

## addenda and errata

Systematic prediction of new ferroelec-  
trics 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  $\text{Cu}_2\text{BaGeS}_4$  at room temperature (Teske, 1979), with hypothetical  $x'$ ,  $y'$  and  $z'$  coordinates and  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u^{33}$
Cu1	3(a) 6(c)†	0.2587 (6)	0.2487 (6)	0.2487 (2)	0.2960	0.3099	0.2565	−0.232	−0.380	−0.121	0.09
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) 6(c)	0.3703 (9)	0.1870 (9)	0.1076 (3)	0.2586	0.2971	0.0863	0.694	−0.684	0.331	0.07
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) 6(c)	0.0035 (9)	0.4292 (9)	−0.0023 (3)	−0.1183	0.5466	0.0034	0.758	−0.730	−0.089	0.10
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  $\text{K}_2\text{HCr}_2\text{AsO}_{10}$  at room temperature (Averbuch-Pouchot *et al.* 1978), with hypothetical  $x'$ ,  $y'$  and  $z'$  coordinates and  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  and  $u_{\text{eq}}$  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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u_{\text{eq}}$
Cr1	3(a) 6(c)†	0.4278 (3)	0.4243 (3)	0.2403	0.4242	0.4217	0.2460	0.028	0.020	−0.083	0.14
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) 6(c)	0.356 (2)	0.186 (2)	0.2975 (8)	0.3465	0.188	0.3077	0.073	−0.015	−0.149	0.17
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) 6(c)	0.625 (2)	0.480 (2)	0.1805 (11)	0.6148	0.4615	0.1794	0.078	0.143	0.016	0.21
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) 6(c)	0.469 (3)	0.594 (2)	0.3163 (9)	0.487	0.584	0.3198	−0.139	0.077	−0.051	0.22
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) 6(c)	0.245 (2)	0.390 (2)	0.1713 (10)	0.237	0.398	0.1835	0.066	−0.062	−0.179	0.20
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) 6(c)	0.087 (2)	0.097 (2)	0.4436 (8)	0.023	0.057	0.4170	0.497	0.312	0.390	0.19
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.

