$$c'_{ij}=\begin{bmatrix}\frac{1}{4}(3c_{11}+c_{12}+2c_{44}) & \frac{1}{4}(c_{11}+3c_{12}-2c_{44}) & c_{12} & 0 & 0 & 0\\ \frac{1}{4}(c_{11}+3c_{12}-2c_{44}) & \frac{1}{4}(3c_{11}+c_{12}+2c_{44}) & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}-c_{12})\end{bmatrix}, \qquad (5{\cdot}2)$$

where c_{11}, c_{12}, and c_{44} are the elastic constants of the cubic tensor.

References

Hearmon, R. F. S. (1961). *An Introduction to Applied Anisotropic Elasticity*, p. 72. Oxford University Press.

Love, A. E. H. (1944). *A Treatise on the Mathematical Theory of Elasticity*. New York: Dover Publications, 4th ed., pp. 157–160.

Weyl, H. (1946). *The Classical Groups*. Princeton, N. J.: Princeton University Press.

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Stereochemistry of Arsenic. IX. Diiodomethylarsine*

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Crystals of diiodomethylarsine, CH_3AsI_2, are monoclinic with eight molecules in a unit cell of dimensions $a=14{\cdot}45$, $b=4{\cdot}60$, $c=19{\cdot}97$ Å, $\beta=114°20'$, space group $C2/c$. The structure has been determined from partial three-dimensional data in normal and generalized projections along b, and values of the bond distances, valency angles, and intermolecular separations have been obtained.

As part of a series of investigations of compounds containing arsenic, the crystal and molecular structure of diiodomethylarsine has been determined; it is one of the few simple arsenic derivatives which are solid at room temperature.

Experimental

Crystals of diiodomethylarsine, which are yellow-orange, are volatile and melt at about room temperature. For recording the X-ray data, crystals were sealed in capillaries and cooled by a stream of nitrogen which was first passed through a coil immersed in an ice-bath. The unit-cell dimensions and space group were determined from various rotation, oscillation, Weissenberg (Cu $K\alpha$) and precession (Mo $K\alpha$) films.

Crystal data (at 5–10 °C; $\lambda(\text{Cu }K\alpha) = 1{\cdot}5418$ Å, $\lambda(\text{Mo }K\alpha) = 0{\cdot}7107$ Å).

Diiodomethylarsine, CH_3AsI_2; M, 343·85; m.p. 26 °C.

Monoclinic,

$a=14{\cdot}45$, $b=4{\cdot}60$, $c=19{\cdot}97$ Å, $\beta=114°\,20'$.

$U=1209{\cdot}5$ Å^3.

D_x (with $Z=8$) $=3{\cdot}8$ g.cm^{-3}.

Absorption coefficient, $\mu(\text{Cu }K\alpha)=939$ cm^{-1}.

$F(000)=1184$.

Absent reflexions: hkl when $(h+k)$ is odd, $h0l$ when l is odd.

Space group is Cc or $C2/c$. Analysis has proceeded satisfactorily in $C2/c$.

No suitable flotation medium was available for measuring the density; the density of the liquid, measured at room temperature by means of a density bottle, was 3·1 g.cm^{-3}, and, since it seemed likely that the solid at slightly reduced temperatures would have a higher density, $Z=8$ was assumed. This was confirmed by the structure analysis.

Intensity data for the $h0l$ and $h1l$ reflexions were recorded on Weissenberg films and estimated visually, and the structure amplitudes were derived as usual, the absolute scale being established later by correlation with the calculated structure factors. The crystal used was a needle, elongated along b, with a rectangular cross-section $0{\cdot}4\times0{\cdot}13$ mm, the (001) face being developed. The films were textbook examples (Buerger, 1960) of severe absorption effects, and corrections were applied (Howells, 1950). These absorption correction factors applied to the intensities varied from 1 to about 150, and since they are approximate, the accuracy of the measured structure amplitudes is probably rather limited. 140 independent $h0l$ reflexions (77% of the possible) and 213 $h1l$ reflexions (62%) were observed.

