gen bond is 2·647 Å, which is in good agreement with the values observed in other carboxyl groups: 2·676 and 2·669 Å in 5-hydroxy-2,3-norbornanedicarboxylic γ-lactone (Chapuis, Zalkin & Templeton, 1973), 2·699 and 2·656 Å in itaconic acid (Harlow & Pfluger, 1973).

The program *FMLS* (Ashida, 1973) was used with some modifications for the full-matrix least-squares calculations. The computations were made on a FACOM 230-60 computer at Nagoya University and a HITAC 8450 computer at the Research Institute for Polymers and Textiles.

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# 2,2′-Bis(dimethylarsino)octafluorobi-1-cyclobuten-1-ylmolybdenum Tetracarbonyl

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**Abstract.** $C_{16}H_{12}As_2F_8O_4Mo$, $M_r = 666{\cdot}1$, $P\bar{1}$, $a = 9{\cdot}174\,(2)$, $b = 15{\cdot}692\,(4)$, $c = 9{\cdot}681\,(3)$ Å, $\alpha = 115{\cdot}93\,(1)$, $\beta = 68{\cdot}98\,(1)$, $\gamma = 114{\cdot}48\,(1)°$, $V = 1114$ Å$^3$, $d_o = 1{\cdot}93\,(4)$ (by flotation), $Z = 2$, $d_c = 1{\cdot}99$ g cm$^{-3}$, Mo $K\alpha$ radiation ($\lambda = 0{\cdot}70926$ Å), $\mu$(Mo $K\alpha$) = 36·8 cm$^{-1}$, $F(000) = 640$, $T = 20 \pm 1$ °C; final $R$ for 2764 observed reflexions 0·069. Approximate octahedral coordination is found about Mo which is bonded to four carbonyl groups and the two As atoms of a puckered, seven-membered chelate.

**Introduction.** Crystals of the title compound were deep red. Weissenberg photographs of the layers *hk*0 and *hkl*, and precession photographs of the *h*0*k* and 0*kl* zones were taken with Cu radiation ($\lambda = 1{\cdot}5418$ Å), from which triclinic Laue symmetry was established. A cleaved fragment 0·18 × 0·23 × 0·15 mm was mounted for data collection. Accurate cell dimensions were determined from counter measurements and least-squares refinement of 12 of the strongest reflexions having $2\theta > 25°$, on a Picker FACS-1 computer-controlled four-circle diffractometer with Mo $K\alpha$ radiation ($\lambda = 0{\cdot}70926$ Å). The take-off angle was 1·0°, and the crystal was mounted with **b** approximately parallel to the $\varphi$ axis of the diffractometer. Intensities were collected with a symmetrical $\theta$–$2\theta$ scan, a base width of 1·4°, Nb-filtered Mo $K\alpha$ radiation and a take-off angle of 1·3°. Background counts of 10 s were measured at each of the scan limits, and after each 70 reflexions, two standard reflexions were measured; their variation was ±5%. The intensities of 3949 unique reflexions were measured and corrected for Lorentz and polarization effects but not for absorption. 2764 were classed as observed $\{I > 2{\cdot}3\sigma(I)$, where $\sigma(I) = [(T) + (t_b/t_s)^2(B_1 + B_2) + (kI)^2]^{1/2}$ where $T$ = total count, $B_1$ and $B_2$ are background counts, $t_s$ = scan time, $t_b$ = total background time, $k$ is a constant set to 0·03, and $I$ is the net count$\}$.

Solution of the Patterson function yielded positions of the Mo and two As atoms. Full-matrix least-squares refinement of scale factor and positional and isotropic thermal parameters for these three atoms gave $R = 0{\cdot}256$. A subsequent difference map served to locate all remaining non-hydrogen atoms. Refinement of all positional and isotropic thermal parameters reduced $R$ to 0·096. Introduction of anisotropic temperature factors for all atoms and further refinement lowered $R$ to 0·081.* The eight C atoms of the two cyclobutene rings showed little indication of anisotropy and were treated isotropically in further refinement. With a reduced sphere of data ($\sin\theta/\lambda_{\max}$ cut off at 0·4 Å$^{-1}$) a difference map located several H atoms; all other H atom positions were calculated. Final refinement of all non-hydrogen atom positional and thermal motion parameters gave a final $R$ of 0·069 for the observed data. In the early stages of refinement, unit weights were used; in the final stages weights $= 1/\sigma_{F^2}$ were used, where $\sigma_F = \sigma_I/L_p(2F_o)$.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32004 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Fractional atomic coordinates* ($\times 10^4$; *for* Mo *and* As $\times 10^5$) *and thermal motion parameters* ($\times 10^3$; *for* Mo *and* As $\times 10^4$ Å$^2$)

