.5886	0.6126	-0.06	-0.14	0.01	0.18	0.18	1
O15	9(*b*)	0.0180(8)	0.4046(9)	0.3425(3)	0.1142	0.3423	0.3787	-1.16	0.75	-1.22	1.27	0.20	1
	18(*f*)												
O22	9(*b*)	0.280(12)	0.132(11)	0.585(3)	0.3423	0.228	0.621	-0.75	-1.16	-1.22	2.07	0.44	0.5
O16	3(*a*),3(*a*)	0.	0.	0.996(3)	0.	0.	0.0	0.	0.	-0.14	0.14	0.44	0.5
O17w	3(*a*),3(*b*)	0.	0.	0.4545(6)	0.	0.	0.5	0.	0.	-1.55	1.55	0.23	1
O18w	9(*b*)	0.1666(14)	0.6470(17)	0.4832(4)	0.1641	0.6409	0.4826	0.03	0.07	0.02	0.09	0.28	1
	18(*f*)												
O20w	9(*b*)	0.5293(17)	0.1616(14)	0.5179(5)	0.5232	0.1641	0.5174	0.07	-0.03	0.02	0.06	0.30	1
O19w	3(*a*)	0.	0.	0.7398(5)	0.	0.	0.7388	0.	0.	0.03	0.03	0.28	1
	6(*c*)												
O21w	3(*a*)	0.	0.	0.2623(5)	0.	0.	0.2612	0.	0.	0.04	0.04	0.21	1

Table S37(*b*)

Modified atomic positions for $2Zn(H_2O)_4 \bullet H_2As_6V_{15}O_{42}H_2O \bullet 2H_2O$ (Cui Xiao-Bing *et al.,* 2003) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [99351] $a = 12.0601(10)$, $c = 33.970(7)$ Å. $z^* = z + 0.0438$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3,R\bar{3}m$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occ. $R3,R\bar{3}m$
As1	9(*b*)	0.6524(1)	-0.0544(1)	0.3606(1)	0.6605	-0.1029	0.3611	-0.10	0.58	-0.02	0.54	0.19	1,0.5
	36(*i*)												
As2	9(*b*)	0.7714(1)	0.8485(1)	0.6385(1)	0.7634	0.8971	0.6389	0.10	-0.59	-0.01	0.55	0.19	1,0.5
V1	9(*b*)	0.7174(2)	0.0927(2)	0.2686(1)	0.7254	0.0947	0.2688	-0.10	-0.02	-0.01	0.11	0.17	1,0.5
	36(*i*)												
V2	9(*b*)	0.6287(2)	0.7333(2)	0.7310(1)	0.6306	0.7254	0.7312	-0.02	0.10	-0.01	0.09	0.17	1,0.5
V3	9(*b*)	0.8564(2)	0.3603(2)	0.2443(1)	0.8603	0.3705	0.2445	-0.05	-0.12	-0.01	0.15	0.17	1,0.5
	36(*i*))												
V4	9(*b*)	0.4797(2)	0.8643(2)	0.7553(1)	0.4899	0.8603	0.7555	-0.12	0.05	-0.01	0.10	0.18	1,0.5
V5	9(*b*),18(*h*)	0.2464(2)	0.8796(2)	0.9993(1)	0.1834	0.8166	0.9993	-0.76	0.76	0.02	0.76	0.18	1,0.5
Zn1	3(*a*)	0.	0.	0.7961(1)	0.	0.	0.7948	0.	0.	0.04	0.04	0.28	1,0.5
	6(*c*)												
Zn2	3(*a*)	0.	0.	0.2064(1)	0.	0.	0.2052	0.	0.	0.04	0.04	0.22	1,0.5
O1	9(*b*)	0.7362(10)	-0.0051(10)	0.2400(3)	0.7473	-0.0011	0.2402	-0.13	-0.05	-0.01	0.16	0.21	1,0.5
	36(*i*)												
O4	9(*b*)	0.7444(9)	0.7584(10)	0.7596(3)	0.7484	0.7473	0.7598	-0.05	0.13	-0.01	0.11	0.20	1,0.5
O2	9(*b*)	0.0114(9)	0.1635(9)	0.3319(3)	0.0023	0.1743	0.3325	0.11	-0.13	-0.02	0.12	0.21	1,0.5
	36(*i*)												
O8	9(*b*)	0.8172(11)	0.9932(11)	0.6669(4)	0.8280	0.0023	0.6675	-0.13	-0.11	-0.02	0.21	0.16	0.64,0.32
O3	9(*b*)	0.8750(10)	0.6112(10)	0.4614(3)	0.8879	0.6049	0.4625	0.16	0.08	-0.04	0.22	0.21	1,0.5
	36(*i*)												
O5	9(*b*)	0.5987(10)	0.7042(11)	0.5364(3)	0.6049	0.7171	0.5375	-0.07	-0.16	-0.04	0.21	0.22	1,0.5
O6	9(*b*)	0.9713(9)	0.5050(8)	0.2796(3)	0.9669	0.5143	0.2804	0.05	-0.11	-0.03	0.10	0.19	1,0.5
	36(*i*)*j*)												
O11	9(*b*)	0.5236(8)	0.5517(8)	0.7189(3)	0.5143	0.5473	0.7196	0.11	0.05	-0.02	0.14	0.19	1,0.5
O7	9(*b*)	0.6292(8)	0.4430(9)	0.4281(3)	0.5869	0.3991	0.4276	0.53	0.53	0.02	0.92	0.19	1,0.5
	36(*i*))												
O12	9(*b*)	0.3551(9)	0.5447(8)	0.5728(3)	0.3991	0.5869	0.5724	-0.53	-0.51	0.01	0.90	0.19	1,0.5
O9	9(*b*)	0.0324(17)	0.5703(18)	0.3328(6)	0.0142	0.5901	0.3380	0.22	-0.24	-0.18	0.29	0.13	0.36,0.18
	36(*i*)												
O14	9(*b*)	0.4060(8)	0.3902(8)	0.6568(3)	0.4241	0.4099	0.6620	-0.22	-0.24	-0.18	0.44	0.18	1,0.5
O10	9(*b*)	0.5998(9)	0.0352(9)	0.3877(3)	0.5886	0.0403	0.3874	0.14	-0.06	0.01	0.12	0.19	1,0.5
	36(*i*)												
O13	9(*b*)	0.5432(9)	0.5774(9)	0.6130(2)	0.5483	0.5886	0.6126	-0.06	-0.14	0.01	0.18	0.18	1,0.5
O15	9(*b*)	0.0180(8)	0.4046(9)	0.3425(3)	0.075	0.342	0.3787	-0.69	0.75	-1.22	1.42	0.20	1,0.5
	36(*i*)												
O22	9(*b*)	0.280(12)	0.132(11)	0.585(3)	0.342	0.075	0.621	-0.75	0.69	-1.22	1.42	0.44	0.5,0.17
O16	3(*a*),3(*a*)	0.	0.	0.996(3)	0.	0.	1.0	0.	0.	-0.14	0.14	0.44	0.5,0.17
O17w	3(*a*),3(*b*)	0.	0.	0.4545(6)	0.	0.	0.5	0.	0.	-1.55	1.55	0.23	1,0.5
O18w	9(*b*)	0.1666(14)	0.6470(17)	0.4832(4)	0.1641	0.6409	0.4826	0.03	0.07	0.02	0.09	0.28	1,0.5
	36(*i*))												
O20w	9(*b*)	0.5293(17)	0.1616(14)	0.5179(5)	0.5232	0.1641	0.5174	0.07	-0.03	0.02	0.06	0.30	1,0.5
O19w	3(*a*)	0.	0.	0.7398(5)	0.	0.	0.7388	0.	0.	0.03	0.03	0.28	1,0.5
	6(*c*)												
O21w	3(*a*)	0.	0.	0.2623(5)	0.	0.	0.2612	0.	0.	0.04	0.04	0.21	1,0 .5