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* Part VIII: Camerman & Trotter (1963).

Table 1. *Measured and calculated structure factors*

H	K	L	F OBS	F CALC
0	0	2	255.9	-286.5
0	0	4	610.1	-710.7
0	0	6	553.3	598.5
0	0	8	123.2	167.3
0	0	10	316.4	-410.8
0	0	12	58.4	75.5
0	0	14	109.3	134.4
0	0	16	73.6	- 88.0
0	0	18	13.1	- 19.2
0	0	20	21.8	30.1
2	0	-24	11.0	13.8
2	0	-22	51.1	49.4
2	0	-20	94.8	- 83.8
2	0	-18	39.4	- 39.1
2	0	-16	185.8	188.3
2	0	-14	82.4	- 83.1
2	0	-12	219.4	-219.8
2	0	-10	256.6	287.5
2	0	- 8	109.5	111.4
2	0	- 6	315.0	-292.9
2	0	- 4	115.9	113.1
2	0	- 2	158.1	133.3
2	0	0	72.9	- 64.7
2	0	2	15.3	- 10.8
2	0	4	141.3	-150.3
2	0	6	43.7	31.9
2	0	8	96.2	122.8
2	0	10	126.9	-130.7
2	0	12	42.3	- 36.3
2	0	14	103.5	98.9
2	0	16	27.0	- 19.4
2	0	18	13.1	- 33.2
2	0	20	21.1	23.0
4	0	-22	6.6	3.8
4	0	-20	10.3	- 4.4
4	0	-18	24.8	- 28.3
4	0	-16	35.7	73.5
4	0	-14	43.0	37.8
4	0	-12	161.1	-194.3
4	0	-10	97.6	103.4
4	0	- 8	256.6	255.3
4	0	- 6	293.0	-365.4
4	0	- 4	159.9	-134.5
4	0	- 2	309.0	386.9
4	0	0	153.8	-155.2
4	0	2	148.0	-226.1
4	0	4	158.9	166.2
4	0	6	0.0	39.1
4	0	8	13.1	- 40.9
4	0	10	19.0	6.4
4	0	12	31.4	- 9.6
4	0	14	28.4	30.6
4	0	16	13.8	7.2
4	0	18	39.4	- 29.9
6	0	-24	10.3	13.8
6	0	-22	0.0	- 18.4
6	0	-20	0.0	- 4.8
6	0	-18	18.3	25.1
6	0	-16	0.0	- 7.7
6	0	-14	27.3	- 0.9
6	0	-12	71.5	- 59.5
6	0	-10	0.0	- 30.1
6	0	- 8	188.8	188.6
6	0	- 6	99.9	-133.5
6	0	- 4	188.6	-263.3
6	0	- 2	349.9	396.4
6	0	0	112.5	97.6
6	0	2	391.0	-427.4
6	0	4	207.1	186.6
6	0	6	271.2	254.3
6	0	8	242.0	-242.7
6	0	10	39.4	- 39.2
6	0	12	203.4	146.8
6	0	14	54.7	- 46.6
6	0	16	56.1	- 49.4