Estimated standard deviations are given in parentheses. The anisotropic temperature factor is of the form:
$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$.
Isotropic temperature factors are $\times 10^3$ Å.

| | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Mo | 50877 (14) | 32010 (8) | 65689 (13) | 381 (7) | 284 (7) | 250 (7) | 124 (5) | −105 (5) | 20 (5) |
| As(1) | 20934 (16) | 32628 (10) | 76922 (15) | 417 (8) | 342 (8) | 202 (7) | 180 (7) | −50 (6) | 28 (6) |
| As(2) | 48421 (16) | 22814 (10) | 36652 (15) | 351 (8) | 341 (8) | 220 (7) | 152 (6) | −24 (6) | 40 (6) |
| F(1) | −1540 (12) | 1127 (7) | 8299 (11) | 89 (7) | 84 (7) | 72 (7) | 11 (6) | −9 (6) | 57 (6) |
| F(2) | −2352 (10) | 2195 (7) | 8177 (9) | 54 (5) | 93 (7) | 39 (5) | 41 (5) | 13 (4) | 4 (5) |
| F(3) | −1750 (10) | −6 (6) (6) | 5324 (11) | 69 (6) | 32 (5) | 88 (7) | 11 (4) | −15 (5) | 23 (5) |
| F(4) | −2664 (9) | 1012 (6) | 5209 (10) | 44 (5) | 60 (6) | 72 (6) | 25 (4) | −21 (4) | 9 (5) |
| F(5) | −187 (12) | 162 (7) | 1714 (11) | 96 (7) | 66 (7) | 51 (6) | 12 (6) | −40 (6) | −5 (5) |
| F(6) | −198 (12) | 1608 (8) | 2046 (11) | 88 (7) | 119 (9) | 61 (9) | 60 (7) | 21 (5) | −25 (6) |
| F(7) | 3006 (12) | 633 (7) | 273 (9) | 115 (8) | 94 (8) | 24 (5) | 70 (6) | −6 (5) | −9 (6) |
| F(8) | 2976 (12) | 2115 (7) | 714 (10) | 113 (8) | 90 (7) | 43 (5) | 44 (6) | −13 (5) | 32 (5) |
| O(1) | 3976 (14) | 1137 (8) | 7093 (12) | 93 (9) | 45 (7) | 49 (7) | 22 (6) | −3 (6) | 16 (6) |
| O(2) | 6312 (17) | 5318 (9) | 6213 (15) | 118 (11) | 43 (7) | 85 (9) | 15 (7) | −12 (8) | 27 (7) |
| O(3) | 8759 (14) | 3264 (9) | 5350 (15) | 61 (8) | 90 (9) | 90 (10) | 31 (7) | −8 (7) | 32 (8) |
| O(4) | 5868 (16) | 4215 (9) | 9891 (13) | 136 (11) | 64 (8) | 58 (8) | 33 (7) | −64 (8) | −6 (6) |
| C(1) | 4361 (17) | 1862 (11) | 6886 (15) | 54 (9) | 38 (9) | 20 (7) | 1 (7) | −8 (6) | 2 (7) |
| C(2) | 5811 (17) | 4547 (12) | 6331 (17) | 49 (9) | 46 (10) | 36 (9) | 8 (8) | −13 (7) | 3 (8) |
| C(3) | 7354 (19) | 3235 (10) | 5822 (17) | 53 (10) | 39 (9) | 40 (9) | 12 (7) | −21 (8) | 9 (7) |
| C(4) | 5541 (16) | 3849 (10) | 8665 (19) | 46 (9) | 32 (8) | 59 (11) | 8 (7) | −30 (8) | 4 (7) |
| C(13) | 1099 (21) | 3321 (13) | 9855 (16) | 93 (13) | 85 (13) | 21 (8) | 48 (11) | 10 (8) | 14 (8) |
| C(14) | 1505 (21) | 4300 (10) | 7655 (20) | 98 (13) | 30 (9) | 75 (12) | 31 (9) | −37 (10) | 2 (8) |
| C(15) | 5498 (20) | 1067 (12) | 2561 (19) | 68 (11) | 60 (11) | 61 (11) | 47 (9) | −2 (9) | −2 (9) |
| C(16) | 6236 (19) | 3024 (12) | 2274 (18) | 62 (10) | 57 (10) | 41 (9) | 12 (8) | 11 (8) | 23 (8) |

