Acta Crystallographica Section B
Structural Science
ISSN 0108-7681

addenda and errata

Systematic prediction of new ferroelectrics in space groups $P3_1$ and $P3_2$. Erratum

S. C. Abrahams

Physics Department, Southern Oregon University, Ashland, OR 97520, USA.
Correspondence e-mail: sca@mind.net

The alignment in Tables 1–4 of the paper by Abrahams (2003) was incorrect. The corrected tables are reproduced herein.

Table 1
Atomic positions for Cu_2BaGeS_4 at room temperature (Teske, 1979), with hypothetical x', y' and z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

a = 6.215 and c = 15.534 Å. Uncertainties not reported. $z^* = z - 0.0907$, $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$, $P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Cu1	3(*a*)	0.2587 (6)	0.2487 (6)	0.2487 (2)	0.2960	0.3099	0.2565	−0.232	−0.380	−0.121	0.09
	6(*c*)†										
Cu2	3(*a*)	−1/3	0.0750 (3)	0.0690 (2)	−0.2960	0.0139	0.0768	−0.232	0.380	−0.121	0.15
Ge	3(*a*), 3(*a*)	1/3	0.3807 (3)	−0.0083 (2)	0.3570	0.3570	0	−0.147	0.147	−0.129	0.14
Ba	3(*a*), 3(*b*)	−0.1029 (2)	2/3	0.1593	0	∼0.6667	0.1667	−0.639	∼0	−0.115	0.08
S1	3(*a*)	0.3703 (9)	0.1870 (9)	0.1076 (3)	0.2586	0.2971	0.0863	0.694	−0.684	0.331	0.07
	6(*c*)										
S2	3(*a*)	−0.1468 (9)	0.1486 (9)	0.2683 (3)	−0.2586	0.0385	0.2470	0.695	0.684	0.331	0.10
S3	3(*a*)	0.0035 (9)	0.4292 (9)	−0.0023 (3)	−0.1183	0.5466	0.0034	0.758	−0.730	−0.089	0.10
	6(*c*)										
S4	3(*a*)	0.6639 (9)	0.7598 (9)	−0.0091 (3)	0.5466	0.8817	−0.0034	0.729	−0.758	−0.089	0.10

† See footnote **1** for equivalent positions.

Table 2
Atomic positions for $K_2HCr_2AsO_{10}$ at room temperature (Averbuch-Pouchot *et al.* 1978), with hypothetical x', y' and z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

a = 7.712 (3) and c = 14.644 (8) Å. $z^* = z - 0.0046$, $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$, $P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Cr1	3(*a*)	0.4278 (3)	0.4243 (3)	0.2403	0.4242	0.4217	0.2460	0.028	0.020	−0.083	0.14
	6(*c*)†										
Cr2	3(*a*)	0.4191 (3)	0.4205 (4)	0.7484 (2)	0.4217	0.4242	0.7540	−0.020	−0.028	−0.082	0.14
As	3(*a*), 3(*a*)	0.1281 (2)	0.0199 (2)	0.3447 (2)	0.1281	0	0.3333	0	0.153	0.167	0.14
K1	3(*a*), 3(*b*)	0.5520 (5)	−0.0182 (5)	0.8343 (3)	0.5520	0	0.8333	0	−0.140	0.015	0.17
K2	3(*a*), 3(*a*)	0.6083 (5)	0.0061 (5)	0.3277 (3)	0.6083	0	0.3333	0	0.047	−0.082	0.17
O1	3(*a*)	0.356 (2)	0.186 (2)	0.2975 (8)	0.3465	0.188	0.3077	0.073	−0.015	−0.149	0.17
	6(*c*)										
O5	3(*a*)	0.190 (2)	0.337 (2)	0.6821 (8)	0.188	0.3465	0.6923	0.015	−0.073	−0.149	0.17
O2	3(*a*)	0.625 (2)	0.480 (2)	0.1805 (11)	0.6148	0.4615	0.1794	0.078	0.143	0.016	0.21
	6(*c*)										
O7	3(*a*)	0.143 (2)	0.557 (2)	0.4885 (9)	0.1533	0.5385	0.4874	−0.079	0.143	0.016	0.19
O3	3(*a*)	0.469 (3)	0.594 (2)	0.3163 (9)	0.487	0.584	0.3198	−0.139	0.077	−0.051	0.22
	6(*c*)										
O8	3(*a*)	0.495 (2)	0.087 (2)	0.0101 (9)	0.513	0.097	0.0136	−0.139	−0.077	−0.051	0.20
O4	3(*a*)	0.245 (2)	0.390 (2)	0.1713 (10)	0.237	0.398	0.1835	0.066	−0.062	−0.179	0.20
	6(*c*)										
O6	3(*a*)	0.772 (2)	0.170 (2)	0.1376 (12)	0.763	0.162	0.1498	0.066	0.062	−0.179	0.22
O9	3(*a*)	0.087 (2)	0.097 (2)	0.4436 (8)	0.023	0.057	0.4170	0.497	0.312	0.390	0.19
	6(*c*)										
O10	3(*a*)	0.016 (2)	−0.042 (2)	0.6096 (9)	0.057	0.023	0.5830	−0.312	−0.497	0.390	0.19