Table S38(*a*)

Modified atomic positions in $Bi_{11.23}IrCl_{12.23}$ (Ruck & Hampel, 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [412014]

a = 12.666(2), c = 15.860(3) Å. $z^* = z - 0.00828$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
	$R3, R\bar{3}$												
Bi1	9(*b*)	0.19383(9)	0.13884(9)	0.09207(13)	0.19328	0.13909	0.09916	0.01	-0.00	-0.11	0.11	0.12	1.
	18(*f*)												
Bi2	9(*b*)	-0.19272(10)	-0.13933(10)	-0.10624(13)	-0.19328	-0.13909	-0.09916	0.01	-0.00	-0.11	0.11	0.14	1.
Bi3	9(*b*)	0.15161(17)	0.12261(18)	0.57792(14)	0.15617	0.12623	0.57974	-0.06	-0.05	-0.03	0.10	0.20	0.75
	18(*f*)												
Bi4	9(*b*)	-0.16073(14)	-0.12985(15)	-0.58155(14)	-0.15617	-0.12623	-0.57974	-0.06	-0.05	-0.03	0.10	0.23	1.
Ir1	3(*a*),3(*a*)	0	0	0.00828	0	0	0	0	0	-0.13	0.13	0.09	1.
Cl1	9(*b*)	0.3425(6)	0.0652(5)	0.0046(4)	0.3461	0.0778	0.0067	-0.05	-0.16	-0.03	0.19	0.15	1.
	18(*f*)												
Cl2	9(*b*)	-0.3498(6)	-0.0903(6)	-0.0088(4)	-0.3461	-0.0778	-0.0067	-0.05	-0.16	-0.03	0.19	0.17	1.
Cl3	9(*b*)	0.1415(7)	-0.0534(7)	0.2057(4)	0.1494	-0.0589	0.2039	-0.10	0.07	0.03	0.09	0.20	0.77
Cl3	9(*b*)	0.1415(7)	-0.0534(7)	0.2057(4)	0.1605	-0.0729	0.1924	-0.24	0.25	0.21	0.32	0.20	0.23
	18(*f*)[†]												
Cl4	9(*b*)	-0.1573(7)	0.0643(7)	-0.2022(5)	-0.1494	0.0589	-0.2039	0.10	0.07	0.03	0.15	0.13	0.77
Cl5	9(*b*)	-0.1795(13)	0.0924(14)	-0.1790(11)	-0.1605	0.0729	-0.1924	-0.24	0.25	0.21	0.32	0.14	0.23
Cl6	3(*a*)	0	0	-0.2335(12)	0	0	-0.2335	0	0	0	0	0.12	0.118
	6(*c*)[‡]												
Cl6A	*3(a)*	*0*	*0*	*0.2335*	*0*	*0*	*0.2335*	*0*	*0*	*0*	*0*	*0.12*	*0.118*

[†] **A**toms related over more than two positions are marked by braces.

[‡] If *Cl6A* is not assumed, Δz(Cl6) = $\Delta\xi$(Cl6) = 3.70 Å and occ.(Cl6) = 0.235(14); if assumed, the summed occupancy of both is likely that of the original site.

Table S38(*b*)

Modified atomic positions in $Bi_{11.7}RhCl_{12.7}$ (Ruck & Hampel, 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [412015]

a = 12.612(1), c = 15.917(2) Å. $z^* = z - 0.00601$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
	$R3,R\bar{3}$												
Bi1	9(*b*)	0.19366(7)	0.13847(7)	0.09223(18)	0.19204	0.13853	0.09929	0.02	-0.00	-0.11	0.11	0.13	1.
	18(*f*)												
Bi2	9(*b*)	-0.19042(7)	-0.13858(8)	-0.10635(18)	-0.19204	-0.13853	-0.09929	0.02	-0.00	-0.11	0.11	0.14	1.
Bi3	9(*b*)	0.15984(10)	0.12383(10)	0.57686(19)	0.15719	0.13008	0.58013	0.03	-0.08	-0.05	0.09	0.18	0.951
	18(*f*)												
Bi4	9(*b*)	-0.15454(10)	-0.13632(10	-0.58339(19)	-0.15719	-0.13008	-0.58013	0.03	-0.08	-0.05	0.09	0.18	0.947
Rh1	3(*a*),3(*a*)	0	0	-0.00601	0	0	0	0	0	-0.10	0.10	0.10	1.
Cl1	9(*b*)	0.3458(5)	0.0712(6)	0.0041(4)	0.3478	0.0812	0.0049	-0.02	-0.13	-0.01	0.14	0.17	1.
	18(*f*)												
Cl2	9(*b*)	-0.3497(5)	-0.0912(6)	-0.0058(4)	-0.3478	-0.0812	-0.0049	-0.02	-0.13	-0.01	0.14	0.17	1.
Cl3	9(*b*)	0.1441(4)	-0.0581(4)	0.1997(3)	0.1606	-0.0691	0.1967	-0.21	0.14	0.05	0.19	0.17	0.28
Cl3	9(*b*)	0.1441(4)	-0.0581(4)	0.1997(3)	0.1693	-0.0731	0.1856	-0.31	0.19	0.22	0.35	0.17	0.72
	18(*f*)†												
Cl4	9(*b*)	-0.177(2)	0.0801(19)	-0.1936(16)	-0.1606	0.0691	-0.1967	-0.21	0.14	0.05	0.19	0.18	0.28
Cl5	9(*b*)	-0.1944(7)	0.0881(7)	-0.1714(6)	-0.1693	0.0731	-0.1856	-0.32	0.19	0.22	0.36	0.17	0.72
Cl6	3(*a*)	0	0	-0.2412(6)	0	0	-0.2412	0	0	0	0	0.17	0.36
	6(*c*)												
Cl6A	*3(a)*	*0*	*0*	*0.2412*	*0*	*0*	*0.2412*	*0*	*0*	*0*	*0*	*0.17*	*0.36*

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† **A**toms related over more than two positions are marked by braces.

