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Refinement of the crystal structure of arsenic tribromide

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Auszug

Bericht über eine Verfeinerung der Kristallstruktur von $AsBr_3$ (bis zu $R = 0.143$).

Abstract

Refinement of the crystal structure of arsenic tribromide is reported.

A single crystal of arsenic tribromide was obtained by crystallizing the specimen in a sealed thin-walled capillary tube[1] (radius 0.31 mm). The intensity data were collected using equi-inclination Weissenberg technique. The intensities were measured visually and corrected for absorption and Lorentz-polarisation factors.

The coordinates reported by Singh and Swaminathan[2] gave an R factor of 0.26. Further refinement by the method of least squares was attempted on the Elliott 803B computer. The analytical expression of Forsyth and Wells[3] was used for atomic scattering factors. Only individual isotropic temperature factors were used. After four cycles of refinement the R factor dropped to 0.143. No attempt was made to apply anisotropic temperature factors.

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[1] A. K. Singh and S. Ramaseshan, A low temperature attachment to the Weissenberg goniometer. Proc. Indian Acad. Sci. **60** (1964) 20–24.

[2] A. K. Singh and S. Swaminathan, The crystal and molecular structure of arsenic tribromide at −10 °C. Curr. Sci. **33** (1964) 429–430.

[3] J. B. Forsyth and M. M. Wells, On an analytic approximation to the atomic scattering factor. Acta Crystallogr. **12** (1959) 412–415.

The observed and calculated structure amplitudes are listed in Table 1. The final positional and thermal parameters together with those reported by BRAEKKEN[4] and TROTTER[5] are given in Table 2.

Table 1. *Observed and calculated structure amplitudes*

h k l	$\|F_c\|$	F_o	h k l	$\|F_c\|$	F_o	h k l	$\|F_c\|$	F_o	h k l	$\|F_c\|$	F_o	h k l	$\|F_c\|$	F_o
2 0 0	89	86	1 7 0	67	77	2 3 1	99	97	9 9 1	19	11	0 5 2	3	< 20
4	10	60	2	17	14	3	61	63	0 10 1	42	27	1	50	57
6	155	188	3	88	98	4	92	93	1	39	30	2	15	< 17
8	18	13	4	18	14	5	54	54	2	70	75	3	36	42
10	62	56	5	7	< 10	6	39	40	3	26	10	4	24	29
12	37	22	6	88	98	7	49	51	4	26	28	5	32	32
14	13	12	7	24	16	8	39	34	5	5	< 7	6	89	96
1 1 0	19	16	8	23	21	9	21	27	6	33	27	7	12	25
2	59	57	9	89	87	10	27	19	7	31	26	8	9	< 12
3	97	104	10	7	6	11	34	23	8	59	49	9	41	26
4	100	110	11	10	6	12	22	13	9	19	11	10	6	< 8
5	27	27	0 8 0	169	200	0 4 1	20	14	0 11 1	24	12	11	6	< 6
6	160	180	1	17	15	1	91	103	1	68	68	0 6 2	3	< 17
7	5	11	2	11	10	2	33	27	2	28	22	1	20	< 17
8	31	31	3	39	37	3	88	90	3	20	19	2	20	35
9	82	89	4	8	8	4	51	58	4	34	31	3	101	105
10	6	< 9	5	21	15	5	147	161	5	29	20	4	23	17
11	1	< 10	6	67	65	6	42	46	6	18	14	5	52	61
12	64	46	7	35	31	7	59	59	7	22	16	6	7	< 15
0 2 0	103	97	8	25	19	8	12	< 9	8	21	14	7	3	< 10
1	21	17	9	6	8	9	40	36	2 0 2	64	60	8	3	< 10
2	59	38	10	14	7	10	12	< 8	3	2	< 20	9	11	< 10
3	242	242	1 9 0	36	37	11	52	37	4	3	< 16	10	5	< 8
4	26	19	2	14	8	12	13	< 6	5	3	< 14	0 7 2	11	< 15
5	50	61	3	33	35	0 5 1	46	47	6	69	52	1	49	66
6	29	19	4	25	22	1	95	104	7	8	< 12	2	11	14
7	14	14	5	30	24	2	101	110	8	59	58	3	19	16
8	37	31	6	42	42	3	50	60	9	3	< 12	4	20	15
9	16	13	7	2	< 9	4	93	100	10	1	< 12	5	13	14
10	28	26	8	10	< 8	5	54	53	11	5	< 10	6	75	79
11	35	25	0 10 0	43	53	6	19	18	12	12	< 10	7	29	25
12	7	< 7	1	10	7	7	49	48	1 1 2	24	17	8	21	21
1 3 0	61	44	2	58	68	8	19	15	2	58	50	9	27	16
2	67	52	3	88	102	9	25	21	3	84	89	10	7	10
3	61	64	4	20	17	10	12	30	4	54	55	0 8 2	161	154
4	42	52	5	30	24	11	34	28	5	18	17	1	47	62
5	18	16	6	8	< 6	0 6 1	69	73	6	48	46	2	13	15
6	74	98	7	3	< 8	1	70	70	7	14	< 14	3	41	47
7	25	15	8	23	20	2	118	140	8	13	< 14	4	13	< 12
8	8	< 12	9	9	< 6	3	31	44	9	82	69	5	52	70
9	58	59	1 0 1	76	66	4	21	23	10	12	< 11	6	64	69
10	4	5	2	65	61	5	9	< 10	11	9	< 10	7	11	16
11	13	10	3	93	80	6	44	40	12	26	10	8	7	< 9
12	33	23	4	79	73	7	38	35	0 2 2	66	60	9	7	< 7
0 4 0	258	242	5	177	182	8	93	89	1	8	< 18	10	21	10
1	57	56	6	45	44	9	22	21	2	66	61	0 9 2	4	< 12
2	43	28	7	60	59	10	39	20	3	222	206	1	41	52
3	64	65	8	16	11	11	15	18	4	22	25	2	17	20
4	9	10	9	32	30	0 7 1	15	23	5	14	< 16	3	62	68
5	72	91	10	9	< 9	1	105	114	6	21	17	4	16	31
6	88	106	11	57	43	2	46	49	7	39	42	5	19	13
7	19	15	12	12	6	3	43	46	8	34	35	6	59	68
8	48	62	0 1 1	90	100	4	64	71	9	13	< 12	7	31	20
9	6	4	1	151	137	5	59	58	10	21	11	8	9	< 8
10	10	9	2	140	150	6	21	21	11	17	10	9	63	50
11	11	8	3	36	32	7	38	37	12	10	8	0 10 2	16	14
12	17	5	4	109	114	8	23	20	0 3 2	3	< 24	1	10	12
1 5 0	85	86	5	30	31	9	11	17	1	58	70	2	13	20
2	24	22	6	34	35	10	14	16	2	29	45	3	113	118
3	122	130	7	53	68	11	28	16	3	87	101	4	27	21
4	25	22	8	47	46	0 8 1	17	12	4	63	55	5	16	19
5	20	27	9	23	22	1	65	68	5	19	17	6	9	10
6	73	83	10	28	22	2	16	12	6	126	134	7	24	22
7	50	36	11	38	32	3	57	63	7	23	15	8	5	6
8	8	< 7	12	20	14	4	35	38	8	30	27	9	6	6
9	112	114	0 2 1	109	98	5	101	115	9	87	79	0 11 2	2	< 10
10	12	8	1	49	48	6	20	24	10	10	< 10	1	16	12
11	28	20	2	172	190	7	46	42	11	11	7	2	25	23
0 6 0	24	22	3	31	34	8	7	< 7	0 4 2	263	252	3	33	23
1	25	19	4	76	76	9	32	26	1	25	25	4	6	< 9
2	44	49	5	4	< 9	10	15	8	2	32	43	5	8	< 9
3	251	221	6	77	85	0 9 1	33	35	3	40	51	6	33	30
4	22	19	7	21	23	1	51	56	4	21	< 17	7	4	6
5	46	42	8	113	117	2	69	65	5	30	29	0 12 2	15	20
6	2	< 8	9	26	26	3	43	50	6	97	99	1	7	< 9
7	54	50	10	46	36	4	60	63	7	31	29	2	3	< 9
8	14	11	11	9	< 8	5	34	37	8	1	< 12	3	1	< 7
9	11	11	12	19	10	6	13	< 8	9	3	< 10	4	1	< 7
10	2	< 7	0 3 1	93	64	7	35	24	10	36	25	5	3	< 5
11	10	8	1	141	137	8	12	< 7	11	12	12	6	7	6