† See footnote **1** for equivalent positions.

Table 3
(*a*) Atomic positions for $RbNO_3$ in phase IV (Shamsuzzoha & Lucas, 1982) at room temperature, with hypothetical x', y' and z' coordinates and Δx, Δy, Δz and u_{eq} displacements in Å.

a = 10.55 (2) and c = 7.47 (2) Å; $z^* = z - 0.0949$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$, $P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Rb1	3(*a*), 3(*b*)	0.4566 (3)	0.5691 (3)	0.5287 (5)	0.5129	0.5129	0.5	−0.59	0.59	0.21	0.19
Rb2	3(*a*)	0.1184 (3)	0.2192 (3)	−0.0949	0.1706	0.3056	−0.1524	−0.55	−0.91	0.43	0.22
	6(*c*)†										
Rb3	3(*a*)	−0.2228 (4)	0.2214 (3)	0.5432 (6)	−0.1706	0.1350	0.4857	−0.55	0.91	0.43	0.24
N1	3(*a*), 3(*a*)	0.4388 (4)	0.5668 (4)	0.0104 (6)	0.5028	0.5028	0	−0.68	0.68	0.08	0.22
N2	3(*a*)	0.0962 (3)	0.2042 (3)	0.4369 (6)	0.1771	0.2935	0.3742	−0.85	−0.94	0.47	0.20
	6(*c*)										
N3	3(*a*)	−0.2580 (3)	0.2057 (3)	0.0219 (7)	−0.1771	0.1164	−0.0408	−0.85	0.94	0.47	0.20
O1	3(*a*)	0.3371 (6)	0.5582 (5)	−0.0855 (8)	0.2773	0.6062	−0.0023	0.63	−0.51	−0.62	0.25
	6(*c*)										
O9	3(*a*)	0.6541 (5)	0.2174 (5)	−0.0809 (7)	0.6062	0.2773	0.0023	0.51	−0.63	−0.62	0.25
O2	3(*a*)	0.3964 (5)	0.4704 (5)	0.1331 (8)	0.3521	0.4717	0.1555	0.47	−0.01	−0.17	0.25
	6(*c*)										
O7	3(*a*)	0.6922 (5)	0.1208 (5)	0.1554 (7)	0.6479	0.1196	0.1778	0.47	0.01	−0.17	0.25
O3	3(*a*), 3(*a*)	0.5646 (5)	0.6512 (5)	−0.0285 (9)	0.6079	0.6079	0	−0.46	0.46	−0.21	0.26
O4	3(*a*), 3(*b*)	−0.0011 (4)	0.1089 (4)	0.5296 (7)	0.0550	0.0550	0.5	−0.58	0.58	0.22	0.21
O5	3(*a*), 3(*b*)	0.2309 (5)	0.2495 (5)	0.4688 (8)	0.2402	0.2402	0.5	−0.10	0.10	−0.23	0.25
O6	3(*a*)	0.0581 (5)	0.2465 (5)	0.3000 (8)	0.0930	0.3085	0.3191	−0.37	−0.65	−0.14	0.25
	6(*c*)										
O8	3(*a*)	−0.1279 (6)	0.2774 (6)	−0.0052 (8)	−0.0930	0.2155	0.0140	−0.37	0.65	−0.14	0.26

