Table 1. *Indexing of selected lines*

	NBS			Present work		
Line no.	Observed $\sin\theta/\lambda$	I/I_0	*hkl*	Calculated $\sin\theta/\lambda$	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
61	0·3242	< 1	{555, 2,6,10}	0·3243	62	2,6,10
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 2·9σ, larger than his value.

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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.*

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

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Table 1. *Interplanar spacings for* BiAlCl$_4$

(Hexagonal indices)

h k l	d_c	d_o	I_0
0 0 3	9·997 Å		
1 0 1	9·699		
0 1 2	8·462	8·456 Å	100*
Impurity		6·970	~5†
1 0 4	6·051		
1 1 0	5·918	5·913	32*
0 1 5	5·177		
1 1 3	5·092	5·090	7*
0 2 1	5·051		
0 0 6	4·998	5·001	7
2 0 2	4·849	4·852	31*
Impurity		4·699	~5†
0 2 4	4·231		
1 0 7	3·953		
2 0 5	3·896		
2 1 1	3·842	3·840	15
1 1 6	3·818		
1 2 2	3·751		
0 1 8	3·521		
2 1 4	3·442	3·440	7*
3 0 0	3·416		
Impurity		3·336	~5†
0 0 9	3·332		
0 2 7	3·287		
1 2 5	3·254	3·254	10*
3 0 3	3·233		
2 0 8	3·026	3·025	13*
2 2 0	2·959		
1 1 9	2·904		
1 0 10	2·878 Å	2·877 Å	7
2 1 7	2·873		
2 2 3	2·837	2·839	36
1 3 1	2·830		
3 0 6	2·821		
3 1 2	2·793		
1 2 8	2·694	2·695	5*
1 3 4	2·658	2·659	16*
0 1 11	2·635		
0 2 10	2·588		
3 1 5	2·569		
4 0 1	2·553		
2 2 6	2·546	2·546	14
0 4 2	2·526		
0 0 12	2·499	2·500	8*
4 0 4	2·425		
2 0 11	2·407		
3 0 9	2·385		
2 1 10	2·371		
1 3 7	2·369		
0 4 5	2·356		
3 2 1	2·344	2·346	7*
2 3 2	2·323		
1 1 12	2·302		
3 1 8	2·265	2·264	7*
1 0 13	2·251		
3 2 4	2·244		
4 1 0	2·237	2·236	5
1 2 11	2·230		

* Observations that were used in the least squares refinement of the cell.

† The three reflections ascribed to impurity appeared with varying intensity on different patterns.

Single crystal diffraction patterns prepared on the precession camera showed the crystal to be rhombohedral. Powder patterns obtained using Cu $K\alpha$ radiation with a special diffractometer ordinarily used for liquids (Agron, Danford, Bredig, Levy & Sharrah, 1957) were indexed on the basis of the cell found from the single crystal data. The powder data, corrected for instrumental errors by the use of Y_2O_3 ($a_0 = 10{\cdot}594$ Å) as an internal standard, were used to obtain a least squares refinement of the cell dimensions. (The cell constant of Y_2O_3 had previously been refined using powdered Ni metal ($a_0 = 3{\cdot}525$ Å) as an internal standard). The hexagonal unit cell of BiAlCl$_4$ is

$$a = 11{\cdot}835 \pm 0{\cdot}003,\ c = 29{\cdot}991 \pm 0{\cdot}009\ \text{Å}\ ,$$

corresponding to the rhombohedral cell

$$a = 12{\cdot}109 \pm 0{\cdot}002\ \text{Å},\ \alpha = 58^\circ\ 29' \pm 2'.$$

The observed interplanar spacings are compared with those calculated on the basis of this cell in Table 1.

The usual methods of density measurement were not feasible because of the instability of the compound in the presence of most supporting liquids. A rough value of 2·9 g.cm.$^{-3}$ (probably a lower limit) was obtained by weighing and measuring, in the dry box, a cylinder cast from the melt. This value indicates that the number of molecules in the rhombohedral cell is probably 6, for which the calculated density is 3·11 g.cm.$^{-3}$.

Precession patterns of the hexagonal levels $h0l$, $h1l$, and $h2l$ show the systematic absences

$$h\bar{h}l \text{ absent if } l \neq 2n\ ,$$
$$hkl \text{ absent if } -h+k+l \neq 3n\ .$$

The space groups consistent with these absences are $R3c$ and $R\bar{3}c$. Since the general positions of $R\bar{3}c$ are 12-fold (rhombohedral cell), and the 6-fold special positions have at most one variable parameter, it is not possible, on the basis of this space group, to find positions for the aluminum and chlorine ions that accommodate the expected tetrahedra of $AlCl_4^-$. The probable space group is, then, $R3c$.

Diffraction studies of the melt and considerations of the probable arrangement of bismuth(I) in a trimeric ion in both the solid and liquid states are reported elsewhere (Levy, Bredig, Danford & Agron, 1960).

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