| | $x$ | $y$ | $z$ | $U_{iso}$ | | $x$ | $y$ | $z$ |
|---|---|---|---|---|---|---|---|---|
| C(5) | 427 (15) | 2151 (9) | 6741 (15) | 37 (3) | H13(3) | 1176 | 2783 | 10055 |
| C(6) | −1300 (17) | 1615 (10) | 7378 (17) | 45 (4) | H14(1) | 186 | 4183 | 8015 |
| C(7) | −1483 (16) | 980 (10) | 5667 (16) | 42 (3) | H14(2) | 1675 | 4126 | 6440 |
| C(8) | 203 (14) | 1578 (9) | 5237 (14) | 31 (3) | H14(3) | 2420 | 4985 | 8307 |
| C(9) | 1239 (15) | 1552 (9) | 3661 (15) | 33 (3) | H15(1) | 6913 | 1365 | 2535 |
| C(10) | 654 (18) | 1135 (11) | 2158 (18) | 50 (4) | H15(2) | 5293 | 728 | 1507 |
| C(11) | 2425 (18) | 1397 (11) | 1377 (18) | 50 (4) | H15(3) | 4925 | 593 | 3141 |
| C(12) | 2831 (15) | 1784 (9) | 2987 (15) | 33 (3) | H16(1) | 6483 | 2568 | 1232 |
| H13(1) | −250 | 3248 | 10072 | † | H16(2) | 7255 | 3461 | 2649 |
| H13(2) | 1630 | 3955 | 10592 | | H16(3) | 5690 | 3446 | 2289 |

† Anisotropic temperature factor of 0·063 Å$^2$ was assigned to each of the hydrogen atoms on C(13)–C(16).

Scattering factors for Mo and As were those given by Cromer & Waber (1965), and for the other non-hydrogen atoms, those from *International Tables for X-ray Crystallography* (1962). The H scattering factors were from Stewart, Davidson & Simpson (1965). Anomalous dispersion corrections for Mo and As were from Cromer (1965). Computer programs were those described by Einstein & Jones (1972).

Final atomic coordinates and thermal parameters are listed in Table 1 and bond lengths and angles in Table 2. The atom labelling is illustrated in Fig. 1, drawn with *ORTEP* (Johnson, 1970).

Table 2. *Interatomic distances* (Å) *and angles* (°)

| | | | |
|---|---|---|---|
| Mo–C(1) | 2·05 (2) | C(1)–O(1) | 1·13 (2) |
| Mo–C(2) | 2·03 (2) | C(2)–O(2) | 1·15 (2) |
| Mo–C(3) | 1·94 (2) | C(3)–O(3) | 1·19 (2) |
| Mo–C(4) | 1·93 (2) | C(4)–O(4) | 1·16 (2) |
| As(1)–Mo | 2·593 (2) | As(2)–Mo | 2·584 (2) |
| As(1)–C(5) | 1·90 (1) | As(2)–C(12) | 1·92 (1) |
| As(1)–C(13) | 1·94 (1) | As(2)–C(15) | 1·96 (1) |
| As(1)–C(14) | 1·93 (1) | As(2)–C(16) | 1·93 (1) |
| C(5)–C(8) | 1·37 (2) | C(12)–C(9) | 1·33 (2) |
| C(5)–C(6) | 1·50 (2) | C(12)–C(11) | 1·53 (2) |
| C(6)–C(7) | 1·54 (2) | C(11)–C(10) | 1·49 (2) |
| C(6)–F(1) | 1·32 (2) | C(11)–F(7) | 1·37 (2) |
| C(6)–F(2) | 1·39 (2) | C(11)–F(8) | 1·37 (2) |
| C(7)–F(3) | 1·36 (2) | C(10)–F(5) | 1·34 (2) |
| C(7)–F(4) | 1·34 (2) | C(10)–F(6) | 1·34 (2) |
| C(7)–C(8) | 1·46 (2) | C(10)–C(9) | 1·51 (2) |
| C(8)–C(9) | 1·47 (2) | | |