Table S38(*c*)

Modified atomic positions in $Bi_{11.28}RhBr_{12.28}$ (Ruck & Hampel, 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [412016]

a = 12.961(7), c = 16.416(8) Å. $z^* = z - 0.00372$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
	$R3,R\bar{3}$												
Bi1	9(*b*)	0.1886(3)	0.1359(3)	0.0934(8)	0.1889	0.1364	0.0958	-0.00	-0.01	-0.04	0.04	0.15	1.
	18(*f*)												
Bi2	9(*b*)	-0.1893(3)	-0.1369(3)	-0.0983(8)	-0.1889	-0.1364	-0.0958	-0.01	-0.01	-0.04	0.04	0.13	1.
Bi3	9(*b*)	0.1540(3)	0.1318(3)	0.5754(8)	0.1512	0.1304	0.5770	0.04	0.02	-0.03		0.18	0.67
	18(*f*)												
Bi4	9(*b*)	-0.1484(4)	-0.1289(4)	-0.5786(8)	-0.1512	-0.1304	-0.5770	0.04	0.02	-0.03	0.06	0.27	1.
Rh1	3(*a*),3(*a*)	0	0	-0.0037	0	0	0	0	0	-0.06	0.06	0.11	1.
Br1	9(*b*)	0.3516(7)	0.0803(7)	0.0027(9)	0.3522	0.0817	0.0059	-0.01	-0.02	-0.05	0.06	0.18	1.
	18(*f*)												
Br2	9(*b*)	-0.3529(7)	-0.0832(8)	-0.0092(9)	-0.3522	-0.0817	-0.0059	-0.01	-0.02	-0.05	0.06	0.18	1.
Br3	9(*b*)	0.1496(9)	-0.0605(9)	0.2014(10)	0.1517	-0.0603	0.2055	-0.02	-0.00	-0.07	0.07	0.24	0.715
Br3	9(*b*)	0.1496(9)	-0.0605(9)	0.2014(10)	0.1725	-0.0764	0.1880	-0.30	0.21	0.22	0.35	0.24	0.285
	18(*f*)[†]												
Br4	9(*b*)	-0.1538(9)	0.0601(9)	-0.2097(11)	-0.1517	0.0603	-0.2055	-0.03	-0.00	-0.07	0.08	0.18	0.715
Br5	3(*a*)	-0.1954(9)	0.0923(10)	-0.1746(11)	-0.1725	0.0764	-0.1880	-0.30	0.21	0.22	0.35	0.18	0.285
Br6	3(a)	0	0	-0.2407(13)	0	0	-0.2407	0	0	0	0	0.17	0.142
	6(*c*)												
Br6A	*3(a)*	*0*	*0*	*0.2407(13)*	*0*	*0*	*0.2407*	*0*	*0*	*0*	0	*0.17*	*0.142*

[†] **A**toms related over more than two positions are marked by braces.

6. Structures most likely to remain in space group *R*3 without phase change

6.1 $Na_3VO_4{\cdot}3H_2O$ [62533]

Kato & Takayama-Muromachi (1987). Mo$K\alpha$; 494 independent $I_{obs} > 3\sigma(I_{obs})$; extinction but not absorption corrections; u_{aniso}, $R = 0.017$, $wR = 0.016$; 7 independent atoms including two H. The apex O atom of the VO_4 tetrahedron lies on, with the equilateral base normal to, the trigonal axis. Spontaneous polarization reversal requires a full orientation reversal by the tetrahedron. In consequence, oxygen atoms would be required to undero displacements greater than the 1.5 Å maximum as O···H bonds were broken and new such bonds made. Additionally, the atomic coordinates do not approach supergroup symmetry, see Table S39. Thus, whereas $Na_3VO_4{\cdot}H_2O$ is polar, it is not ferroelectric and a thermally dependent phase change is not expected.

6.2.1 $LiGaSiO_4$ [65125]

Fleet, (1987). Mo$K\alpha$, graphite monochromator; absorption and extinction corrections; 583 independent $I_{obs} > 3\sigma(I_{obs})$; $R = 0.041$, $wR = 0.022$ in space group *R*3, all metal ion u_{aniso} coefficients varied, u_{iso}(O) only refinable; $R = 0.043$, $wR = 0.073$ in space group $R\bar{3}$, neither u_{aniso}(Li) nor u_{aniso}(O) refinable. *R*3 selected based on the superior fit and the ordered Li and Si atoms. The condition $0.3 \geq \Delta\xi \geq 0.05$ Å in Table S40 would satisfy the criteria for ferroelectricity if the Li and Si atoms were disordered over both Li/Si 18(*f*) sites in the polar space group. The difference between $\langle d_{Li\text{-}O}\rangle = 1.978$ Å and $\langle d_{Si\text{-}O}\rangle = 1.637$ Å in space group *R*3, however, is almost identical to the 0.33 Å difference between Shannon's (1976) ionic radii for Li^+ and Si^{4+}, and is hence strongly indicative of the ordering expected by the highly stable SiO_4^{-4} ion. $LiGaSiO_4$ is thus expected to remain polar over its thermal stability range. By contrast, the Al and Ge atoms in isotypic $LiAlGeO_4$, and the Ga and Ge atoms in isotypic $LiGaGeO_4$, are fully disordered at the corresponding 18(*f*) sites at ambient temperature and both closely approach the hypothetical *x*',*y*',*z*' structures of Tables S40, S41 with space group $R\bar{3}$, in accord with Fleet's (1987) report.