6	0	18	35.0	35.4
8	0	-24	47.4	41.4
8	0	-22	25.5	- 34.7
8	0	-20	94.8	- 76.0
8	0	-18	145.0	136.8
8	0	-16	43.0	25.8
8	0	-14	351.4	-274.3
8	0	-12	177.8	165.0
8	0	-10	261.1	280.6
8	0	- 8	290.0	-374.7
8	0	- 6	43.0	- 44.9
8	0	- 4	352.7	411.8
8	0	- 2	169.1	-164.4
8	0	0	217.2	-197.4
8	0	2	239.8	190.2
8	0	4	28.4	11.4
8	0	6	81.6	- 95.2
8	0	8	0.0	22.2
8	0	10	11.0	12.6
8	0	12	8.7	- 8.2
10	0	-24	43.7	- 30.3
10	0	-22	0.0	- 2.9
10	0	-20	33.5	45.1
10	0	-18	28.4	- 22.5
10	0	-16	0.0	- 20.5
10	0	-14	26.3	28.9
10	0	-12	0.0	0.0
10	0	-10	24.4	33.7
10	0	- 8	24.8	- 28.0
10	0	- 6	53.4	- 72.9
10	0	- 4	87.9	97.9
10	0	- 2	14.6	12.4
10	0	0	123.6	-130.1
10	0	2	55.7	48.2
10	0	4	68.3	64.9
10	0	6	77.7	- 62.7
10	0	8	0.0	- 6.5
10	0	10	48.1	33.8
10	0	12	40.8	- 6.9
10	0	14	13.8	- 6.6
12	0	-22	19.7	- 16.1
12	0	-20	26.3	35.0
12	0	-18	15.3	5.9
12	0	-16	83.1	- 59.5
12	0	-14	25.5	30.9
12	0	-12	80.2	43.5
12	0	-10	78.8	- 61.7
12	0	- 8	0.0	- 12.5
12	0	- 6	37.1	28.2
12	0	- 4	0.0	- 1.2
12	0	- 2	0.0	5.5
12	0	0	27.7	- 25.6
12	0	2	0.0	3.8
12	0	4	51.8	44.6
12	0	6	22.6	- 23.3
12	0	8	45.2	- 22.5
12	0	10	56.1	29.5
14	0	-22	13.1	- 16.1
14	0	-20	13.8	15.8
14	0	-18	24.8	22.6
14	0	-16	67.8	- 60.2
14	0	-14	0.0	- 0.1
14	0	-12	132.7	95.4
14	0	-10	75.8	- 67.8
14	0	- 8	123.2	- 71.8
14	0	- 6	130.7	126.1
14	0	- 4	0.0	2.5
14	0	- 2	155.8	-104.6
14	0	0	89.6	57.0
14	0	2	83.8	44.6
14	0	4	108.6	- 55.6
16	0	-18	61.9	- 41.4
16	0	-16	36.4	32.3
16	0	-14	38.7	28.6
16	0	-12	53.9	- 45.1
16	0	-10	0.0	4.5
16	0	- 8	39.4	32.2
16	0	- 6	0.0	- 17.2
16	0	- 4	0.0	- 7.8
16	0	- 2	0.0	6.8
16	0	0	0.0	- 2.9
16	0	2	27.0	1.8
18	0	-14	52.5	14.1
