INDEXING POWDER PATTERNS FOR HIGH PRESSURE SULPHUR, PHASES I AND III*

By R. B. Roof†

Three high pressure phases of sulphur have been reported by Geller (1966). The material designated fibrous sulphur (phase II) was indexed by Geller on the basis of single crystal type photographs, first (Geller 1966) as *C*-centered orthorhombic and later (Geller and Lind 1969) as monoclinic. The structure of this material has also been determined (Lind and Geller 1969). However, no unit cells or structures have been proposed for phases I and III.

The present note lists the indexing results obtained for high pressure sulphur, phases I and III, by applying to Geller's original data the methods of Haendler and Cooney (1963) as incorporated in a computer program by Roof (1968). Table 1(*a*) lists the d values, the relative intensities I_{rel}, and the derived Q_0 values for high pressure sulphur, phase I. A monoclinic cell with $a = 7{\cdot}086 \pm 0{\cdot}011$, $b = 6{\cdot}215 \pm 0{\cdot}009$, $c = 5{\cdot}319 \pm 0{\cdot}008$ Å, and $\beta = 96{\cdot}19° \pm 0{\cdot}09°$ is proposed for this material. The calculated Q_c values and the associated *hkl* indices for this cell are included in Table 1(*a*). The standard deviations of the lattice constants were determined by using the methods of Vogel and Kempter (1961) applied to the monoclinic crystal system.

As reported by Geller (1966) the powder pattern for high pressure sulphur, phase III, is very similar to that obtained for phase I. For phase III the d values 3·53, 2·66, and 2·32 are missing and all reflections with d values less than 2·32 are broader in appearance than for phase I. The cell proposed in this instance is monoclinic with $a = 6{\cdot}299 \pm 0{\cdot}008$, $b = 7{\cdot}240 \pm 0{\cdot}009$, $c = 5{\cdot}673 \pm 0{\cdot}008$ Å, and $\beta = 95{\cdot}51° \pm 0{\cdot}07°$. Table 1(*b*) lists the relevant data for d, I_{rel}, Q_0, Q_c, and *hkl*.

An examination of the indices listed in Table 1 indicates that no specific space group is favoured. The absence of systematic extinctions indicating *C* centering or *c* glide planes leaves the space groups $P2$, $P2_1$, Pm, $P2/m$, or $P2_1/m$ as possible for these materials. The close similarity between the cells proposed for phases I and III of high pressure sulphur would indicate that relatively minor differences may exist in their structures.

References

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† Visiting Lecturer at the Department of Physics, University of Western Australia, Nedlands, W.A.; permanent address: Los Alamos Scientific Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87544, U.S.A.

TABLE 1

INDEXING RESULTS FOR HIGH PRESSURE SULPHUR, PHASES I AND III

d	I_{rel}	Q_0	Q_c	hkl	d	I_{rel}	Q_0	Q_c	hkl
				(*a*) *Phase I*					
4·47	s	0·0500	0·0502	$10\bar{1}$	1·75	m	0·3265	0·3247	$10\bar{3}$
			0·0617	011	1·72	vw	0·3380	0·3378	$23\bar{1}$
4·05	vs	0·0610	0·0618	101				0·3380	321
3·53	vvs	0·0803	0·0806	200				0·3477	013
3·04	vvs	0·1082	0·1065	210	1·69	w–m	0·3501	0·3483	410
			0·1394	021				0·3503	222
2·66	m–s	0·1413	0·1430	002				0·3506	$11\bar{3}$
2·32	m	0·1858	0·1842	220	1·65	vw	0·3673	0·3677	203
			0·1998	$30\bar{1}$				0·3846	$13\bar{2}$
2·24	w	0·1992	0·2005	$20\bar{2}$	1·61	w–m	0·3858	0·3849	312
			0·2007	112				0·3852	113
2·09	m–s	0·2289	0·2264	$21\bar{2}$	1·57	w–m	0·4057	0·4072	411
			0·2316	221				0·4078	132
2·07	m	0·2334	0·2330	030	1·55	w	0·4162	0·4142	040
			0·2344	301				0·4143	330
			0·2466	022	1·53	m	0·4272	0·4260	420
2·02	m	0·2451	0·2467	202				0·4283	$12\bar{3}$
1·93	w–m	0·2685	0·2688	031	1·50	vw	0·4444	0·4450	$41\bar{2}$
			0·2832	$13\bar{1}$				0·4626	322
1·88	w	0·2829	0·2849	320	1·47	vw	0·4628	0·4629	123
			0·3034	$32\bar{1}$				0·4630	213
1·82	m	0·3019	0·3041	$22\bar{2}$				0·4644	$14\bar{1}$
			0·3136	230	1·41	w	0·5030	0·5038	500
1·78	m	0·3156	0·3155	$31\bar{2}$	1·33	m	0·5653	0·5658	$14\bar{2}$
				(*b*) *Phase III*					
4·47	s	0·0500	0·0505	011	1·61	w–m	0·3858	0·3870	302
			0·0514	$10\bar{1}$	1·57	w–m	0·4057	0·4061	312
4·05	vs	0·0610	0·0622	101				0·4070	400
3·04	vvs	0·1082	0·1077	021				0·4158	$33\bar{1}$
2·24*	w	0·1992	0·1986	$22\bar{1}$	1·55	w	0·4162	0·4166	203
2·09	m–s	0·2289	0·2290	300				0·4167	$40\bar{1}$
2·07	m	0·2334	0·2339	131				0·4261	410
2·02	m	0·2451	0·2441	$30\bar{1}$	1·53	m	0·4272	0·4276	$24\bar{1}$
1·93	w–m	0·2685	0·2680	212				0·4277	$22\bar{3}$
			0·2819	$22\bar{2}$	1·50	vw	0·4444	0·4453	$14\bar{2}$
1·88	w	0·2829	0·2822	003				0·4623	$30\bar{3}$
1·82	m	0·3019	0·3013	013	1·47	vw	0·4628	0·4630	$13\bar{3}$
1·78	m	0·3156	0·3158	231				0·4634	322
1·75	m	0·3265	0·3253	222	1·41	w	0·5030	0·5018	004
1·72	vw	0·3380	0·3367	041				0·5026	150
1·69	w–m	0·3501	0·3514	$20\bar{3}$	1·33*	m	0·5653	0·5654	$42\bar{2}$
			0·3675	141					
1·65	vw	0·3673	0·3676	$12\bar{3}$					

* All reflections with $2{\cdot}24 \geqslant d \geqslant 1{\cdot}33$ are broader than for phase I.