6.2.2 $LiAlSiO_4$ [92708]

Daniels & Fyfe, (2001). Mo*K*α, graphite monochromator; empirical absorption corrections; intensity statistics favor $R\bar{3}$ over *R*3; 1,978 independent F_{obs} in $R\bar{3}$ with R = 0.0557, wR = 0.1324 for 64 variables; 3,956 independent F_{obs} in *R*3 with R = 0.0259, wR = 0.0709 for 127 variables and Flack parameter 0.01(6); 14 independent atoms in *R*3. NMR spectroscopy, improved refinement indicators and characteristic $<d_{Si\text{-}O}> = 1.633$ Å, $<d_{Al\text{-}O}> = 1.763$ Å strongly favor the ordering of Si and Al atoms in this α-eucryptite $LiAlSiO_4$ sample as shown in Table S41. All pairs of *positions* effectively satisfy the 18(*f*) condition in $R\bar{3}$ and, with $\Delta\xi \lesssim u_{33}$, identical site occupation would correspond to the lower structural free-energy. It is possible that the Si:Al site occupancy depends on the growth conditions. Atomic locations in fully ordered samples such as the present are not likely to undergo exchange without disruption and hence are not predicted to be ferroelectric; if this site were fully disordered, centrosymmetry above the ferroelectric phase transition temperature T_C would be expected, *cf.* §2.5.

6.3 $Co(CO)_4SnCl_3$ [69685]

Klüfers (1991). Mo *K*α; graphite monochromator; absorption and extinction corrections; 891 independent $F_{obs} > n\sigma(F_{obs})$, *n* not reported; 7 independent atoms, U^{ij}, $R = 0.028$, wR_s = 0.028. Alignment of the linear Sn-Co-C1-O1 molecular axis in $SnCl_3Co[(CO)_4]$ with the polar axis, together with the three Cl, three C and 3 O atoms normal to it, does not allow the practical possibility of polarization reversal, as examination of the atomic positions in Table S42 confirms. In the absence of a first-order phase transition, $Co(CO)_4SnCl_3$ is hence predicted to remain polar at higher T without the possibility of ferroelectricity developing.

6.4 $Sn_{1.008}P_2S_6$ [79818]

Wang *et al.* (1995). Mo$K\alpha$, graphite monochromator; $T \approx 296$ K; 333 independent $F_{\mathrm{obs}} > 3\sigma(F_{\mathrm{obs}})$, ψ-scan absorption, extinction corrections, U^{ij}, $R = 0.0158$, $wR = 0.0207$; 6 independent atoms including a partially occupied second Sn atom site; $Sn_{1.008}P_2S_6$ generates second harmonics (Cleary, 2006) with nearly zero temperature dependence between 225 and 425 K. The given atomic coordinates depart only slightly from zero polarity in supergroup $P312$, as may be seen in Table S43. There is, however, no phase transition below 425 K nor is one likely at higher temperatures. Ferroelectricity in the related $Sn_2P_2S_6$ was reported by Carpentier & Nitsche (1974), with $T_C = 339(2)$ K at the transition from Pn to $P2_1/n$ (Cleary *et al.*, 1993); Gamernyk *et al.* (2006) report $T_C \simeq 337$ K.

6.5 $KNi(PO_3)_3$ [91527]

Kapshuk *et al.*, (2000). Mo$K\alpha$, graphite monochromator; no absorption correction; 409 independent $F^2_{\mathrm{obs}} > n\sigma(F^2_{\mathrm{obs}})$, n unspecified, U_{eq}, $R = 0.026$; 6 independent atoms. The near-centrosymmetric relationship between O1 and O3 and the close approach of K and Ni to 0,0,½ and 0,0,0 respectively, required if the space group were $R\bar{3}$, are notable, see Table

S44. Although the coordinates of P and O2 are within 1.50 Å of satisfying centrosymmetry, with P occupying a PO_4 tetrahedron these two atoms are not interchangeable under normal conditions, hence the symmetry of $KNi(PO_3)_3$ most likely remains $R3$ over the thermal stability range.

6.6 La_2MgGeO_6 [97016]

Swaffer *et al.* (2002). Time-of-flight neutron powder diffraction, λ unstated; Rietveld profile refinement; atom positions, B and site occupancies varied, $R_{wp} = 0.0703$, $R_p = 0.0494$; 4 independent metal, 2 O atoms. Space group $R3$, allowing ordered Mg and Ge sites, gave the best fit among the unspecified space groups examined. Table S45 shows that, if the Mg and Ge sites were comparably occupied, then the structure would more likely be in space group $R3c$ since that gives $0.02 \lesssim \Delta\xi \lesssim 0.11$ Å for all atoms, with $0.04 \lesssim u_{iso} \lesssim 0.08$ Å. The nominal $d_{Mg\text{-}O} = 2.09$, 2.04 Å and $d_{Ge\text{-}O} = 1.87$, 1.86 Å in the present structure are comparable to the $d_{Mg\text{-}O} = 2.12$, $d_{Ge\text{-}O} = 1.93$ Å given by Shannon's (1976) atomic radii, whereas $d_{Mg,Ge\text{-}O} = 1.98$, 1.95 Å. Space group $R3$ is hence confirmed, *cf.* §6.2, and although $R3c$ symmetry is approached a transition is unlikely below ~1500 K.

6.7 $Tl_2(MoO_3)_3PO_3CH_3$ [150170]

Harrison *et al.*, (1998). Mo$K\alpha$, graphite monochromator; ψ- scan absorption corrections; 824 $I_{obs} > 3\sigma(I_{obs})$, U_{eq}, $R = 0.0476$, $wR = 0.0535$; 9 independent atoms, excluding the unreported H atom. Table S46 shows that all atoms except Mo approach the symmetry of supergroup $R\bar{3}$ with $0.16 \lesssim \Delta\xi \lesssim 1.28$ Å, except for $\Delta\xi$(Mo) = 2.79 Å, provided the P and C atoms can achieve equivalence in the Wyckoff 6(c) site. The Mo atom displacement is sufficiently large that such a phase transition is highly unlikely, as is the possibility of equivalence between the P and C atoms, hence the material is expected to remain in space group *R*3 within its thermal stability limits.

6.8 $Cs_4SrSn_3Se_9$ [171013]

Almsick & Sheldrick, (2005). Mo*K*α, graphite monochromator; *ψ*-scan absorption corrections; 792 independent $F^2_{obs} > 2\sigma(F^2_{obs})$ at 293 K, U^{ij}, $R(F^2) = 0.0376$, $wR(F^2) = 0.102$. Four of the 7 independent atoms approach the symmetry of *R*3*m* with $0 \lesssim \Delta\xi \lesssim 0.80$ Å but the remaining three have $1.6 \lesssim \Delta\xi \lesssim 2.0$ Å, see Table S47. Unless $Cs_4SrSn_3Se_9$ remains stable well above the preparation temperature of 463 K, the three largest $\Delta\xi$ at 293 K are unlikely to become comparable to u_{eq} and hence result in a possible transition to *R*3*m*.

