might appear that such errors could frequently be absorbed in the random errors in intensity measurement, it must be noted that they are calculable, systematic errors which can generate measurable effects upon the refined structure. In a particular case where the corrections were applied (Parkes & Hughes, 1963), there resulted not only an improvement in R but also a statistically significant change in the structure.

References

Parkes, A. S. & Hughes, R. E. (1963). *Acta Cryst.* **16**, 734.

Waser, J. (1951). *Rev. Sci. Instrum.* **22**, 563.

Acta Cryst. (1963). **16**, 1187

Stereochemistry of Arsenic. X. Tri-*p*-xylylarsine*

By J. Trotter

Department of Chemistry, University of British Columbia, Vancouver 8, B. C., Canada

(*Received* 14 *January* 1963)

Crystals of tri-*p*-xylylarsine are monoclinic, with four molecules in a unit cell of dimensions $a = 10{\cdot}81$, $b = 33{\cdot}4$, $c = 5{\cdot}72$ Å, $\beta = 96°\ 28'$, space group $P2_1/a$. The structure has been determined from projections along the a and c axes. Within experimental error the molecule has symmetry C_3, the arsenic being pyramidal with mean C–As–C angles of 102°, and each ring being rotated about its As–C bond, in the same sense, 37° from the position it would occupy in an ideal model with maximum interaction between the lone pair and the aromatic π-electrons. Overcrowded intramolecular distances are thereby increased to the usual van der Waals separations. Values of the bond distances, valency angles and intermolecular contacts have been obtained.

Introduction

Tri-*p*-xylylarsine has methyl substituents *ortho* to the arsenic atom, and its structure has been investigated for comparison with that of tri-*p*-tolylarsine, which has no *ortho* substituents (Trotter, 1963).

Experimental

Crystals of tri-*p*-xylylarsine are colourless prisms elongated along the c axis. The density was measured by flotation in aqueous potassium iodide, and 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

Tri-*p*-xylylarsine, $C_{24}H_{27}As$; $M = 390{\cdot}4$; m.p. 161 °C.
Monoclinic, $a = 10{\cdot}81$, $b = 33{\cdot}4$, $c = 5{\cdot}72$ Å; $\beta = 96°\ 28'$.
Volume of the unit cell $= 2052$ Å^3.
D_x (with $Z = 4$) $= 1{\cdot}256$, $D_m = 1{\cdot}24$ g.cm^{-3}.
Absorption coefficients for X-rays, $\lambda = 1{\cdot}542$ Å, $\mu = 24$ cm^{-1}.
$\lambda = 0{\cdot}7107$ Å, $\mu = 17$ cm^{-1}.
$F(000) = 816$.
Absent spectra: $h0l$ when h is odd, $0k0$ when k is odd. Space group is $P2_1/a$.

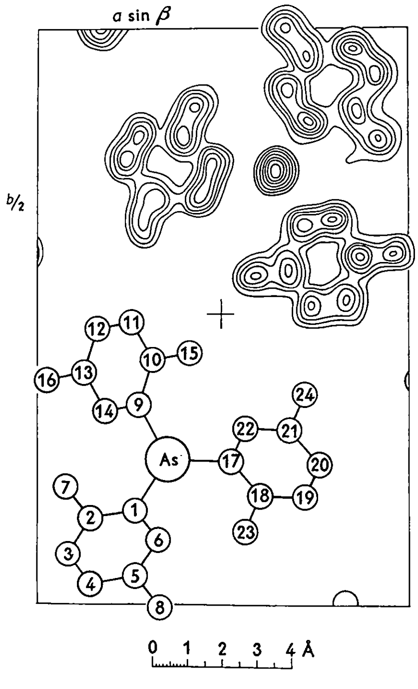

Fig. 1. Electron-density projection along the c axis. Contours at intervals of 1 e.Å^{-2} (starting at 2) for the C atoms, and 5 e.Å^{-2} for the As atom.

$hk0$ (Weissenberg films, Cu $K\alpha$) and $0kl$ (precession films, Mo $K\alpha$) intensity data were recorded and estimated visually, and the structure amplitudes derived. No absorption corrections were applied, and the absolute scale was established later by correlation

---

* Part IX. Camerman & Trotter (1963).