18	0	-12	24.1	- 10.2
18	0	-10	32.8	- 12.5
18	0	- 8	61.9	16.2
1	1	-23	9.8	13.4
1	1	-22	0.0	15.1
1	1	-21	5.1	- 8.9
1	1	-20	12.0	11.0
1	1	-19	19.0	- 28.8
1	1	-18	34.8	- 57.7
1	1	-17	36.1	46.2
1	1	-16	0.0	35.0
1	1	-15	11.1	24.2
1	1	-14	93.7	117.1
1	1	-13	92.8	-105.6
1	1	-12	93.7	-163.6
1	1	-11	42.2	54.7
1	1	-10	65.4	- 76.1
1	1	- 9	116.8	157.7
1	1	- 8	213.7	306.8
1	1	- 7	133.1	-170.6
1	1	- 6	130.3	-133.7
1	1	- 5	92.8	- 76.6
1	1	- 4	272.3	-308.4
1	1	- 3	184.6	263.1
1	1	- 2	[illegible]	251.6
1	1	- 1	[illegible]	- 92.1
1	1	0	[illegible]	59.4
1	1	1	[illegible]	-223.1
1	1	2	124.7	-173.3
1	1	3	157.2	136.6
1	1	4	31.0	33.4
1	1	5	27.8	43.7
1	1	6	9.3	6.5
1	1	7	65.9	-119.7
1	1	8	61.7	58.9
1	1	9	14.4	17.2
1	1	10	42.7	35.0
1	1	11	19.9	46.6
1	1	12	93.2	- 96.9
1	1	13	0.0	- 20.3
1	1	14	13.0	32.6
1	1	15	0.0	- 5.2
1	1	16	73.3	65.3
1	1	17	0.0	12.6
1	1	18	54.8	- 52.9
1	1	19	0.0	- 0.1
1	1	20	15.8	- 14.4
1	1	21	0.0	- 2.5
1	1	22	21.4	31.3
3	1	-23	10.6	- 11.6
3	1	-22	0.0	- 2.0
3	1	-21	0.0	- 5.3
3	1	-20	0.0	- 0.5
3	1	-19	21.4	29.6
3	1	-18	7.4	- 10.5
3	1	-17	7.9	- 7.4
3	1	-16	0.0	- 12.5
3	1	-15	17.1	- 32.1
3	1	-14	54.8	77.1
3	1	-13	18.5	35.0
3	1	-12	48.3	- 61.1
3	1	-11	0.0	15.4
3	1	-10	226.2	-192.9
3	1	- 9	30.6	- 50.6
3	1	- 8	330.9	289.3
3	1	- 7	0.0	- 9.6
3	1	- 6	80.7	117.2
3	1	- 5	0.0	5.7
3	1	- 4	488.8	-573.0
3	1	- 3	24.1	- 19.8
3	1	- 2	259.3	260.9
3	1	- 1	0.0	- 12.5
3	1	0	613.7	549.8
3	1	1	74.7	- 9.6
3	1	2	466.4	-538.0
3	1	3	19.5	12.5
3	1	4	164.6	-133.5
3	1	5	0.0	21.3
3	1	6	491.4	489.6
3	1	7	0.0	2.5
3	1	8	108.9	-142.1
3	1	9	0.0	1.2
3	1	10	206.9	-219.8
3	1	11	8.4	3.2
3	1	12	142.3	164.2