6.9 Hematolite, $Mn_{10.39}Mg_{2.53}Al_{1.89}Fe_{0.19}(OH)_{23}(AsO_3)(AsO_4)_2$ [200324]

Moore & Araki, (1978). Mo*K*α, graphite monochromator; 1,345 independent F_{obs}, absorption corrections, U_{iso}, $R = 0.09$, $wR = 0.10$; 10 independent metal sites, 14 independent O atoms. All atomic sites are within 1.1 Å of locations consistent with *R*32 symmetry, see Table S48(*a*), except for the 'Al2' site shared by Al, Fe and Mn in a ratio ~0.6:0.2:0.2 and four O atoms. The 'Al2' site at 00*z* is 2.96 Å, the four sites are ~1.9 Å, distant from *R*32 symmetry. In addition to these large displacements, the possible location of a comparable but overlooked Al, Fe, Mn (*i.e., Al2A*) atom at $0,0,\bar{z}$, which might allow the possibility of ferroelectricity at higher temperatures, is eliminated by the 4 rather than the expected 6 oxygen nearest neighbors about the site. The structure is hence most likely to remain in space group *R*3 over its thermal stability range. It is noted that, excluding Al2, *Al2A*,O1,O6 and O7 from the origin determination as in Table S48(*b*), all other $\Delta\xi$ become significantly smaller, suggesting the possibility of error in one or more of these four atomic coordinates and the advisability of a more accurate redetermination.

Tables for Appendix 4

Table S39

Atomic positions for $Na_3VO_4 \cdot 3H_2O$ at 298 K (Kato & Takayama-Muromachi, 1987) [62533]

a = 8.5099(3), c = 7.7876(3) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position *R*3	*x*	*y*	*z*	u_{iso}
Na1	9(*b*)	0.10110(7)	0.64996(18)	0.07713(15)	0.14
V1	3(*a*)	0	0	0	0.10
O1	3(*a*)	0	0	0.21770(33)	0.13
O2	9(*b*)	0.13335(19)	0.21469(18)	-0.08283(19)	0.12
O3	9(*b*)	0.31006(29)	-0.12621(28)	0.27244(24)	0.12
H1	9(*b*)	0.372(4)	0.875(4)	0.364(5)	0.11
H2	9(*b*)	0.331(5)	0.997(5)	0.275(4)	0.19

Table S40

Modified atomic positions for $LiGaSiO_4$ at 293 K (Fleet, 1987) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [65125]

a = 13.6427(11), *c* = 9.0965(7) Å. $z^* = z + 0.0002$; $\Delta x = (x - x')a, \Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
	$R3$, $R\bar{3}$											
Ga1	9(*b*)	0.4510(1)	0.1375(1)	0.0836	0.4543	0.1377	0.0834	-0.05	-0.00	0.00	0.05	0.07
	18(*f*)											
Ga2	9(*b*)	0.5424(1)	0.8622(1)	0.9169(1)	0.5457	0.8623	0.9166	-0.05	-0.00	0.00	0.05	0.07
Li1	9(*b*)	0.1249(11)	0.4763(13)	0.0784(19)	0.1229	0.4734	0.0804	0.03	0.04	-0.02	0.06	0.10
	18(*f*)											
Si1	9(*b*)	0.8792(2)	0.5294(2)	0.9175(2)	0.8771	0.5266	0.9196	0.03	0.04	-0.02	0.06	0.08
Si2	9(*b*)	0.0126(2)	0.2103(2)	0.0844(2)	0.0162	0.2097	0.0881	-0.05	0.01	-0.03	0.05	0.08
	18(*f*)											
Li2	9(*b*)	0.9803(10)	0.7909(10)	0.9083(18)	0.9838	0.7903	0.9119	-0.05	0.01	-0.03	0.05	0.09
O1	9(*b*)	0.5450(2)	0.4254(2)	0.0588(3)	0.5438	0.4204	0.0818	0.02	0.07	-0.21	0.23	0.10
	18(*f*)											
O2	9(*b*)	0.4574(2)	0.5845(2)	0.8951(3)	0.4562	0.5796	0.9182	0.02	0.07	-0.21	0.23	0.09
O3	9(*b*)	0.0018(3)	0.3245(3)	0.0849(4)	0.0040	0.3349	0.0827	-0.03	-0.14	0.02	0.16	0.09
	18(*f*)											
O4	9(*b*)	0.9939(3)	0.6548(3)	0.9195(4)	0.9960	0.6651	0.9173	-0.03	-0.14	0.02	0.16	0.10
O5	9(*b*)	0.2195(2)	0.1168(2)	0.0953(3)	0.2111	0.1233	0.0818	0.11	-0.09	0.12	0.16	0.09
	18(*f*)											
O6	9(*b*)	0.7973(2)	0.8702(2)	0.9318(3)	0.7889	0.8767	0.9182	0.11	-0.09	0.12	0.16	0.09
O7	9(*b*)	0.2616(3)	0.4637(2)	0.0964(3)	0.2452	0.4571	0.0837	0.22	0.09	0.12	0.30	0.10
	18(*f*)											
O8	9(*b*)	0.7713(2)	0.5495(2)	0.9291(3)	0.7548	0.5429	0.9163	0.22	0.09	0.12	0.30	0.09