[4] H. BRAEKKEN, Die Kristallstruktur von Arsen- und Antimontribromid. Kgl. Norske Videnskab Selskab 8 (1935) Nr. 10.

[5] J. TROTTER, The crystal structure of arsenic tribromide. Z. Kristallogr. **122** (1965) 230–236.

Table 2. *The final positional and thermal parameters*

Atom	Author	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	B
As	B	0.300	0.215	0.000	—	—	—	—
	T	0.3030	0.2118	0.0004	0.0013	0.0008	0.0059	1.16 Å^2
	A	0.3047	0.2129	0.0085	0.0007	0.0007	0.0050	3.44
Br(1)	B	0.307	0.377	−0.262	—	—	—	—
	T	0.3010	0.3794	−0.2824	0.0010	0.0007	0.0045	1.49
	A	0.3022	0.3799	−0.2643	0.0008	0.0007	0.0040	2.67
Br(2)	B	0.133	0.123	−0.262	—	—	—	—
	T	0.1380	0.1198	−0.2752	0.0010	0.0008	0.0053	1.79
	A	0.1387	0.1198	−0.2604	0.0008	0.0007	0.0060	3.00
Br(3)	B	0.482	0.123	−0.250	—	—	—	—
	T	0.4825	0.1307	−0.2504	0.0010	0.0008	0.0071	1.96
	A	0.4831	0.1318	−0.2611	0.0008	0.0008	0.0062	2.97

The present coordinates and those reported by TROTTER[5] have been transformed to the set of axes chosen by BRAEKKEN[4].

The axes of coordinates chosen by the different authors are related by

$$\begin{aligned} a_B &= \quad b_T = -b_A \\ b_B &= -c_T = \quad a_A \\ c_B &= -a_T = \quad c_A \end{aligned}$$

and the coordinates by

$$\begin{aligned} x_B &= y_T = \tfrac{3}{4} - y_A \\ y_B &= \tfrac{1}{2} - z_T = -\tfrac{1}{4} + x_A \\ z_B &= -x_T = -\tfrac{1}{4} + z_A \end{aligned}$$

B — BRAEKKEN[4], T — TROTTER[5] and A — the present author

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