Table 1 (*cont.*)

3	1	13	0.0	5.2
3	1	14	30.1	29.1
3	1	15	0.0	2.2
3	1	16	74.7	- 83.7
3	1	17	0.0	- 6.8
3	1	18	14.9	17.6
3	1	19	0.0	- 0.7
3	1	20	0.0	20.5
3	1	21	8.4	4.1
5	1	-24	27.4	34.9
5	1	-23	0.0	1.0
5	1	-22	6.5	12.0
5	1	-21	0.0	0.7
5	1	-20	102.9	-100.8
5	1	-19	0.0	- 1.3
5	1	-18	51.0	57.8
5	1	-17	0.0	- 0.9
5	1	-16	135.8	144.4
5	1	-15	0.0	- 4.9
5	1	-14	181.8	-222.5
5	1	-13	0.0	- 9.7
5	1	-12	80.7	- 58.1
5	1	-11	0.0	- 4.6
5	1	-10	294.2	364.5
5	1	- 9	0.0	13.7
5	1	- 8	132.2	-149.2
5	1	- 7	0.0	- 4.9
5	1	- 6	237.5	-265.0
5	1	- 5	0.0	- 33.5
5	1	- 4	257.4	310.4
5	1	- 3	10.2	53.0
5	1	- 2	51.5	54.9
5	1	- 1	59.8	59.8
5	1	0	245.3	-197.3
5	1	1	66.3	- 72.1
5	1	2	0.0	45.5
5	1	3	0.0	1.2
5	1	4	0.0	22.0
5	1	5	101.1	88.2
5	1	6	0.0	- 7.4
5	1	7	49.2	- 42.3
5	1	8	0.0	6.1
5	1	9	46.9	- 49.3
5	1	10	42.2	- 46.6
5	1	11	42.7	47.7
5	1	12	15.8	15.6
5	1	13	13.0	3.8
5	1	14	22.3	30.6
5	1	15	28.8	- 32.1
5	1	16	23.1	- 24.1
5	1	17	0.0	9.4
5	1	18	0.0	- 4.3
5	1	19	0.0	10.3
7	1	-24	8.4	- 7.1
7	1	-23	0.0	- 0.5
7	1	-22	0.0	- 8.6
7	1	-21	12.5	- 19.5
7	1	-20	14.4	8.5
7	1	-19	0.0	15.0
7	1	-18	0.0	- 0.5
7	1	-17	19.5	28.1
7	1	-16	20.9	33.2
7	1	-15	101.1	- 58.7
7	1	-14	0.0	- 21.9
7	1	-13	0.0	- 4.4
7	1	-12	102.4	- 78.3
7	1	-11	156.6	117.6
7	1	-10	131.7	143.6
7	1	- 9	76.0	- 61.7
7	1	- 8	60.7	38.5
7	1	- 7	96.4	-102.2
7	1	- 6	198.5	-262.3
7	1	- 5	128.0	164.3
7	1	- 4	71.9	109.9
7	1	- 3	18.5	25.4
7	1	- 2	172.1	195.5
7	1	- 1	203.1	-171.6
7	1	0	258.8	-235.3
7	1	1	123.3	64.5
7	1	2	51.5	- 45.2
7	1	3	120.6	85.8
7	1	4	158.1	171.8
7	1	5	135.4	- 96.8
7	1	6	82.1	- 51.0
7	1	7	0.0	- 16.5
7	1	8	35.3	- 58.1
7	1	9	47.8	55.2
7	1	10	38.5	45.1
7	1	11	11.6	- 16.8
7	1	12	0.0	7.0
7	1	13	0.0	- 18.1
7	1	14	10.6	- 8.7
7	1	15	7.0	15.0
7	1	16	7.0	0.4
9	1	-24	7.4	4.0
9	1	-23	10.2	- 14.0
9	1	-22	25.0	- 31.7
9	1	-21	27.8	28.3
9	1	-20	0.0	21.8
9	1	-19	0.0	6.6
9	1	-18	40.8	39.5
9	1	-17	47.8	- 48.1
9	1	-16	93.7	- 59.1
9	1	-15	82.1	31.8
9	1	-14	0.0	- 12.7
9	1	-13	65.9	51.6
9	1	-12	57.0	52.6
9	1	-11	59.4	- 68.5
9	1	-10	0.0	- 21.8
9	1	- 9	0.0	- 15.0
9	1	- 8	0.0	- 11.5
9	1	- 7	48.7	68.9
9	1	- 6	25.0	- 31.1
9	1	- 5	16.6	- 34.9
9	1	- 4	0.0	- 5.9
9	1	- 3	18.5	- 45.7
9	1	- 2	106.2	103.8
9	1	- 1	0.0	32.9