Table 1. *Measured and calculated structure factors*

Unobserved reflexions, which are listed as 0·0, have threshold values in the ranges 4–7 for *hk*0 and 13–28 for 0*kl* reflexions

h	k	l	F_o	F_c
0	2	0	*	5.4
0	4	0	139.8	-142.5
0	6	0	22.4	11.5
0	8	0	82.5	76.8
0	10	0	28.1	-26.5
0	12	0	48.4	-56.8
0	14	0	13.8	-0.0
0	16	0	71.7	72.7
0	18	0	0.0	1.6
0	20	0	63.6	-49.9
0	22	0	13.3	10.5
0	24	0	68.1	51.2
0	26	0	18.9	6.3
0	28	0	30.1	-39.2
0	30	0	7.0	1.7
0	32	0	22.1	30.9
0	34	0	9.6	-4.9
0	36	0	19.5	-23.6
0	38	0	8.1	0.2
0	40	0	14.8	17.0
0	42	0	5.3	-5.7
1	1	0	*	75.3
1	2	0	*	-132.8
1	3	0	77.5	-84.7
1	4	0	5.4	2.8
1	5	0	75.6	-81.6
1	6	0	61.4	-50.7
1	7	0	69.5	76.6
1	8	0	3.3	-7.2
1	9	0	62.8	58.1
1	10	0	84.0	-89.6
1	11	0	3.8	-10.2
1	12	0	4.0	-11.1
1	13	0	80.3	-73.7
1	14	0	50.5	38.7
1	15	0	13.9	11.5
1	16	0	7.6	1.5
1	17	0	25.5	14.4
1	18	0	81.3	-66.0
1	19	0	43.7	-41.8
1	20	0	5.6	11.2
1	21	0	25.3	-23.5
1	22	0	50.8	51.2
1	23	0	8.8	19.6
1	24	0	6.4	-12.1
1	25	0	21.7	23.2
1	26	0	48.1	-41.7
1	27	0	0.0	-3.9
1	28	0	17.7	-17.0
1	29	0	8.5	-11.9
1	30	0	10.0	7.6
1	31	0	23.3	30.4
1	32	0	0.0	-0.5
1	33	0	9.7	10.5
1	34	0	11.2	-0.2
1	35	0	11.8	-18.3
1	36	0	8.9	-11.2
1	37	0	5.2	-5.6
1	38	0	6.3	5.6
1	39	0	5.4	4.2
1	40	0	0.0	-1.4
1	41	0	4.4	5.7
1	42	0	10.4	-9.7
2	0	0	131.0	-148.4
2	1	0	16.4	9.8
2	2	0	5.6	-8.8
2	3	0	28.7	-26.3
2	4	0	5.6	3.4
2	5	0	23.0	36.3
2	6	0	10.0	9.8
2	7	0	76.5	75.8
2	8	0	36.4	-34.6
2	9	0	85.6	-93.5
2	10	0	7.8	-3.7
2	11	0	80.4	-81.1
2	12	0	51.4	-37.2
2	13	0	61.8	57.7
2	14	0	21.2	-17.5
2	15	0	72.6	77.0
2	16	0	12.1	-16.3
2	17	0	77.9	-63.0
2	18	0	0.0	-4.9
2	19	0	23.2	-25.6
2	20	0	29.4	32.9
2	21	0	52.2	51.5
2	22	0	5.3	-1.8
2	23	0	51.3	57.6
2	24	0	21.5	-25.0
2	25	0	19.9	-20.7
2	26	0	15.9	-10.5
2	27	0	18.9	-17.1
2	28	0	0.0	6.9
2	29	0	24.3	17.8
2	30	0	0.0	-4.7
2	31	0	17.8	13.9
2	32	0	0.0	-0.5
2	33	0	19.3	-21.5
2	34	0	5.8	10.4
2	35	0	10.2	-4.3
2	36	0	0.0	1.9
2	37	0	0.0	-0.9
2	38	0	0.0	4.3
2	39	0	14.7	8.2
2	40	0	0.0	-4.0
2	41	0	0.0	-4.6
3	1	0	76.2	-73.3
3	2	0	52.5	-44.6
3	3	0	70.0	65.8
3	4	0	18.4	-17.0
3	5	0	66.4	69.6
3	6	0	20.1	24.7
3	7	0	32.8	-40.7
3	8	0	29.9	-30.9
3	9	0	21.0	-22.0
3	10	0	60.3	-55.6
3	11	0	57.8	57.4
3	12	0	19.9	33.5
3	13	0	62.1	55.6