Table S41 LiAlSiO$_4$

Atomic positions for LiAlSiO$_4$ (Daniels & Fyfe, 2001) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [92708]
a = 13.532(4), *c* = 9.044(3) Å. $\Delta x = (x - x')a, \Delta y = (y - y')a, \Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{33}
Li1	9(*b*)	-0.0172(2)	0.1889(2)	0.2514(4)	-0.0190	0.1886	0.2489	0.02	0.00	0.02	0.03	0.11
Li2	18(*f*) 9(*b*)	0.0208(2)	0.8117(2)	0.7535(4)	0.0190	0.8114	0.7511	0.02	0.00	0.02	0.03	0.12
Si1	9(*b*)	0.53003(2)	0.87978(2)	0.74976(2)	0.53018	0.88069	0.74944	0.00	-0.01	0.00	0.01	0.10
Al1	18(*f*) 9(*b*)	0.46967(3)	0.11840(3)	0.25088(3)	0.46982	0.11931	0.25056	0.00	-0.01	0.00	0.01	0.10
Si2	9(*b*)	0.87557(2)	0.34416(2)	0.91628(2)	0.87533	0.34446	0.91604	0.00	0.00	0.00	0.00	0.10
Al2	18(*f*) 9(*b*)	0.12492(3)	0.65525(3)	0.08420(3)	0.12467	0.65554	0.08396	0.00	0.00	0.00	0.00	0.10
O1	9(*b*)	0.24713(6)	0.79009(6)	0.10959(9)	0.24080	0.78696	0.10559	0.09	0.04	0.04	0.12	0.10
O2	18(*f*) 9(*b*)	0.76554(6)	0.21616(6)	0.89841(8)	0.75920	0.21304	0.89441	0.09	0.04	0.04	0.12	0.11
O3	9(*b*)	0.26720(6)	0.80088(6)	0.40671(7)	0.26737	0.80080	0.41514	0.00	0.00	-0.08	0.08	0.10
O4	18(*f*) 9(*b*)	0.73246(6)	0.19928(6)	0.57644(7)	0.73263	0.19920	0.58486	0.00	0.00	-0.08	0.08	0.09
O5	9(*b*)	0.89552(6)	0.11202(6)	0.06308(8)	0.89959	0.11571	0.05839	-0.06	-0.05	0.04	0.10	0.10
O6	18(*f*) 9(*b*)	0.09633(6)	0.88060(6)	0.94630(8)	0.10041	0.88429	0.94161	-0.06	-0.05	0.04	0.10	0.10
O7	9(*b*)	0.33574(5)	0.99138(6)	0.25101(9)	0.34058	0.99756	0.25059	-0.07	-0.08	0.00	0.13	0.12
O8	18(*f*) 9(*b*)	0.65458(7)	-0.00374(5)	0.74982(9)	0.65942	0.00244	0.74941	-0.07	-0.08	0.00	0.13	0.12

Table S42

Atomic positions for $Co(CO)_4SnCl_3$ at ambient temperature (Klüfers, 1991) with hypothetical $x'y'\,z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [69685]

a = 10.1606(9), c = 9.294(2) Å. $z^* = z + 0.0000$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff Position $R3$, $R\bar{3}$	x	y	z
Sn	3(a)	0	0	0
Co	3(a)	0	0	0.2665(1)
Cl	9(b)	0.2091(2)	0.0063(2)	0.8935(2)
C1	3(a)	0	0	0.4623(12)
O1	3(a)	0	0	0.5818(9)
C2	9(b)	0.1431(7)	0.1961(7)	0.2520(6)
O2	9(b)	0.2342(6)	0.3206(5)	0.2437(6)

Table S43 $Sn_{1.008}P_2S_6$

Modified atomic positions in $Sn_{1.008}P_2S_6$ (Wang *et al.*, 1995) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [79818]

a = 5.999(2), c = 19.424(4) Å. $z^* = z - 0.1107$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$

	Wyckoff position $R3$,$P312$[†]	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}	occ.
Sn1	3(a) 2(g)	0	0	0.7774	0	0	0.8326	0	0	-1.07	1.07	0.10	1.
Sn2	3(a)	0	0	0.1121(27)	0	0	0.1674	0	0	-1.07	1.07	0.19	0.008
S1	9(b) 6(l)	0.3428(3)	0.3455(3)	0.1953(1)	0.3411	0.3446	0.0848	0.01	0.01	2.15	2.15	0.12	1.
S2	9(b)	0.6562(3)	0.6607(3)	0.0258(1)	0.6554	0.6589	-0.0848	0.01	0.01	2.15	2.15	0.10	1.
P1	3(a) 2(g)	0	0	0.5017(1)	0	0	0.5569	0	0	-1.07	1.07	0.09	1.
P2	3(a)	0	0	0.3879(1)	0	0	0.4431	0	0	-1.07	1.07	0.10	1.

[†] For a possible transition through $R32$ to $P312$ as the rhombohedral centering relaxes and each independent atom in $R3$ becomes three atoms. Each Wyckoff position in $P312$ is then related to one-third of the corresponding atoms in $R3$.

Table S44 KNi(PO$_3$)$_3$

Modified atomic positions for KNi(PO$_3$)$_3$ (Kapshuk *et al.*, 2000) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{eq} displacements in Å [91527]

a = 10.076(2), c = 6.9623(5) Å. $z^* = z - 0.0096$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R\bar{3}$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Ni	3(a),3(a)	0	0	-0.0096	0	0	0	0	0	-0.07	0.07	0.08
K	3(a),3(b)	0	0	0.4837(1)	0	0	0.5000	0	0	-0.11	0.11	0.13
P	9(b)	0.3435(1)	0.2386(1)	0.1264(2)	0.3219	0.1038	0.1069	0.22	1.36	0.14	1.49	0.08
	18(f)											
O2	9(b)	0.3530(4)	0.3004(4)	-0.0875(5)	0.2182	0.3219	-0.1069	1.36	-0.22	0.14	1.27	0.10
O1	9(b)	0.1875(1)	0.1092(5)	0.1682(3)	0.1878	0.1117	0.1748	0.00	-0.03	-0.05	0.06	0.10
	18(f)											
O3‡	9(b)	0.8118(4)	0.8858(4)	0.8187(6)	0.8122	0.8883	0.8252	0.00	-0.03	-0.05	0.06	0.09

Table S45

Atomic positions for La$_2$MgGeO$_6$ (Swaffer *et al.,* 2002) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso}displacements in Å [97016]

a = 5.5125(1), c = 13.3295(2) Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position $R3$, $R3c$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}
La1	3(a)	0.	0.	0.248(3)	0.	0.	0.250	0.	0.	-0.03	0.03	0.06
	6(a)											
La2	3(a)	0.	0.	0.752(2)	0.	0.	0.750	0.	0.	0.03	0.03	0.06
Mg	3(a)	0.	0.	0.	0.	0.	0.0015	0.	0.	-0.02	0.02	0.04
	6(a)†											
Ge	3(a)	0.	0.	0.503(3)	0.	0.	0.5015	0.	0.	0.02	0.02	0.05
O1	9(c)	0.119(2)	0.354(2)	0.089(2)	0.1155	0.3404	0.0835	0.02	0.08	0.07	0.11	0.08
	18(b)											
O2	9(c)	0.112(2)	0.789(2)	0.578(2)	0.1155	0.7754	0.5835	-0.02	0.08	-0.07	0.11	0.06

† Assuming the Mg and Ge sites are identically occupied; if not, then space group $R3c$ cannot be a possible structural choice for La$_2$MgGeO$_6$.