9	1	0	63.0	- 57.6
9	1	1	0.0	4.1
9	1	2	103.5	- 86.5
9	1	3	0.0	- 19.4
9	1	4	133.3	123.2
9	1	5	0.0	7.2
9	1	6	33.7	15.8
9	1	7	0.0	7.0
9	1	8	141.0	- 96.5
9	1	9	0.0	- 2.2
9	1	10	40.4	37.8
9	1	11	0.0	1.4
9	1	12	47.8	38.2
9	1	13	0.0	2.1
9	1	14	46.4	- 36.9
11	1	-24	11.6	12.3
11	1	-23	0.0	6.7
11	1	-22	35.3	- 32.1
11	1	-21	0.0	- 2.8
11	1	-20	11.6	- 4.9
11	1	-19	0.0	- 4.4
11	1	-18	104.8	76.1
11	1	-17	0.0	4.1
11	1	-16	70.9	- 60.7
11	1	-15	0.0	- 2.1
11	1	-14	99.8	- 95.0
11	1	-13	0.0	- 4.1
11	1	-12	188.2	167.1
11	1	-11	11.1	- 1.8
11	1	-10	13.0	17.0
11	1	- 9	12.5	- 5.9
11	1	- 8	212.0	-213.8
11	1	- 7	0.0	0.2
11	1	- 6	119.2	124.5
11	1	- 5	0.0	5.4
11	1	- 4	157.7	142.3
11	1	- 3	14.9	1.1
11	1	- 2	199.9	-175.7
11	1	- 1	0.0	- 2.5
11	1	0	14.4	- 9.8
11	1	1	0.0	3.1
11	1	2	165.6	120.2
11	1	3	0.0	10.5
11	1	4	56.1	- 50.5
11	1	5	0.0	- 1.9
11	1	6	37.5	- 40.7
11	1	7	0.0	- 7.8
11	1	8	35.8	35.7
13	1	-22	21.4	19.9
13	1	-21	0.0	0.6
13	1	-20	27.4	25.2
13	1	-19	0.0	5.0
13	1	-18	52.4	- 43.4
13	1	-17	0.0	- 9.1
13	1	-16	12.5	1.8
13	1	-15	0.0	- 6.3
13	1	-14	53.3	44.2
13	1	-13	0.0	21.4
13	1	-12	0.0	- 20.4
13	1	-11	0.0	- 2.5
13	1	-10	0.0	- 10.1
13	1	- 9	25.0	- 26.9
13	1	- 8	0.0	8.0
13	1	- 7	18.1	27.2
13	1	- 6	0.0	- 4.9
13	1	- 5	25.0	22.1
13	1	- 4	38.5	20.9
13	1	- 3	39.9	- 37.7
13	1	- 2	29.3	- 16.8
13	1	- 1	0.0	2.4
13	1	0	42.7	- 26.5
13	1	1	42.7	31.5
13	1	2	63.0	31.4
13	1	3	17.6	- 19.1
13	1	4	0.0	2.9
13	1	5	18.1	- 14.3
13	1	6	45.9	- 25.6
13	1	7	23.1	16.9
13	1	8	19.0	10.2
15	1	-21	7.9	7.8
15	1	-20	37.5	19.6
15	1	-19	22.5	- 17.8
15	1	-18	9.3	- 14.5
15	1	-17	0.0	2.5
15	1	-16	39.9	- 21.7
15	1	-15	41.3	27.4
15	1	-14	78.8	37.9
15	1	-13	21.4	- 18.6
15	1	-12	0.0	0.8
15	1	-11	21.4	- 18.0
15	1	-10	77.9	- 45.4
15	1	- 9	45.0	32.5
15	1	- 8	20.9	21.8
15	1	- 7	0.0	- 1.5
15	1	- 6	36.6	21.8
15	1	- 5	36.6	- 28.8
15	1	- 4	42.2	- 26.1
15	1	- 3	15.8	14.0
15	1	- 2	0.0	- 1.3
15	1	- 1	16.3	10.9
15	1	0	15.3	10.5
15	1	1	11.6	- 15.7
17	1	-16	24.1	- 12.2
17	1	-15	26.0	- 7.9
17	1	-14	17.6	12.2
17	1	-13	0.0	- 0.1
17	1	-12	34.8	13.3
17	1	-11	0.0	5.0
17	1	-10	55.7	- 30.1
17	1	- 9	0.0	- 4.2
17	1	- 8	0.0	3.0
17	1	- 7	0.0	- 2.1
17	1	- 6	81.7	35.2
17	1	- 5	0.0	2.8
17	1	- 4	47.8	- 22.5
17	1	- 3	0.0	- 0.5