3	14	0	65.6	59.6
3	15	0	33.0	-44.8
3	16	0	0.0	-6.0
3	17	0	15.3	-19.4
3	18	0	0.0	-7.3
3	19	0	14.8	11.8
3	20	0	0.0	-5.1
3	21	0	36.4	30.5
3	22	0	16.1	13.4
3	23	0	9.2	-12.5
3	24	0	0.0	9.2
3	25	0	31.8	-25.5
3	26	0	11.9	-9.6
3	27	0	7.8	10.4
3	28	0	0.0	12.8
3	29	0	21.2	13.4
3	30	0	12.1	8.4
3	31	0	22.0	-26.0
3	32	0	9.7	7.6
3	33	0	10.6	-11.2
3	34	0	7.3	-8.3
3	35	0	8.3	11.6
3	36	0	0.0	-1.9
3	37	0	6.9	7.4
3	38	0	6.5	8.0
3	39	0	0.0	-4.8
3	40	0	0.0	-1.7
3	41	0	7.3	-7.4
4	0	0	69.1	-63.8
4	1	0	92.2	88.9
4	2	0	19.9	23.4
4	3	0	4.6	10.0
4	4	0	32.6	40.9
4	5	0	51.4	-46.1
4	6	0	5.3	-7.7
4	7	0	9.3	-17.8
4	8	0	60.6	-57.1
4	9	0	31.4	28.4
4	10	0	6.7	6.5
4	11	0	18.6	29.6
4	12	0	72.9	63.2
4	13	0	43.6	-45.0
4	14	0	41.3	29.6
4	15	0	42.7	-43.8
4	16	0	44.1	-30.6
4	17	0	14.1	25.9
4	18	0	0.0	11.8
4	19	0	5.3	-0.9
4	20	0	17.2	17.0
4	21	0	11.2	-9.3
4	22	0	6.6	-0.0
4	23	0	12.5	-15.0
4	24	0	17.4	-22.6
4	25	0	12.0	13.5
4	26	0	0.0	0.6
4	27	0	6.1	11.1
4	28	0	16.5	19.8
4	29	0	10.0	-6.2
4	30	0	9.2	6.1
4	31	0	10.2	-13.2
4	32	0	14.2	-10.6
4	33	0	13.0	10.7
4	34	0	6.3	-4.7
4	35	0	0.0	3.5
4	36	0	19.6	13.5
4	37	0	7.1	-4.7
4	38	0	0.0	0.3
4	39	0	6.7	-6.1
4	40	0	5.3	-7.1
5	1	0	15.4	14.5
5	2	0	113.7	106.5
5	3	0	14.6	-20.6
5	4	0	4.8	-6.8
5	5	0	5.9	12.2
5	6	0	79.1	-72.8
5	7	0	21.5	-20.1
5	8	0	5.0	3.0
5	9	0	0.0	-5.7
5	10	0	76.3	62.1
5	11	0	0.0	-4.3
5	12	0	13.4	15.2
5	13	0	5.6	5.2
5	14	0	77.0	-69.3
5	15	0	0.0	2.3
5	16	0	6.0	-5.0
5	17	0	5.3	-1.9
5	18	0	63.8	61.2
5	19	0	5.6	10.2
5	20	0	16.1	-13.9
5	21	0	0.0	1.4
5	22	0	31.9	-32.9
5	23	0	0.0	-1.3
5	24	0	0.0	2.4
5	25	0	0.0	1.2
5	26	0	29.9	31.6
5	27	0	0.0	4.6
5	28	0	0.0	2.3
5	29	0	0.0	5.8
5	30	0	19.2	-26.1
5	31	0	0.0	-0.8
5	32	0	0.0	2.6
5	33	0	8.8	-6.2
5	34	0	18.8	18.4
5	35	0	0.0	-0.8
5	36	0	0.0	-3.7
5	37	0	0.0	-3.7
5	38	0	14.0	-14.7
6	0	0	29.9	30.0
6	1	0	16.7	25.2
6	2	0	10.0	4.0
6	3	0	61.4	51.6
6	4	0	25.2	-27.1
6	5	0	36.7	-37.6
6	6	0	25.1	-26.7
6	7	0	51.8	-42.1
6	8	0	40.3	44.0
6	9	0	14.0	13.1
6	10	0	5.0	4.3
6	11	0	36.1	27.9
6	12	0	38.3	-34.3
6	13	0	17.2	-24.3
6	14	0	16.9	-22.3
6	15	0	17.9	-20.5
6	16	0	50.3	48.2
6	17	0	19.6	27.8
6	18	0	9.4	-5.9
6	19	0	15.1	12.4
6	20	0	17.4	-22.0
6	21	0	6.0	-5.3
6	22	0	6.1	5.1
6	23	0	16.4	-12.2
6	24	0	15.0	19.8