# addenda and errata

**Table 3**

(a) Atomic positions for RbNO<sub>3</sub> in phase IV (Shamsuzzoha & Lucas, 1982) at room temperature, with hypothetical  $x'$ ,  $y'$  and  $z'$  coordinates and  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u_{eq}$
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) 6(c)†	0.1184 (3)	0.2192 (3)	-0.0949	0.1706	0.3056	-0.1524	-0.55	-0.91	0.43	0.22
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) 6(c)	0.0962 (3)	0.2042 (3)	0.4369 (6)	0.1771	0.2935	0.3742	-0.85	-0.94	0.47	0.20
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) 6(c)	0.3371 (6)	0.5582 (5)	-0.0855 (8)	0.2773	0.6062	-0.0023	0.63	-0.51	-0.62	0.25
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) 6(c)	0.3964 (5)	0.4704 (5)	0.1331 (8)	0.3521	0.4717	0.1555	0.47	-0.01	-0.17	0.25
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) 6(c)	0.0581 (5)	0.2465 (5)	0.3000 (8)	0.0930	0.3085	0.3191	-0.37	-0.65	-0.14	0.25
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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u_{eq}$
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) 6(c)	0.1231 (1)	0.2201 (1)	-0.1049	0.1696	0.3098	-0.1455	-0.49	-0.94	0.30	0.18
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) 6(c)	0.1009 (8)	0.2047 (8)	0.4167 (15)	0.1673	0.2990	0.3795	-0.85	-0.99	0.28	0.17
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) 6(c)	0.2283 (7)	0.5505 (7)	-0.1669 (8)	0.2799	0.6630	-0.1969	-0.54	1.18	-0.22	0.22
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) 6(c)	0.3927 (8)	0.4597 (7)	0.0886 (10)	0.3328	0.4692	0.1499	0.63	-0.10	-0.45	0.25
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) 6(c)	0.0637 (7)	0.2519 (7)	0.2870 (8)	0.0836	0.3223	0.3350	-0.21	-0.74	-0.36	0.22
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<sub>4</sub> at room temperature (Le Fur *et al.*, 1992), with hypothetical  $x'$ ,  $y'$  and  $z'$  coordinates and  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u^{33}$
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) 6(c)†	0.1050 (2)	0.3945 (3)	-0.0331 (4)	0.0851	0.4247	-0.0034	0.280	-0.425	-0.300	0.17
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) 6(c)	0.6111 (2)	0.8778 (2)	0.0028 (3)	0.5851	0.9122	0.0021	0.366	-0.484	0.005	0.13
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) 6(c)	0.12871 (6)	0.88764 (6)	-0.0135	0.09321	0.91451	0.0018	0.499	-0.378	-0.155	0.09
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 $P3_1, P3_121$	$x$	$y$	$z^*$	$x'$	$y'$	$z'$	$\Delta x$	$\Delta y$	$\Delta z$	$u^{33}$
Y2	3(a) 6(c)	0.28157 (7)	0.73104 (7)	-0.0238 (8)	0.24375	0.75554	-0.0082	0.531	-0.344	-0.158	0.09
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) 6(c)	0.45256 (7)	0.54579 (7)	-0.0215 (1)	0.41959	0.57477	-0.0096	0.464	-0.407	-0.120	0.11
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) 6(c)	0.1304 (7)	0.9342 (7)	-0.2280 (9)	0.095	0.967	-0.270	0.50	-0.46	0.42	0.16
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) 6(c)	0.0692 (8)	0.8779 (8)	0.199 (1)	0.096	0.963	0.197	-0.38	-1.20	0.02	0.17
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) 6(c)	0.2105 (8)	0.5934 (8)	0.125 (1)	0.2366	0.5162	0.123	-0.37	1.09	0.02	0.18
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) 6(c)	0.334 (1)	0.7286 (7)	0.309 (1)	0.301	0.7594	0.263	0.46	-0.43	0.46	0.21
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) 6(c)	0.3954 (6)	0.5413 (6)	0.1908 (8)	0.4257	0.6267	0.1695	-0.43	-1.20	0.22	0.13
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) 6(c)	0.4618 (7)	0.5950 (6)	0.7645 (8)	0.4281	0.6799	0.7172	0.47	-1.19	0.48	0.14
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) 6(c)	0.7727 (6)	0.7346 (6)	-0.283 (1)	0.7495	0.7740	-0.256	0.33	-0.55	-0.27	0.14
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) 6(c)	0.2533 (6)	0.2289 (6)	0.2593 (1)	0.2242	0.2625	0.253	0.41	-0.47	0.06	0.15
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) 6(c)	0.1339 (6)	0.3916 (6)	0.2234 (8)	0.1094	0.4193	0.2565	0.34	-0.39	-0.33	0.12
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) 6(c)	0.0941 (7)	0.4031 (8)	-0.284 (1)	0.0817	0.4431	-0.254	0.17	-0.56	-0.30	0.16
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) 6(c)	0.1535 (6)	0.7561 (7)	0.0808 (9)	0.1073	0.7188	0.0790	0.65	0.53	0.02	0.14
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) 6(c)	0.5874 (6)	0.8816 (7)	0.2576 (9)	0.5595	0.9127	0.2555	0.39	-0.44	0.02	0.13
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.* **B59**, 541–556.  
 Averbuch-Pouchot, M. T., Durif, A. & Guitel, J. C. (1978). *Acta Cryst.* **B34**, 3725–3727.  
 Le Fur, Y., Khaidukov, N. M. & Aléonard, S. (1992). *Acta Cryst.* **C48**, 978–982.  
 Pohl, J., Pohl, D. & Adiwidjaja, G. (1992). *Acta Cryst.* **B48**, 160–166.  
 Shamsuzzoha, M. & Lucas, B. W. (1982). *Acta Cryst.* **B38**, 2353–2357.  
 Teske, Ch. L. (1979). *Z. Naturforsch. Teil B*, **34**, 386–389.