(*b*) As in Table 3(*a*) but based on the atomic coordinates of Pohl *et al.* (1992), with atom O1 in an equivalent position.† a = 10.474 (1) and c = 7.443 (1) Å; $z^* = z - 0.1049$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z^* - z')c$.

	Wyckoff position $P3_1$, $P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u_{eq}
Rb1	3(*a*), 3(*b*)	0.4474 (2)	0.5575 (2)	0.5434 (4)	0.5024	0.5024	0.5	−0.58	0.58	0.32	0.18
Rb2	3(*a*)	0.1231 (1)	0.2201 (1)	−0.1049	0.1696	0.3098	−0.1455	−0.49	−0.94	0.30	0.18
	6(*c*)										
Rb3	3(*a*)	−0.2161 (1)	0.2299 (1)	0.5193 (1)	−0.1696	0.1402	0.4788	−0.49	0.94	0.30	0.17
N1	3(*a*), 3(*a*)	0.4612 (7)	0.5915 (7)	0.0579 (15)	0.5264	0.5264	0	−0.68	0.68	0.43	0.17
N2	3(*a*)	0.1009 (8)	0.2047 (8)	0.4167 (15)	0.1673	0.2990	0.3795	−0.85	−0.99	0.28	0.17
	6(*c*)										
N3	3(*a*)	−0.2337 (9)	0.2260 (6)	−0.0090 (14)	−0.1673	0.1317	−0.0462	−0.85	0.99	0.28	0.15
O1	3(*a*)	0.2283 (7)	0.5505 (7)	−0.1669 (8)	0.2799	0.6630	−0.1969	−0.54	1.18	−0.22	0.22
	6(*c*)										
O9	3(*a*)	0.6685 (6)	0.2246 (7)	−0.1064 (8)	0.6169	0.3370	−0.1364	0.54	−1.18	0.22	0.21
O2	3(*a*)	0.3927 (8)	0.4597 (7)	0.0886 (10)	0.3328	0.4692	0.1499	0.63	−0.10	−0.45	0.25
	6(*c*)										
O7	3(*a*)	0.7271 (9)	0.1458 (8)	0.1220 (9)	0.6672	0.1552	0.1834	0.63	−0.10	−0.46	0.24
O3	3(*a*), 3(*a*)	0.5465 (7)	0.6419 (8)	−0.0660 (9)	0.5942	0.5942	0	−0.50	0.50	−0.49	0.23
O4	3(*a*), 3(*b*)	0.0022 (6)	0.1101 (6)	0.5152 (9)	0.0562	0.0562	0.5	−0.58	0.58	0.11	0.21
O5	3(*a*), 3(*b*)	0.2310 (6)	0.2476 (7)	0.4519 (10)	0.2393	0.2393	0.5	−0.07	0.06	−0.36	0.23
O6	3(*a*)	0.0637 (7)	0.2519 (7)	0.2870 (8)	0.0836	0.3223	0.3350	−0.21	−0.74	−0.36	0.22
	6(*c*)										
O8	3(*a*)	−0.1034 (6)	0.3091 (7)	−0.0496 (11)	−0.0836	0.2387	−0.0017	−0.21	0.74	−0.36	0.24

† See footnote **1** for equivalent positions.

Table 4
Atomic positions for KYF_4 at room temperature (Le Fur *et al.*, 1992), with hypothetical x', y' and z' coordinates and Δx, Δy, Δz and u^{33} displacements in Å.

a = 14.060 (10) and c = 10.103 (10) Å; $z^* = z - 0.3195$, with $\Delta x = (x - x')a$, $\Delta y = (y - y')a$ and $\Delta z = (z^* - z)c$.