Average C–H in methyl groups 1·04

**Discussion.** The title compound is one of a series of metal carbonyl complexes containing ditertiary (phosphine or arsine) ligands with bialicyclic bridging

Table 2 (*cont.*)

| | | | |
|---|---|---|---|
| Mo—C(1)—O(1) | 178·3 (1) | Mo—C(2)—O(2) | 175·7 (1) |
| Mo—C(3)—O(3) | 179·1 (1) | Mo—C(4)—O(4) | 176·8 (1) |
| As(1)—Mo—C(1) | 89·9 (4) | As(2)—Mo—C(1) | 90·2 (4) |
| As(1)—Mo—C(2) | 90·0 (4) | As(2)—Mo—C(2) | 91·7 (4) |
| As(1)—Mo—C(3) | 176·6 (4) | As(2)—Mo—C(3) | 86·4 (4) |
| As(1)—Mo—C(4) | 91·1 (4) | As(2)—Mo—C(4) | 172·4 (4) |
| As(1)—Mo—As(2) | 96·3 (1) | C(3)—Mo—C(4) | 86·3 (6) |
| C(1)—Mo—C(4) | 88·0 (5) | C(1)—Mo—C(3) | 92·4 (6) |
| C(2)—Mo—C(4) | 90·1 (6) | C(2)—Mo—C(3) | 87·8 (6) |
| C(1)—Mo—C(2) | 178·1 (6) | | |
| Mo—As(1)—C(13) | 118·3 (5) | Mo—As(2)—C(15) | 116·5 (5) |
| Mo—As(1)—C(14) | 120·3 (5) | Mo—As(2)—C(16) | 114·9 (5) |
| Mo—As(1)—C(5) | 117·5 (4) | Mo—As(2)—C(12) | 123·8 (4) |
| C(13)—As(1)—C(14) | 100·4 (7) | C(15)—As(2)—C(16) | 99·9 (7) |
| C(13)—As(1)—C(5) | 97·9 (7) | C(15)—As(2)—C(12) | 98·1 (6) |
| C(14)—As(1)—C(5) | 98·0 (6) | C(16)—As(2)—C(12) | 99·6 (6) |
| As(1)—C(5)—C(8) | 136·6 (10) | As(2)—C(12)—C(9) | 135·8 (10) |
| As(1)—C(5)—C(6) | 133·4 (10) | As(2)—C(12)—C(11) | 133·4 (10) |
| C(6)—C(5)—C(8) | 89·8 (10) | C(11)—C(12)—C(9) | 90·6 (10) |
| C(5)—C(6)—C(7) | 88·3 (10) | C(12)—C(11)—C(10) | 88·3 (11) |
| C(5)—C(6)—F(1) | 118·5 (12) | C(12)—C(11)—F(7) | 115·2 (12) |
| C(5)—C(6)—F(2) | 117·0 (11) | C(12)—C(11)—F(8) | 113·4 (12) |
| F(1)—C(6)—F(2) | 105·2 (12) | F(7)—C(11)—F(8) | 106·1 (12) |
| F(1)—C(6)—C(7) | 116·5 (12) | F(7)—C(11)—C(10) | 117·1 (13) |
| F(2)—C(6)—C(7) | 113·0 (11) | F(8)—C(11)—C(10) | 116·4 (13) |
| C(6)—C(7)—C(8) | 85·9 (10) | C(11)—C(10)—C(9) | 85·8 (17) |
| C(6)—C(7)—F(3) | 113·1 (12) | C(11)—C(10)—F(5) | 115·7 (13) |
| C(6)—C(7)—F(4) | 117·0 (11) | C(11)—C(10)—F(6) | 114·8 (13) |
| F(1)—C(6)—F(2) | 105·2 (12) | F(7)—C(11)—F(8) | 106·1 (12) |
| F(1)—C(6)—C(7) | 116·5 (12) | F(7)—C(11)—C(10) | 117·1 (13) |
| F(2)—C(6)—C(7) | 113·0 (11) | F(8)—C(11)—C(10) | 116·4 (13) |
| C(6)—C(7)—C(8) | 85·0 (10) | C(11)—C(10)—C(9) | 85·8 (17) |
| C(6)—C(7)—F(3) | 113·1 (12) | C(11)—C(10)—F(5) | 115·7 (13) |
| C(6)—C(7)—F(4) | 117·0 (11) | C(11)—C(10)—F(6) | 114·8 (13) |
| F(3)—C(7)—F(4) | 105·3 (11) | F(5)—C(10)—F(6) | 107·0 (12) |
| F(3)—C(7)—C(8) | 116·9 (11) | F(5)—C(10)—C(9) | 115·8 (12) |
| F(4)—C(7)—C(8) | 119·1 (12) | F(6)—C(10)—C(9) | 117·0 (12) |
| C(7)—C(8)—C(9) | 129·1 (11) | C(10)—C(9)—C(8) | 126·5 (11) |
| C(7)—C(8)—C(5) | 96·9 (11) | C(10)—C(9)—C(12) | 95·3 (11) |
| C(5)—C(8)—C(9) | 134·0 (12) | C(12)—C(9)—C(8) | 138·1 (12) |