* Cut off by beam stop.

Table 1 (*cont.*)

6	25	0	8.6	8.9	9	3	0	0.0	9.5	12	1	0	7.9	10.4
6	26	0	0.0	-6.3	9	4	0	0.0	1.2	12	2	0	0.0	-2.3
6	27	0	9.2	4.5	9	5	0	11.0	14.1	12	3	0	8.3	14.2
6	28	0	14.4	-20.3	9	6	0	17.0	21.4	12	4	0	0.0	2.9
6	29	0	8.1	-13.6	9	7	0	0.0	-4.0	12	5	0	8.3	-11.5
6	30	0	0.0	-3.8	9	8	0	0.0	3.7	12	6	0	0.0	4.2
6	31	0	10.9	-14.4	9	9	0	12.1	-14.1	12	7	0	10.6	-15.2
6	32	0	0.0	6.8	9	10	0	14.0	-15.3	12	8	0	0.0	6.7
6	33	0	6.4	11.8	9	11	0	8.6	6.2	12	9	0	7.8	9.6
6	34	0	0.0	-2.3	9	12	0	0.0	1.7	12	10	0	0.0	4.2
6	35	0	5.0	8.1	9	13	0	28.2	33.7	12	11	0	6.5	8.3
6	36	0	7.3	-5.1	9	14	0	14.0	13.8	12	12	0	0.0	-0.1
6	37	0	4.0	-6.0	9	15	0	0.0	-8.8	12	13	0	8.8	-10.8
7	1	0	10.2	2.4	9	16	0	13.9	14.1	12	14	0	0.0	-0.2
7	2	0	7.3	-9.9	9	17	0	0.0	-5.1	12	15	0	0.0	-4.1
7	3	0	38.1	-39.3	9	18	0	21.7	-25.5	12	16	0	0.0	-0.0
7	4	0	0.0	-4.7	9	19	0	0.0	5.6	12	17	0	8.1	8.2
7	5	0	49.4	-45.5	9	20	0	6.6	-7.1	12	18	0	0.0	3.8
7	6	0	0.0	5.0	9	21	0	0.0	-5.9	12	19	0	9.5	9.7
7	7	0	41.4	49.4	9	22	0	7.9	4.8	13	1	0	0.0	8.4
7	8	0	17.5	-12.9	9	23	0	0.0	-6.1	13	2	0	8.1	5.0
7	9	0	44.5	47.3	9	24	0	0.0	-8.7	13	3	0	0.0	-3.7
7	10	0	0.0	0.8	9	25	0	5.9	1.0	13	4	0	0.0	-0.4
7	11	0	39.5	-37.9	9	26	0	8.8	-10.8	13	5	0	4.5	-7.3
7	12	0	6.5	7.7	9	27	0	0.0	5.9	13	6	0	10.0	-11.1
7	13	0	42.2	-38.9	9	28	0	0.0	0.4	0	0	1	221.5	215.0
7	14	0	5.8	11.9	9	29	0	0.0	2.4	0	1	1	29.4	-23.4
7	15	0	48.4	46.2	9	30	0	7.6	9.8	0	2	1	0.0	-13.9
7	16	0	11.8	-8.4	9	31	0	3.8	-5.4	0	3	1	67.1	-56.4
7	17	0	10.9	8.7	10	0	0	25.3	-33.5	0	4	1	58.2	-74.8
7	18	0	0.0	-6.1	10	1	0	0.0	-5.6	0	5	1	149.1	143.7
7	19	0	13.9	-18.2	10	2	0	0.0	5.7	0	6	1	89.5	85.6
7	20	0	11.6	0.6	10	3	0	0.0	-3.6	0	7	1	26.0	-23.4
7	21	0	19.8	-20.5	10	4	0	18.7	19.2	0	8	1	50.6	33.3
7	22	0	0.0	2.2	10	5	0	0.0	11.7	0	9	1	68.2	-78.6
7	23	0	14.0	16.5	10	6	0	0.0	-2.1	0	10	1	28.5	41.6
7	24	0	0.0	6.2	10	7	0	9.8	12.3	0	11	1	45.0	-50.2
7	25	0	13.8	17.8	10	8	0	27.8	-27.5	0	12	1	15.1	-10.7
7	26	0	5.9	-7.1	10	9	0	0.0	6.7	0	13	1	38.3	46.0
7	27	0	16.2	-16.8	10	10	0	0.0	-5.0	0	14	1	18.5	13.0
7	28	0	0.0	-4.9	10	11	0	6.0	-9.1	0	15	1	40.6	54.0
7	29	0	10.8	-11.8	10	12	0	21.6	15.4	0	16	1	14.0	1.9