	Wyckoff position $P3_1$, $P3_121$	x	y	z^*	x'	y'	z'	Δx	Δy	Δz	u^{33}
K1	3(*a*), 3(*a*)	0.7818 (2)	0.7190 (2)	−0.0282 (2)	0.7504	0.7504	0	0.442	−0.442	−0.285	0.12
K2	3(*a*), 3(*a*)	0.2677 (2)	0.2208 (3)	0.0057 (3)	0.2443	0.2443	0	0.329	−0.330	0.046	0.16
K3	3(*a*)	0.1050 (2)	0.3945 (3)	−0.0331 (4)	0.0851	0.4247	−0.0034	0.280	−0.425	−0.300	0.17
	6(*c*)†										
K6	3(*a*)	0.4549 (3)	0.0652 (3)	−0.0264 (4)	0.4247	0.0851	0.0034	0.425	−0.280	−0.301	0.15
K4	3(*a*)	0.6111 (2)	0.8778 (2)	0.0028 (3)	0.5851	0.9122	0.0021	0.366	−0.484	0.005	0.13
	6(*c*)										
K5	3(*a*)	0.9466 (3)	0.5591 (2)	−0.0018 (3)	0.9122	0.5851	−0.0021	0.484	−0.366	0.005	0.16
Y1	3(*a*)	0.12871 (6)	0.88764 (6)	−0.0135	0.09321	0.91451	0.0018	0.499	−0.378	−0.155	0.09
	6(*c*)										
Y4	3(*a*)	0.94137 (7)	0.05770 (7)	−0.0171 (2)	0.91451	0.09321	−0.0018	0.378	−0.499	−0.155	0.12

Table 4 (continued)