Table 3. *Atomic displacements from selected least-squares planes*

The orthogonal system of axes has $X$ along **a**, $Y$ in the *ab* plane, and $Z$ along **c***. Weights used in the calculation are given by $W_i = W_{i1}/\sigma^2 = 3/[(\sigma_{x_i})^2 + (\sigma_{y_i})^2 + (\sigma_{z_i})^2]$.

| | | $\chi^2$† |
|---|---|---|
| $A$ | $0{\cdot}7466X - 0{\cdot}6653Y - 0{\cdot}0001Z - 0{\cdot}3105$ | 1·82 |
| $B$ | $0{\cdot}3352X - 0{\cdot}9189Y - 0{\cdot}2078Z - 1{\cdot}1906$ | 0·64 |

Displacements

| Plane $A$ | | | | Plane $B$ | | | |
|---|---|---|---|---|---|---|---|
| As(1) | C(5) | C(8) | C(9) | As(2) | C(12) | C(9) | C(8) |
| 0 | 0·014 | −0·014 | 0·005 | 0·007 | −0·007 | 0·008 | 0·003 |

† $\chi^2$ for a plane $lX + mY + nZ - p = 0$ for $N$ atoms is given by $\sum_{i=1}^{i=N} P_i^2/\sigma^2(P_i)]$, where $\sigma^2(P_i) = (\sigma_{x_i})^2 + m^2(\sigma_{y_i})^2 + n^2(\sigma_{z_i})^2$, and $P_i$ is the distance of atom $i$ from the plane.

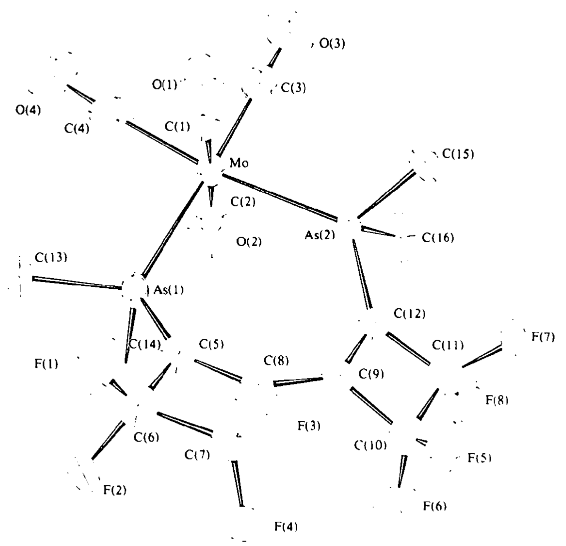

Fig. 1. Perspective view of the title compound illustrating the thermal motion ellipsoids (50%) and labelling.

groups (Cullen, Davis, Einstein, Hazlett & Wu, 1976). The coordination about Mo is nearly octahedral. The bridged diarsine ligand forms a seven-membered chelate in which the puckering can be described in terms of the angle (30·5°) between least-squares planes containing As(1), C(5), C(8), C(9) and As(2), C(12), C(9), C(8) (Fig. 1 and Table 3). The Mo—As lengths of 2·593 (2) and 2·584 (2) Å are comparable to values determined previously for a bridged dimethylarsine ligand bonded to Mo (Nowell & Trotter, 1971), and indicate some back-donation of electrons from Mo to As ($d_\pi \rightarrow d_\pi$). The differences in Mo—C lengths for carbonyl groups *cis* [2·03 (2), 2·05 (2) Å] and *trans* [1·93 (2), 1·94 (2) Å] to the As atoms reflect the greater $\pi$-acidity of the carbonyl group. The C—O bond lengths are consistent with this effect.