7	30	0	0.0	6.6	10	13	0	0.0	-4.8	0	17	1	47.8	-49.6
7	31	0	10.0	6.9	10	14	0	5.9	2.9	0	18	1	0.0	8.3
7	32	0	0.0	1.0	10	15	0	0.0	-11.7	0	19	1	42.5	-29.7
7	33	0	12.5	11.3	10	16	0	23.6	-27.5	0	20	1	40.8	-31.6
7	34	0	0.0	-1.3	10	17	0	0.0	-2.4	0	21	1	54.8	53.1
7	35	0	6.0	-5.6	10	18	0	6.3	-4.7	0	22	1	0.0	10.6
8	0	0	11.2	13.2	10	19	0	10.7	-4.4	0	23	1	75.2	60.9
8	1	0	21.6	-23.1	10	20	0	7.4	18.3	0	24	1	33.8	44.0
8	2	0	6.5	-1.5	10	21	0	0.0	5.0	0	25	1	24.3	-11.8
8	3	0	14.5	-13.3	10	22	0	6.8	-6.0	0	26	1	17.3	15.3
8	4	0	19.6	-16.3	10	23	0	0.0	-2.4	0	27	1	17.9	-15.3
8	5	0	33.5	37.3	10	24	0	5.2	-9.3	0	28	1	18.2	-29.0
8	6	0	11.4	8.8	10	25	0	0.0	-3.9	0	29	1	0.0	3.3
8	7	0	16.3	24.0	10	26	0	4.7	3.6	0	30	1	0.0	0.9
8	8	0	29.4	24.5	10	27	0	0.0	-0.8	0	31	1	32.7	20.1
8	9	0	12.6	-19.7	10	28	0	6.5	10.7	0	32	1	0.0	2.2
8	10	0	10.7	-14.7	11	1	0	6.7	-11.1	0	33	1	0.0	-13.3
8	11	0	10.8	-11.7	11	2	0	9.5	15.2	0	34	1	0.0	-0.9
8	12	0	16.9	-16.4	11	3	0	10.6	14.1	0	35	1	33.8	-25.2
8	13	0	18.3	25.8	11	4	0	8.2	-8.4	0	0	2	62.4	-60.0
8	14	0	6.9	11.8	11	5	0	9.4	10.5	0	1	2	31.3	-40.3
8	15	0	8.5	13.6	11	6	0	6.6	-11.9	0	2	2	0.0	0.3
8	16	0	14.0	22.2	11	7	0	8.0	-7.7	0	3	2	36.4	-51.0
8	17	0	13.2	-17.2	11	8	0	7.3	4.5	0	4	2	63.5	61.1
8	18	0	8.6	18.0	11	9	0	12.1	-10.9	0	5	2	32.2	38.5
8	19	0	0.0	0.4	11	10	0	10.2	15.1	0	6	2	18.7	17.4
8	20	0	15.6	-22.4	11	11	0	0.0	2.3	0	7	2	19.0	27.3
8	21	0	0.0	-3.9	11	12	0	0.0	-1.1	0	8	2	66.3	-74.1
8	22	0	0.0	1.0	11	13	0	5.4	-3.9	0	9	2	33.6	-43.7
8	23	0	17.9	20.4	11	14	0	6.0	-3.9	0	10	2	0.0	-7.8
8	24	0	10.4	12.6	11	15	0	7.8	-12.7	0	11	2	0.0	-6.8
8	25	0	6.5	-3.9	11	16	0	0.0	4.2	0	12	2	97.9	94.9
8	26	0	0.0	-0.6	11	17	0	0.0	-4.8	0	13	2	25.5	36.8
8	27	0	9.2	-7.8	11	18	0	7.1	10.8	0	14	2	36.6	31.6
8	28	0	11.7	-11.9	11	19	0	0.0	6.4	0	15	2	56.8	64.2
8	29	0	5.6	5.5	11	20	0	0.0	3.9	0	16	2	43.6	-29.5
8	30	0	0.0	1.2	11	21	0	12.6	11.1	0	17	2	25.2	-23.9
8	31	0	14.1	11.4	11	22	0	4.5	-7.1	0	18	2	0.0	4.3
8	32	0	6.1	2.6	11	23	0	4.2	-4.6	0	19	2	39.2	-37.4
8	33	0	6.5	-8.9	11	24	0	0.0	-2.1	0	20	2	28.5	35.4
9	1	0	0.0	-1.0	11	25	0	4.2	-5.6	0	21	2	25.2	24.1
9	2	0	24.9	-28.1	12	0	0	0.0	9.8	0	22	2	37.2	-35.3