***** Cut off by beam stop

Structure analysis

The x- and z-parameters were determined from $h0l$ Patterson and electron-density projections, and the y-coordinates by some trials with $0k0$ and $h1l$ reflexions. Structure factors were calculated by means of the scattering factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for As and C, and of Thomas & Umeda (1957) for I, and with an overall temperature factor $B=5{\cdot}1$ Å^2 determined from a plot of $\ln\{|F_c|/|F_o|\}$ against $\sin^2\theta/\lambda^2$. Refinement proceeded by $h0l(F_o-F_c)$ syntheses and $h1l$ cosine and sine difference generalized projections, refining all parameters simultaneously (Rossmann & Shearer, 1958). Refinement was complete after four cycles; measured and calculated structure factors are listed in Table 1, the final R values for the observed reflexions being 0·18 for $h0l$ and 0·22 for $h1l$. The final electron-density projection is shown in Fig. 1, and the $h1l$ cosine and sine generalized projections in Fig. 2.

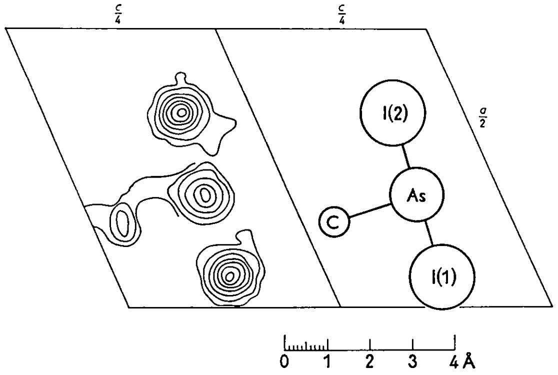

Fig. 1. Electron-density projection along the b-axis; contours at intervals of 5, 10, 20, 30, ... e.Å^{-2} at As and I atoms, and 3, 4, 5 e.Å^{-2} at the C atom.

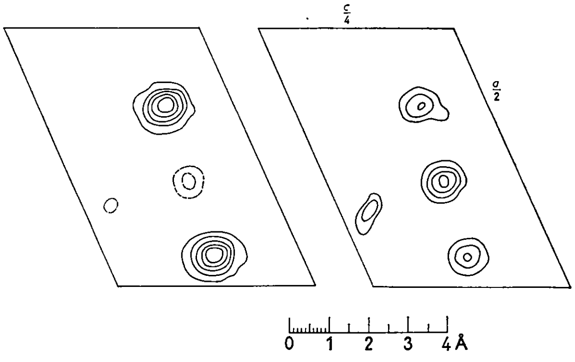

Fig. 2. Cosine and sine $h1l$ generalized projections.

The final positional parameters are listed in Table 2; the standard deviations (Cruickshank, 1949) are $\sigma(x)=\sigma(y)=\sigma(z)=0{\cdot}006$ Å for I, 0·010 Å for As, and 0·07 Å for C. The bond lengths and valency angles are shown in Fig. 3, and the shorter intermolecular contacts, all of which correspond to van der Waals interactions, in Fig. 4.

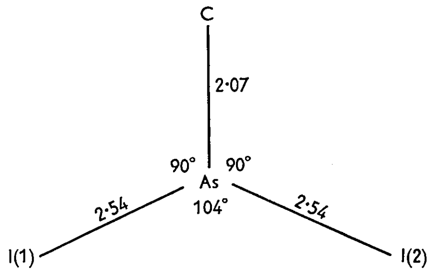

Fig. 3. Bond lengths and valency angles in $MeAsI_2$.

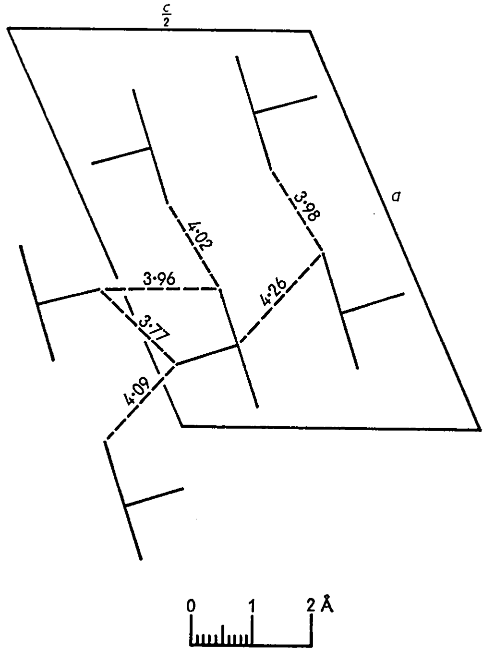

Fig. 4. Projection of the structure onto (010), showing the shorter intermolecular contacts.