Table S46 $Tl_2(MoO_3)_3PO_3CH_3$

Modified atomic positions in $Tl_2(MoO_3)_3PO_3CH_3$ (Harrison *et al.*, 1998) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å.[150170]

$a = 7.281(1)$, $c = 18.932(2)$ Å. $z^* = z + 0.088677$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$

	Wyckoff position $R3$, $R\bar{3}$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Tl1	3(*a*)	0.	0.	0.26379(9)	0.	0.	0.30760	0.	0.	-0.83	0.83	0.23
	6(*c*)											
Tl2	3(*a*)	0	0	0.64859(8)	0	0	0.69240	0	0	-0.83	0.83	0.17
Mo	9(*b*),9(*e*)	0.0067(1)	0.5404(1)	0.14612(9)	0	0.5	0	0.05	0.29	2.77	2.79	0.11
P	3(*a*)	0	0	0.94548(2)	0	0	0.95405	0.	0.	-0.16	0.16	0.12
	6(*c*)											
C	3(*a*)	0	0	0.0373(1)	0	0	0.0459	0	0	-0.16	0.16	0.13
O1	9(*b*)	0.075(2)	0.541(1)	0.0593(5)	0.097	0.703	0.0697	-0.16	-1.18	-0.20	1.28	0.14
	18(*f*)											
O4	9(*b*)	0.231(1)	0.120(1)	0.9199(5)	0.394	0.097	0.9303	-1.19	0.17	-0.20	1.13	0.14
O2	9(*b*)	0.548(1)	0.464(1)	0.8439(5)	0.565	0.621	0.8542	-0.12	-1.14	-0.20	1.22	0.14
	18(*f*)											
O3	9(*b*)	0.787(1)	0.582(1)	0.1355(5)	0.944	0.565	0.1458	-1.14	0.12	-0.20	1.10	0.13

Table S47 $Cs_4SrSn_3Se_9$

Atomic positions in $Cs_4SrSn_3Se_9$ (Almsick & Sheldrick, 2005) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å. [171013]

$a = 14.528(3)$, $c = 9.685(6)$ Å. $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$

	Wyckoff position $R3$,$R3m$	x	y	z	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{eq}
Cs1	9(*b*)	1.00451(10)	0.56109(9)	0.17713(13)	1.0437	0.5219	0.17713	-0.57	0.57	0	0.57	0.17
Cs2	3(*a*)	0	0	0.8553(3)	0	0	0.8553	0	0	0	0	0.20
Sn	9(*b*)	0.89143(8)	0.23873(9)	0.44014(13)	0.82635	0.17365	0.44014	0.95	0.95	0	1.65	0.13
Se1	9(*b*)	0.90254(14)	0.26040(15)	0.1782(2)	0.82107	0.17893	0.1782	1.18	1.18	0	2.04	0.14
Se2	9(*b*)	0.94565(15)	0.11743(14)	0.5419(2)	0.91411	0.08589	0.5419	0.46	0.46	0	0.80	0.16
Se3	9(*b*)	0.70045(15)	0.17204(15)	0.4813(2)	0.76421	0.23580	0.4813	-0.93	-0.93	0	1.61	0.15
Sr	3(*a*)	0	0	0.3186(3)	0	0	0.3186	0	0	0	0	0.14

Table S48(*a*)

Modified atomic positions in the mineral hematolite (Moore & Araki*,* 1978) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and $u_{\rm iso}$ displacements in Å [200324]

a = 8.275(5), c = 36.60(5) Å. $z^* = z + 0.0436$; $\Delta x = (x - x')a$,$\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	$u_{\rm i\,so}$	occ.
Mn1	3(*a*)	0	0	0.0436	0	0	0.0589	0	0	-0.56	0.56	0.14	1.
	6(*c*)												
Mn2	3(*a*)	0	0	0.9258	0	0	0.9411	0	0	-0.56	0.56	0.15	1.
Mn3	9(*b*)	0.3124(4)	0.4243(4)	0.1175	0.2840	0.3230	0.1326	0.24	0.84	-0.55	1.13	0.14	1.
	18(*f*)												
Mn4	9(*b*)	0.7444(4)	0.7783(4)	0.8522	0.7160	0.6770	0.8674	0.24	0.84	-0.55	1.13	0.14	1.
Mg1,Al1,Mn5	9(*b*)	0.0935(7)	0.4750(7)	0.3183	0.0883	0.4733	0.3325	0.04	0.01	-0.52	0.52	0.15	0.4,0.44,0.16
	18(*f*)												
Mn6,Mg2	9(*b*)	0.9170(5)	0.5284(5)	0.6534	0.9117	0.5267	0.6675	0.04	0.01	-0.52	0.52	0.14	0.56,0.44
Al2,Fe,Mn7†	3(*a*)	0	0	0.1245	0	0	0.1245	0	0	0.00	0	0.14	0.58,0.19,0.23
	6(*c*)												
Al2A,FeA,Mn7A	*3(a)*	*0*	*0*	*-0.1245*	*0*	*0*	*-0.1245*	*0*	*0*	*0.00*	0	*n.d.*	*n.d.*
As1	3(*a*)	0	0	0.2385	0	0	0.2337	0	0	0.18	0.18	0.13	1.
	6(*c*)												
As3	3(*a*)	0	0	0.7711	0	0	0.7663	0	0	0.18	0.18	0.14	1.
O1	3(*a*)	0	0	0.2858	0	0	0.2339	0	0	1.89	1.89	0.13	1.
	6(*c*)												
O4	3(*a*)	0	0	0.8179	0	0	0.7661	0	0	1.89	1.89	0.09	1.
O2	9(*b*)	0.059(2)	0.218(2)	0.2228	0.062	0.2165	0.2338	-0.02	0.01	-0.40	0.40	0.15	1.
	18(*f*)												
O5	9(*b*)	0.934(3)	0.785(3)	0.7552	0.938	0.7835	0.7662	-0.03	0.01	-0.40	0.40	0.20	1.
As2	3(*a*),3(*b*)	0	0	0.5164	0	0	0.5	0	0	0.60	0.6	0.13	1.
O3	3(*a*)	0.139(2)	0.499(2)	0.157	0.147	0.470	0.1686	-0.07	0.24	-0.42	0.47	0.13	1.
	18(*f*)												
O9$_{\rm H}$	9(*b*)	0.559(2)	0.845(2)	0.8198	0.530	0.853	0.8314	0.24	-0.07	-0.42	0.47	0.14	1.
O6$_{\rm H}$	3(*a*)	0	0	0.4223	0	0	0.3723	0	0	1.83	1.83	0.12	1.
	6(*c*)												
O7$_{\rm H}$	3(*a*)	0	0	0.6776	0	0	0.6277	0	0	1.83	1.83	0.17	1.
O8$_{\rm H}$	9(*b*)	0.060(2)	0.211(2)	0.0904	0.0475	0.213	0.1034	0.10	-0.02	-0.48	0.49	0.15	1.
	18(*f*)												
O10$_{\rm H}$	9(*b*)	0.965(2)	0.785(2)	0.8836	0.9525	0.787	0.8966	0.10	-0.02	-0.48	0.49	0.15	1.
O11	9(*b*)	0.286(2)	0.436(2)	0.291	0.2825	0.428	0.3052	0.03	0.07	-0.52	0.53	0.17	1.
	18(*f*)												
O13$_{\rm H}$	9(*b*)	0.721(2)	0.580(2)	0.6806	0.7175	0.572	0.6948	0.03	0.07	-0.52	0.53	0.15	1.
O12$_{\rm H}$	9(*b*)	0.417(2)	0.124(2)	0.287	0.4095	0.193	0.3006	0.06	-0.57	-0.50	0.74	0.16	1.
	18(*f*)												
O14$_{\rm H}$	9(*b*)	0.262(2)	0.402(2)	0.6857	0.193	0.4095	0.6994	0.57	-0.06	-0.50	0.74	0.17	1.