Table 1 (*cont.*)

0	23	2	40.0	37.9
0	24	2	0.0	- 0.5
0	25	2	35.8	- 31.5
0	0	3	65.2	- 62.4
0	1	3	0.0	16.3
0	2	3	0.0	- 1.8
0	3	3	0.0	8.9
0	4	3	41.1	41.3
0	5	3	0.0	- 7.5
0	6	3	33.6	31.5
0	7	3	0.0	- 14.6
0	8	3	50.3	- 49.7
0	9	3	0.0	- 13.9
0	10	3	0.0	- 5.1
0	11	3	0.0	8.2
0	12	3	51.2	49.7
0	13	3	0.0	- 11.0
0	14	3	0.0	12.2
0	15	3	0.0	- 17.5
0	16	3	53.7	- 55.6
0	17	3	29.9	37.5
0	18	3	0.0	1.9
0	19	3	0.0	- 3.7
0	20	3	43.6	44.8
0	21	3	0.0	6.5
0	22	3	0.0	- 12.3
0	23	3	0.0	- 11.3
0	24	3	26.3	- 19.3
0	25	3	0.0	- 1.5
0	26	3	0.0	- 0.1
0	27	3	0.0	7.2
0	28	3	27.1	30.2
0	0	4	0.0	16.2
0	1	4	0.0	1.6
0	2	4	0.0	- 7.1
0	3	4	32.4	27.8
0	4	4	0.0	- 12.7
0	5	4	42.8	- 51.5
0	6	4	0.0	5.1
0	7	4	43.1	- 44.6
0	8	4	0.0	12.0
0	9	4	28.2	18.9
0	10	4	0.0	2.3
0	11	4	33.6	43.1
0	12	4	0.0	- 13.6
0	13	4	28.5	- 32.1
0	14	4	0.0	14.3
0	15	4	18.5	- 26.6
0	16	4	0.0	6.4
0	17	4	26.0	21.4
0	18	4	0.0	5.3
0	19	4	26.3	21.4
0	0	5	34.4	32.4
0	1	5	0.0	0.8
0	2	5	0.0	- 5.7
0	3	5	0.0	5.1
0	4	5	29.9	- 23.1
0	5	5	0.0	- 4.9
0	6	5	0.0	- 7.5
0	7	5	0.0	- 15.6
0	8	5	35.5	42.6
0	9	5	19.0	19.8
0	10	5	0.0	0.1
0	11	5	0.0	2.7
0	12	5	33.0	- 37.1
0	13	5	0.0	- 18.3
0	14	5	0.0	6.7
0	15	5	0.0	- 12.4
0	16	5	30.2	39.2