Table 2. *Final positional parameters*

Atom	x	y	z
As	0·2045	0·3804	0·1501
I_1	0·0590	0·0436	0·1384
I_2	0·3475	0·0349	0·1615
C	0·156	0·380	0·037

Discussion

The structure analysis has utilized a large part of the observable three-dimensional data, and we did not use the rest of the available reflexions since any inaccuracies in the final results (as reflected in the rather high R values) are due not to a lack of data (353 reflexions have been used to determine twelve positional parameters), but to the poor quality of the intensity measurements as a result of the absorption effects. The standard deviations of the atomic positions indicate that the carbon atom has been located rather imprecisely in the presence of the heavier I and As atoms.

The arsenic atom has the usual pyramidal configuration. The As–I distance (2·54 ± 0·01 Å) is similar to corresponding lengths in AsI_3 (2·52 Å), Me_2AsI (2·54 Å), and Ph_2AsI (2·53 Å) (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958; Trotter, 1963). The I–As–I angle (104° ± 0·4°) is a little larger than the angles in AsI_3 (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958). Bonds and angles involving the carbon atom have been determined less precisely, and do not differ significantly from normal values.

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References

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Buerger, M. J. (1960). *Crystal-structure Analysis*, p. 224. New York: Wiley.

Camerman, N. & Trotter, J. (1963). *Canad. J. Chem.* **41**, 460.

Cruickshank, D. W. J. (1949). *Acta Cryst.* **2**, 65.

Howells, R. G. (1950). *Acta Cryst.* **3**, 366.

Rossmann, M. G. & Shearer, H. M. M. (1958). *Acta Cryst.* **11**, 829.

Tables of Interatomic Distances and Configuration in Molecules and Ions (1958). *Special Publ.* No. 11. London: The Chemical Society.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Trotter, J. (1963). *Canad. J. Chem.* **41**, 191.

Acta Cryst. (1963). **16**, 926

Calculation of Atomic Scattering Factors for the Helium Atom by means of the Six-Term Hylleraas Wave Function

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Atomic scattering factors have been calculated for the helium atom by means of the six-term Hylleraas wave function. The results are in good agreement with the calculations of Matsen and collaborators.

Introduction

In their classic work on the atomic scattering factors, James & Brindley (1931) employed the Hartree self-consistent field wave functions which were then available only for a few atoms. These wave functions were also limited in numerical accuracy owing to the lack of computing facilities at that time. In order to extend their work to other atoms for which the Hartree solutions were then not available, James & Brindley (1931) resorted to an interpolation scheme which has been found to be unreliable in the light of some recent experimental and theoretical developments (McWeeny, 1951; Hoerni & Ibers, 1954; Bacon, 1952; Cochran, 1953).

Recently efforts have been made by Matsen and collaborators to improve upon the values of atomic scattering factors of James & Brindley (Hurst, Miller & Matsen, 1958; Hurst & Matsen, 1959; Silverman, Platas & Matsen, 1960; Hurst, 1960). These authors have also studied the effects of radial and angular correlation on the form factor. The effects of aspherical charge distributions on the scattering factor have been studied by McWeeny (1951) and Freeman (1959). In this paper, calculations have been made on the scattering factor for the helium atom by means of the six-term Hylleraas wave function.

The Hylleraas wave function, which is essentially an expansion in terms of the positions of electrons from each other and the nucleus, is given by (Hylleraas, 1929; Bethe & Salpeter, 1957):

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