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# Hydrotris(triphenylphosphine)platinum(II) Hydrogenbis(trifluoroacetate)

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**Abstract.** $[\mathrm{PtH(PPh_3)_3}](\mathrm{CF_3CO_2})_2\mathrm{H}$, triclinic, $P\bar{1}$, $a = 13{\cdot}104\,(7)$, $b = 13{\cdot}134\,(7)$, $c = 16{\cdot}132\,(9)$ Å, $\alpha = 91{\cdot}07\,(2)$, $\beta = 100{\cdot}05\,(3)$, $\gamma = 102{\cdot}02\,(2)^\circ$, $Z = 2$, $\rho_c = 1{\cdot}51$ g cm$^{-3}$. The distances P(1)—Pt, P(2)—Pt, and P(3)—Pt are 2·315 (7), 2·363 (7) and 2·309 (7) Å, and the bond angles P(3)—Pt—P(2) and P(1)—Pt—P(2) are 99·7 (2) and 100·6 (2)° respectively, while the angle between the *trans* P ligands, P(1)—Pt—P(3), is 159·6 (2)°. The proton was not located but its position was inferred from the geometry around the Pt atoms. The distorted square-planar cation does not interact with the hydrogenbis(trifluoroacetate) anion.

**Introduction.** The $^1$H NMR spectra of salts of the $[\mathrm{PtH(PPh_3)_3}]^+$ cation have been interpreted in terms of second-order effects causing the anticipated double triplet splitting to be observed as an apparent pair of double doublets (Thomas, Dumler, Renoe, Nyman & Roundhill, 1972; Dingle & Dixon, 1974). An alternative explanation has been offered, namely that ion pairing may occur, leading to a stereochemical distortion of the square-planar structure, thereby causing the mutually *trans* triphenylphosphines to become nonequivalent (Bird, Harrod & Than, 1974). The single-crystal structure determination of the title compound was carried out to investigate whether any of these triphenylphosphines showed a significant deviation from planarity in the solid state. A triclinic crystal with dimensions 0·47 × 0·30 × 0·06 mm was used. A total of 5549 reflections were collected with a $\theta$–$2\theta$ step scan (20 steps per degree, 2·2° scan) on an automated four-circle Picker diffractometer out to $2\theta = 45^\circ$, with Mo $K\alpha$ radiation and a Zr filter. The structure was solved with the heavy-atom technique and was refined by full-matrix least-squares calculations with anisotropic thermal parameters for the Pt and P atoms. During data collection, the intensities of standard reflections decreased exponentially with time to 88% of the initial intensities as a result of radiation damage. All data were corrected for this effect. Corrections were made for absorption ($\mu = 2{\cdot}91$ mm$^{-1}$) with transmission factors ranging from 0·84 to 0·92. Refinement was carried out for 5549 reflections. The $R$ value decreased to 0·114 ($R = \Sigma|\Delta F|/\Sigma|F_{\mathrm{obs.}}|$). At this point, it was clear that the F atoms were disordered and undergoing large torsional oscillation, and it was decided that the cost of further structural analysis to sort out the disorder/thermal motion interactions was not justified. The final positional and thermal parameters are shown in Table 1.*

**Discussion.** Interatomic distances and bond angles are listed in Table 2, and an *ORTEP* (Johnson, 1965) drawing of the cation is shown in Fig. 1. This figure shows that the cation adopts a distorted square-planar geometrical arrangement with the mutually *trans* triphenylphosphines in equivalent positions. There is no interaction between cation and anion. The bond angles are 99·7 and 100·6° for P—Pt—P. The H atom on Pt has not been located but the third angle of 159·6° about the Pt center confirms the planarity of the cation. The large cone angle of triphenylphosphine causes considerable in-plane distortion from a square geometry; by comparison, the P—Pt—Cl and P—Pt—Br angles in $\mathrm{PtHCl(PPh_2Et)_2}$ and $\mathrm{PtHBr(PEt_3)_2}$ are close to 94° (Eisenberg & Ibers, 1965; Owston, Partridge & Rowe, 1960). Our structural data agree with the concept that the stereochemical influence of the hydride ligand causes the molecule to adopt a square-planar, albeit considerably distorted, geometry, rather than a trigonal

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32006 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.