with the calculated structure factors. 330 $hk0$ and 84 $0kl$ reflexions were observed.

Structure analysis

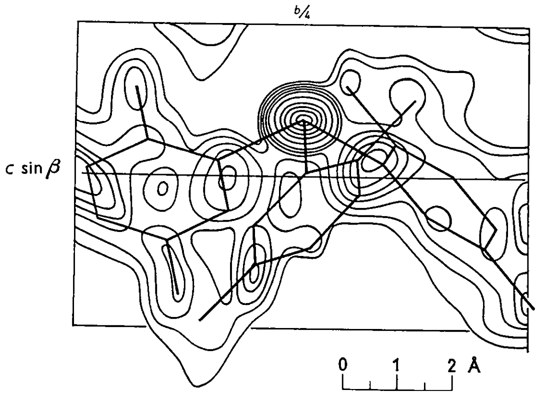

Fig. 2. Electron-density projection along the a axis. Contours at intervals of 2 e.Å^{-2}, except at the As atom, where contours above 10 are at intervals of 5 e.Å^{-2}.

The coordinates of the arsenic atom were determined from c- and a-axis Patterson projections, and Fourier series summed with signs based on the As contributions alone. From the resulting electron-density maps it was possible to determine the positions of all the carbon atoms. Refinement proceeded by successive Fourier and difference syntheses. The final measured and calculated structure factors are listed in Table 1; the discrepancy factors, for the observed reflexions, are $R(hk0)=0{\cdot}18$, $R(0kl)=0{\cdot}15$. The scattering factors used were those listed by Sagel (1958), with $B(hk0)=4{\cdot}5$ Å^2 and $B(0kl)=3{\cdot}5$ Å^2 for all the atoms. The final electron-density projections are shown in Figs. 1 and 2.

Coordinates and molecular dimensions

The final positional parameters, x, y and z, are listed, as fractions of the unit cell edges, in Table 2. The standard deviations (Cruickshank, 1949) are $\sigma(x)=\sigma(y)=\sigma(z)=0{\cdot}008$ Å for As and 0·05 Å for C.

Table 2. *Final positional parameters, and deviations* (Δ) *from the aromatic planes*

Atom	x	y	z	Δ (Å)
As	0·1467	0·1250	0·1893	0
C(1)	0·233	0·169	0·042	0
C(2)	0·355	0·175	0·109	−0·01
C(3)	0·416	0·207	0·006	0
C(4)	0·355	0·232	−0·165	+0·02
C(5)	0·233	0·225	−0·236	0
C(6)	0·172	0·194	−0·132	−0·01
C(7)	0·421	0·148	0·302	0
C(8)	0·168	0·252	−0·427	−0·01
C(9)	0·224	0·078	0·049	−0·01
C(10)	0·187	0·040	0·115	−0·01
C(11)	0·243	0·007	0·020	+0·01
C(12)	0·335	0·013	−0·146	0
C(13)	0·371	0·051	−0·212	0
C(14)	0·316	0·084	−0·114	−0·01
C(15)	0·086	0·033	0·295	0
C(16)	0·473	0·057	−0·391	0
C(17)	−0·024	0·126	0·011	+0·01
C(18)	−0·103	0·155	0·057	−0·02
C(19)	−0·223	0·157	−0·059	+0·01
C(20)	−0·261	0·129	−0·236	0
C(21)	−0·180	0·099	−0·290	−0·01
C(22)	−0·063	0·098	−0·167	0
C(23)	−0·061	0·186	0·255	+0·01
C(24)	−0·222	0·069	−0·477	+0·01

The best planes through the three *p*-xylyl groups have equations:

