

Taking the value of $\Delta H_{298}^0(\text{CN}^-g)$ as 10.6 kg.cal./mole and $\Delta H_{298}^0(\text{CN}g)$ as 92 kg.cal./mole (Skinner, 1958), the electron affinity of the cyanide radical $E_{298}^0(\text{CN})$ is found to be 81.4 kg.cal./mole. This value for the electron affinity is probably reliable to within ± 3 kg.cal.

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Acta Cryst. (1961). **14**, 548

The lattice constants of orthorhombic sulfur and revision of the interatomic distances. By AIMERY CARON and JERRY DONOHUE, *Department of Chemistry, University of Southern California, Los Angeles, California, U.S.A.*

(Received 18 November 1960)

As a part of his careful refinement of the parameters in orthorhombic sulfur, Abrahams (1955) also redetermined the lattice constants from precession photographs corrected for film shrinkage. The values he obtained are:

$$a = 10.437, b = 12.845, c = 24.369 \text{ \AA}, \text{ all } \pm 0.010 \text{ \AA}$$

(at room temperature). These values give a calculated density of 2.086 g.cm.⁻³. Swanson *et al.* (1960), hereinafter called NBS, have recently reported significantly different values, namely,

$$a = 10.468, b = 12.870, c = 24.49 \text{ \AA},$$

at 25°C. These were obtained by a least squares treatment of resolved lines in the latter half of the powder pattern as recorded with a Geiger counter diffractometer. The standard errors were not given. The corresponding calculated density is 2.065 g.cm.⁻³, in far better agreement with the observed value of 2.069 g.cm.⁻³ (Batuecas & Losa, 1951), a fact highly suggestive that the earlier values were subject to systematic error.

As a check on the values reported by NBS, and to obtain a measure of their precision, we have reexamined their data, and have obtained, by least squares, the following values:

$$a = 10.467 \pm 0.001, b = 12.870 \pm 0.001, \\ c = 24.493 \pm 0.003 \text{ \AA}$$

(at 25°C.). These values were obtained in the following way: (i) The lattice constants of NBS were used to calculate values of $\sin \theta/\lambda$ for all reflections within the Cu $K\alpha$ sphere; (ii) values of pF_0^2 were calculated from the single crystal data of Abrahams; (iii) all of the lines observed by NBS were assigned indices on the basis of (i) and (ii); (iv) data for lines which clearly were not unresolved multiplets were then treated by least squares to obtain values for the lattice constants, and their standard errors. This treatment made use of 60 resolved lines. A drift correction was not used because no drift

was found upon comparison of observed and calculated spacings. Our indexing is not always the same as that of NBS as shown in Table 1, which lists all lines where the indexing differs, regardless of whether the line was included in the least squares. It thus appears that their treatment omitted some lines which could have been included, and vice versa. It is interesting that although exactly the same data were not used by us and by NBS, the resulting values for the lattice constants are sensibly the same, due to compensating errors. The very small standard errors of the revised lattice constants do not, of course, include any systematic errors in their experiment, but the high standard of accuracy which characterizes the work from that laboratory together with the much better agreement that the revised lattice constants give with the experimental density leaves little doubt that they are in fact more accurate than those of Abrahams, or, for that matter, than those of earlier investigators cited by NBS.

Abrahams (1961) has very recently reported new values for the positional parameters as obtained from a least squares treatment which allowed for thermal anisotropy. These new parameters differ by an average of 0.004 Å from the old, and the average S-S bond distance changes from 2.037 Å to 2.041 Å. The present revision of the lattice constants leads to the following revised values of the molecular constants:

Bond lengths	Bond angles	Torsion angles
S_1-S_3 2.046 Å	$S'_1-S_1-S_3$ 108° 13'	$S_1-S_3-S_2-S_4$ 101° 6'
S_2-S_3 2.050	$S_3-S_2-S_4$ 107° 58'	$S'_1-S_1-S_3-S_2$ 99° 7'
S_2-S_4 2.048	$S_1-S_3-S_2$ 107° 11'	$S_3-S_2-S_4-S'_4$ 98° 3'
$S_1-S'_1$ 2.044	$S'_4-S_4-S_2$ 108° 54'	$S_3-S_1-S'_1-S'_3$ 97° 19'
$S_4-S'_4$ 2.052		$S_2-S_4-S'_4-S'_2$ 95° 1'
Av. 2.048 \pm 0.002 ₄	107° 54' \pm 36'	98° 37' \pm 2° 9'

The quoted uncertainties are standard errors as calculated on the assumption that we are looking at several measurements of the same quantity, with values involving the primed atoms being given half weight. The angular

Table 1. Indexing of selected lines

Line no.	NBS			Present work		
	Observed sin θ/λ	I/I_0	hkl	Calculated sin θ/λ	pF_0^2	hkl
13	0.1553	50	{ 206 040	0.1553	146	206
				0.1554	50	040
				0.1556	109	117
44	0.2743	2	2,2,12	0.2738	58	2,4,10
				0.2742	116	2,2,12
48	0.2902	7	4,2,10	0.2901	97	0,4,12
				0.2903	53	4,2,10
51	0.3018	2	357*	0.3017	58	537
53	0.3041	3	462	0.3038	22	519
				0.3041	36	3,1,13
				0.3042	2	462
56	0.3108	1	080	0.3107	48	4,0,12
				0.3108	1	080
				0.3109	0	177
57	0.3111	2	{ 177 2,2,14	0.3112	160	2,2,14
				0.3243	4	555
				0.3243	62	2,6,10
61	0.3242	<1	{ 555 2,6,10	0.3474	116	4,4,12
				0.3475	20	286
68	0.3475	1	286	0.3474	116	4,4,12
				0.3475	20	286
69	0.3482	1	646	0.3479	29	5,3,11
				0.3483	44	646
72	0.3594	1	733	0.3591	22	5,1,13
				0.3594	36	733
75	0.3671	<1	{ 573 482	0.3671	10	573
				0.3671	32	482
				0.3674	40	195
76	0.3687	1	0,6,14	0.3685	48	735
				0.3688	34	0,6,14
77	0.3694	2	660	0.3692	96	1,3,17
				0.3694	101	660

* (A typographical error, private communication, H. E. Swanson to co-editor.)

quantities do not differ appreciably from those given by Abrahams, but the average bond distance is 0.007 Å, or 2.9 σ , larger than his value.

This work was supported in part by the Office of Ordnance Research, U.S. Army. Some of the calculations were performed in the Western Data Processing Center. We wish to thank Dr Abrahams for sending us his manuscript in advance of publication.

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Acta Cryst. (1961). **14**, 549

Cell dimensions and space group of bismuth(I) chloro-aluminate. By H. A. LEVY, P. A. AGRON, M. D. DANFORD and R. D. ELLISON, *Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee,* U.S.A.*

(Received 29 November 1960)

The cell dimensions and probable space group of bismuth(I) chloroaluminate were determined from crystals

* Work performed for the U.S. Atomic Energy Commission at the Oak Ridge National Laboratory, operated by the Union Carbide Corporation, Oak Ridge, Tennessee.

of this compound (Corbett & McMullen, 1956) grown from the melt under helium. Because the compound is unstable in the presence of moisture, single crystals were transferred to thin-walled glass capillary tubes under mineral oil; powder diffraction samples were prepared in a dry box and kept in sealed enclosures while being used.