† *Al2A,FeA,Mn7A* postulated as with coordinates 0,0, -*z*(Al2,Fe,Mn7)

Table S48(*b*)

Modified atomic positions in the mineral hematolite (Moore & Araki, 1978) with hypothetical $x'y'z'$ coordinates and the Δx, Δy, Δz and u_{iso} displacements in Å [200324]

$a = 8.275(5)$, $c = 36.60(5)$ Å. $z^* = z + 0.0536$; $\Delta x = (x - x')a$, $\Delta y = (y - y')a$, $\Delta z = (z^* - z')c$.

	Wyckoff position *R*3,*R*32	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	$\Delta\xi$	u_{iso}	occ.
Mn1	3(*a*)	0	0	0.0536	0	0	0.0589	0	0	-0.19	0.19	0.14	1.
	6(*c*)												
Mn2	3(*a*)	0	0	0.9358	0	0	0.9411	0	0	-0.19	0.19	0.15	1.
Mn3	9(*b*)	0.3124(4)	0.4243(4)	0.1275	0.2840	0.3230	0.1326	0.24	0.84	-0.19	1.00	0.14	1.
	18(*f*)												
Mn4	9(*b*)	0.7444(4)	0.7783(4)	0.8622	0.7160	0.6770	0.8674	0.24	0.84	-0.19	1.00	0.14	1.
Mg1,Al1,Mn5	9(*b*)	0.0935(7)	0.4750(7)	0.3283	0.0883	0.4733	0.3325	0.04	0.01	-0.15	0.16	0.15	0.4,0.44,0.16
	18(*f*)												
Mn6,Mg2	9(*b*)	0.9170(5)	0.5284(5)	0.6634	0.9117	0.5267	0.6675	0.04	0.01	-0.15	0.16	0.14	0.56,0.44
Al2,Fe,Mn7†	3(*a*)	0	0	0.1345	0	0	0.	0	0	0.00	0.00	0.14	0.58,0.19,0.23
	6(*c*)												
Al2A,FeA,Mn7A	3(*a*)	*0*	*0*	*0.8655*	*0*	*0*	*0.*	*0*	*0*	*0.00*	*0.00*	*n.d.*	*n.d.*
As1	3(*a*)	0	0	0.2485	0	0	0.2337	0	0	0.54	0.54	0.13	1.
	6(*c*)												
As3	3(*a*)	0	0	0.7811	0	0	0.7663	0	0	0.54	0.54	0.14	1.
O1	3(*a*)	0	0	0.2958	0	0	0.2339	0	0	2.27	2.27	0.13	1.
	6(*c*)												
O4	3(*a*)	0	0	0.8279	0	0	0.7661	0	0	2.26	2.26	0.09	1.
O2	9(*b*)	0.059(2)	0.218(2)	0.2328	0.062	0.2165	0.2338	-0.02	0.01	-0.04	0.04	0.15	1.
	18(*f*)												
O5	9(*b*)	0.934(3)	0.785(3)	0.7652	0.938	0.7835	0.7662	-0.03	0.01	-0.04	0.05	0.20	1.
As2	3(*a*),3(*b*)	0	0	0.5264	0	0	0.5	0	0	0.96	0.96	0.13	1.
O3	3(*a*)	0.139(2)	0.499(2)	0.167	0.147	0.470	0.1686	-0.07	0.24	-0.06	0.22	0.13	1.
	18(*f*)												
$\mathrm{O9_H}$	9(*b*)	0.559(2)	0.845(2)	0.8298	0.530	0.853	0.8314	0.24	-0.07	-0.06	0.22	0.14	1.
$\mathrm{O6_H}$	3(*a*)	0	0	0.4323	0	0	0.3723	0	0	2.20	2.20	0.12	1.
	6(*c*)												
$\mathrm{O7_H}$	3(*a*)	0	0	0.6876	0	0	0.6277	0	0	2.19	2.19	0.17	1.
$\mathrm{O8_H}$	9(*b*)	0.060(2)	0.211(2)	0.1004	0.0475	0.213	0.1034	0.10	-0.02	-0.11	0.14	0.15	1.
	18(*f*)												
$\mathrm{O10_H}$	9(*b*)	0.965(2)	0.785(2)	0.8936	0.9525	0.787	0.8966	0.10	-0.02	-0.11	0.14	0.15	1.
O11	9(*b*)	0.286(2)	0.436(2)	0.301	0.2825	0.428	0.3052	0.03	0.07	-0.15	0.17	0.17	1.
	18(*f*)												
$\mathrm{O13_H}$	9(*b*)	0.721(2)	0.580(2)	0.6906	0.7175	0.572	0.6948	0.03	0.07	-0.15	0.17	0.15	1.
$\mathrm{O12_H}$	9(*b*)	0.417(2)	0.124(2)	0.297	0.4095	0.193	0.3006	0.06	-0.57	-0.13	0.56	0.16	1.
	18(*f*)												
$\mathrm{O14_H}$	9(*b*)	0.262(2)	0.402(2)	0.6957	0.193	0.4095	0.6994	0.57	-0.06	-0.13	0.56	0.17	1.

† Atoms Al2, O1, O4, O6 and O7 are excluded from the origin determination in this table with *Al2A* assumed to occupy equally the location centrosymmetrically related to that of Al2, see text.

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