Letter to the Editor

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Space group and unit cell dimensions of bis(2-methyl benzothiozole) silver(I) perchlorate

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Bis(2-methyl benzothiozole) silver (1) perchlorate $[Ag(C_8H_7NS)_2ClO_4]$ crystals are white in colour and obtainable in the form of microcrystals. As it is not possible to grow suitable single crystals out of it, by ordinary means, the powder method of investigation has been employed to throw some light on its structure.

The finely powdered sample contained in a capillary tube is irradiated by filtered CuK_α radiation from an X-ray tube operated at 15mA and 30KV. The powder pattern was recorded by a 9 cm diameter camera in 10 hours A systematic procedure to fit the data (recorded in the table) to cubic, tetragonal and hexagonal systems after Azaroff *et al* (1958), D'Eye *et al* (1960) and Henry *et al* (1951) and to orthorhombic system after Lipson (1949) led to negative results Therefore the most general procedure due to Ito (1950) applicable to crystals of lower symmetry was applied for indexing the crystal

The equation relating the different parameters of the reciprocal cell of a monoclinic system is given by

$$Q_{hkl} = \frac{1}{d^2_{hkl}} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2lhc^*a^* \cos\beta^*$$

where $$\cos\beta^* = \frac{Q_{h0l} - Q_{h0\bar{l}}}{4lhc^*a^*}$$

The error in Q values are indicated in the table Taking the error into account, after a thorough search, the quantities 0.0196, 0.0356 and 0.0304 were chosen as reasonable choice for Q_{200}, Q_{020} and Q_{002} values. Study of Q_{h0l} and $Q_{h0\bar{l}}$ values shows that $\beta^* = 79°59'$.

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Table 1

No. of line	Intensity	dÅ	$Q_{hkl} = 1/d^2$ observed	Q_{hkl} computed	Indices
1	w	8.5422	0.0138±0 0003	0.0138	110
2	w	7.2546	0.0192±0.0004	0.0193	$11\bar{1}$
				0.0196	200
3	s	5.7176	0 0305±0.0004	0.0304	002
4	s	5.3160	0.0354±0.0004	0.0356	020
5	s	4.6677	0 0454±0.0004	0.0454	$30\bar{1}$
6	s	4.3728	0.0525±0.0005	0.0530	310
7	m	3.8921	0.0660±0 0005	0.0660	022
8	w	3.5391	0.0798±0 0005	0.0796	103
				0.0797	320
				0.0801	030
9	s	3 2963	0.0921±0.0005	0.0920	$40\bar{2}$
10	w	3.0898	0.1045±0.0005	0.1040	043
11	w	2.9508	0.1149±0.0006	0.1152	123
12	vw	2.7696	0.1304±0.0006	0.1305	014
				0.1300	421
				0 1305	$41\bar{3}$
13	s	2.5399	0.1551±0.0006	0.1552	$52\bar{1}$
				0.1555	$23\bar{3}$
14	s	2.4541	0.1659±0.0006	0.1654	$24\bar{1}$
				0.1664	$40\bar{4}$
15	vw	2.2964	0.1896±0.0007	0.1900	005
16	m	2.0904	0.2288±0.0007	0 2295	342
17	m	1.9931	0.2518±0.0007	0.2517	$63\bar{2}$
				0.2515	$63\bar{1}$
				0.2521	433
18	m	1.7830	0 3146±0.0008	0.3140	$64\bar{2}$
				0.3144	443
				0.3145	$45\bar{2}$
				0.3153	$81\bar{2}$
19	w	1.6022	0.3195±0.0008	0.3193	415
				0.3202	730
20	w	1.5824	0.3994±0.0008	0.3988	460
				0.3989	650
				0.4000	163
21	vw	1.3923	0 5156±0.0009	0.5157	173
				0.5157	$32\bar{8}$

Table 1 (*Contd.*)

No of line	Intensity	dÅ	$Q_{hkl} = 1/d^2$ observed	Q_{hkl} computed	Indices
22	w	1 3125	0.5850±0.0009	0 5800	$18\bar{1}$
				0.5804	$56\bar{5}$
				0.5806	308
23	vvw	1.2893	0.6016±0.0009	0.6009	11,1,3
				0.6010	281
				0.6015	546
				0.6016	$10\bar{9}$
				0.6018	11,1,0
				0.6019	706
				0.6020	914
24	w	1.2502	0 6398±0.0009	0.6394	109
				0 6397	$37\bar{5}$
				0 6400	$44\bar{8}$

Therefore the reciprocal cell dimensions are

$$a^* = 0.07000$$

$$b^* = 0.09434 \quad \text{and} \quad \beta^* = 79°59'$$

$$c^* = 0.08718$$

The corresponding values of direct cell dimensions are

$$a = 14.507\text{Å}$$

$$b = 10.600\text{Å} \quad \text{and} \quad \beta = 100°1'$$

$$c = 11.647\text{Å}$$

The Buerger test establishes the cell dimensions to be reduced ones There is a good agreement between the observed density $\rho_0 = 1\ 4041$ gm cm^{-3} and calculated density $\rho_c = 1\ 4282$ gm cm^{-3} The crystal is built up of trimolecular unit cell and the probable space group assigned to it is P_2 or P_2/m or P_m. Thus the crystal is established to be a monoclinic one and happens to be of the same system as that of $[Ag(C_9H_7N)_2ClO_4]$ studied by Ratho *et al* (1967).

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