I. C(1)–C(8):
$$-0\cdot2447X'+0\cdot6291Y+0\cdot7378Z'-2\cdot9076=0\ ,$$
II. C(9)–C(16):
$$+0\cdot7280X'-0\cdot0007Y+0\cdot6855Z'-1\cdot7639=0\ ,$$
III. C(17)–C(24):
$$-0\cdot3388X'-0\cdot5939Y+0\cdot7297Z'+2\cdot3537=0\ ,$$

where X', Y, Z' are coordinates in Å referred to orthogonal axes a', b and c. The deviations of the atoms from the appropriate planes are given in the last column of Table 2; the arsenic atom lies on all three planes.

Table 3. *Bond lengths and valency angles*

	As–C(1)	1·98 Å
	As–C(9)	1·99
	As–C(17)	2·00
Mean	As–C	1·99 Å
	$18C_{ar}$–C_{ar}	1·35–1·46 Å
Mean	C_{ar}–C_{ar}	1·39 Å
	$6C_{ar}$–CH_3	1·51–1·60 Å
Mean	C_{ar}–CH_3	1·55 Å
	C(1)–As–C(9)	100·2°
	C(9)–As–C(17)	102·3
	C(17)–As–C(1)	102·7
Mean	C–As–C	102°
Mean	As–C–C	120°
Mean	C–C–C	120°

The bond lengths and valency angles in the molecule are given in Table 3. The closest intramolecular contacts between the *p*-xylyl groups have mean values: C_{ar}–C_{ar} = C_{ar}–CH_3 = 3·5 Å, H_{ar}–CH_3 = 3·1 Å (assuming that the aromatic hydrogen atoms lie on the ring diagonals with C–H = 1·08 Å; no attempt was made to predict the positions of the methyl hydrogen atoms).

All the intermolecular contacts correspond to van der Waals interactions, the shortest being a C · · · C separation of 3·42 Å.

Discussion

Since the analysis has utilized only two-dimensional data, the bond distances and valency angles, particularly those involving only carbon, have not been measured very accurately, and only mean values are quoted in Table 3. The object of the analysis was the determination of the orientations of the *p*-xylyl groups, so no effort was made to determine the bond distances and angles more precisely by three-dimensional methods; they all appear to be quite normal. The orientation angles, which are calculated from mean planes, have been established more reliably.

The *p*-xylyl groups are planar, the plane of each also passing through the arsenic atom. The rotations of the rings from their positions in an 'ideal' model similar to that described for tri-*p*-tolylarsine (Trotter, 1963) (in this case with the assumption that the lone pair makes equal angles with the three As–C bonds), are 34·6°, 37·0° and 38·0° for rings I, II and III respectively. The differences between these values are not significant, so that each ring is rotated, about its As–C bond, through a mean angle of 37°. The rotations are all in the same sense and are such that the *ortho* methyl groups are displaced in the direction of the lone pair (Fig. 2). The minimum C · · · C and C · · · H non-bonded distances are increased by these displacements to 3·5 Å and 3·1 Å, corresponding to normal van der Waals separations.

The rotations of the rings from their positions in the ideal model are equal within experimental error to the corresponding displacements in the *p*-tolyl derivative (36°). This indicates that the rotation which was required to relieve overcrowding between H atoms in the *p*-tolyl compound is sufficient also to relieve the more severe overcrowding involving the methyl group in the *p*-xylyl derivative.

The author is indebted to Dr W. R. Cullen for suggesting the problem, for the crystal sample and for much helpful discussion, to Dr F. R. Ahmed for kindly making available his IBM 1620 programs, to the staff of the University of British Columbia Computing Centre for assistance with the operation of the computer, and to the National Research Council of Canada and the President's Research Fund, University of British Columbia, for financial support.

References

Camerman, N. & Trotter, J. (1963). *Acta Cryst.* **16**, 922.
Cruickshank, D. W. J. (1949). *Acta Cryst.* **2**, 65.
Sagel, K. (1958). *Tabellen zur Röntgenstrukturanalyse.* Berlin: Springer-Verlag.
Trotter, J. (1963). *Canad. J. Chem.* **41**, 14.