	Wyckoff position $P3_1$, $P3_121$	x	y	z*	x'	y'	z'	Δx	Δy	Δz	u^{33}
Y2	3(*a*)	0.28157 (7)	0.73104 (7)	−0.0238 (8)	0.24375	0.75554	−0.0082	0.531	−0.344	−0.158	0.09
	6(*c*)										
Y3	3(*a*)	0.78003 (7)	0.20592 (6)	−0.0074 (1)	0.75554	0.24375	0.0082	0.344	−0.532	−0.158	0.08
Y5	3(*a*)	0.45256 (7)	0.54579 (7)	−0.0215 (1)	0.41959	0.57477	−0.0096	0.464	−0.407	−0.120	0.11
	6(*c*)										
Y6	3(*a*)	0.60374 (7)	0.38662 (6)	−0.0024 (7)	0.57477	0.41959	0.0096	0.407	−0.464	−0.121	0.07
F1	3(*a*)	0.1304 (7)	0.9342 (7)	−0.2280 (9)	0.095	0.967	−0.270	0.50	−0.46	0.42	0.16
	6(*c*)										
F7	3(*a*)	0.000 (1)	0.059 (1)	0.312 (2)	0.967	0.095	0.270	0.46	−0.51	0.42	0.25
F2	3(*a*)	0.0692 (8)	0.8779 (8)	0.199 (1)	0.096	0.963	0.197	−0.38	−1.20	0.02	0.17
	6(*c*)										
F8	3(*a*)	0.0489 (8)	0.1223 (8)	−0.195 (2)	0.963	0.096	−0.197	1.20	0.37	0.02	0.24
F3	3(*a*)	0.2105 (8)	0.5934 (8)	0.125 (1)	0.2366	0.5162	0.123	−0.37	1.09	0.02	0.18
	6(*c*)										
F5	3(*a*)	0.7372 (5)	0.2023 (5)	0.2133 (8)	0.7634	0.2796	0.211	−0.37	−1.09	0.02	0.11
F4	3(*a*)	0.334 (1)	0.7286 (7)	0.309 (1)	0.301	0.7594	0.263	0.46	−0.43	0.46	0.21
	6(*c*)										
F6	3(*a*)	0.7901 (6)	0.2684 (6)	−0.2163 (9)	0.7594	0.301	−0.263	0.43	−0.46	0.47	0.13
F9	3(*a*)	0.3954 (6)	0.5413 (6)	0.1908 (8)	0.4257	0.6267	0.1695	−0.43	−1.20	0.22	0.13
	6(*c*)										
F11	3(*a*)	0.5440 (6)	0.2863 (6)	0.1852 (8)	0.5743	0.2010	0.1639	−0.43	1.20	0.22	0.13
F10	3(*a*)	0.4618 (7)	0.5950 (6)	0.7645 (8)	0.4281	0.6799	0.7172	0.47	−1.19	0.48	0.14
	6(*c*)										
F12	3(*a*)	0.6057 (7)	0.3368 (7)	0.6637 (1)	0.5720	0.2519	0.6161	0.47	1.19	0.48	0.16
F13	3(*a*)	0.7727 (6)	0.7346 (6)	−0.283 (1)	0.7495	0.7740	−0.256	0.33	−0.55	−0.27	0.14
	6(*c*)										
F14	3(*a*)	0.8133 (9)	0.7262 (6)	0.229 (1)	0.7740	0.7495	0.256	0.55	−0.33	−0.27	0.16
F15	3(*a*)	0.2533 (6)	0.2289 (6)	0.2593 (1)	0.2242	0.2625	0.253	0.41	−0.47	0.06	0.15
	6(*c*)										
F16	3(*a*)	0.8050 (6)	0.0719 (6)	0.0864 (8)	0.7758	0.0383	0.080	0.41	0.47	0.06	0.14
F17	3(*a*)	0.1339 (6)	0.3916 (6)	0.2234 (8)	0.1094	0.4193	0.2565	0.34	−0.39	−0.33	0.12
	6(*c*)										
F24	3(*a*)	0.4469 (7)	0.0849 (6)	−0.2896 (9)	0.4193	0.1094	−0.2565	0.39	−0.34	−0.33	0.15
F18	3(*a*)	0.0941 (7)	0.4031 (8)	−0.284 (1)	0.0817	0.4431	−0.254	0.17	−0.56	−0.30	0.16
	6(*c*)										
F23	3(*a*)	0.4830 (7)	0.0692 (7)	0.2240 (9)	0.4431	0.0817	0.254	0.56	−0.18	−0.30	0.14
F19	3(*a*)	0.1535 (6)	0.7561 (7)	0.0808 (9)	0.1073	0.7188	0.0790	0.65	0.53	0.02	0.14
	6(*c*)										
F21	3(*a*)	0.9390 (6)	0.5741 (7)	0.2561 (9)	0.8927	0.6115	0.2543	0.65	−0.53	0.02	0.14
F20	3(*a*)	0.5874 (6)	0.8816 (7)	0.2576 (9)	0.5595	0.9127	0.2555	0.39	−0.44	0.02	0.13
	6(*c*)										
F22	3(*a*)	0.9438 (6)	0.5316 (6)	−0.2534 (8)	0.9127	0.5595	−0.2555	0.44	−0.39	0.02	0.12

† See footnote **1** for equivalent positions.

References

Abrahams, S. C. (2003). *Acta Cryst.* B**59**, 541–556.

Averbuch-Pouchot, M. T., Durif, A. & Guitel, J. C. (1978). *Acta Cryst.* B**34**, 3725–3727.

Le Fur, Y., Khaidukov, N. M. & Aléonard, S. (1992). *Acta Cryst.* C**48**, 978–982.

Pohl, J., Pohl, D. & Adiwidjaja, G. (1992). *Acta Cryst.* B**48**, 160–166.

Shamsuzzoha, M. & Lucas, B. W. (1982). *Acta Cryst.* B**38**, 2353–2357.

Teske, Ch. L. (1979). *Z. Naturforsch. Teil B*, **34**, 386–389.