Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Di-$\mu$-iodido-bis[iodido(triphenylphosphine-$\kappa P$)platinum(II)]

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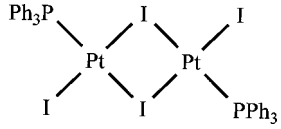
Received 16 October 2007; accepted 23 October 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.023; $wR$ factor = 0.059; data-to-parameter ratio = 16.8.

Each Pt atom in the dimeric iodide-bridged title compound, $[Pt_2I_4(C_{18}H_{15}P)_2]$, is tetracoordinated by a triphenylphosphine P and three I atoms in an approximately square-planar geometry. The *trans* influence of triphenylphosphine is evident from the longer Pt—I bond length.

## Related literature

For related literature, see: Black *et al.* (1969); Chatt (1951); Chatt & Venanzi (1955, 1957); Chatt *et al.* (1964); Jinchao *et al.* (2006).




## Experimental

### *Crystal data*

$[Pt_2I_4(C_{18}H_{15}P)_2]$
$M_r$ = 1422.32
Monoclinic, $P2_1/c$
$a$ = 16.036 (4) Å
$b$ = 15.874 (4) Å
$c$ = 16.882 (4) Å
$\beta$ = 117.980 (4)°
$V$ = 3794.8 (17) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 10.73 mm$^{-1}$
$T$ = 293 (2) K
0.41 × 0.26 × 0.12 mm

### *Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.048, $T_{max}$ = 0.277
35551 measured reflections
6689 independent reflections
6163 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.059
$S$ = 1.09
6689 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.70 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pt1—P1 | 2.2391 (13) | Pt2—P2 | 2.2409 (13) |
| Pt1—I2 | 2.5910 (7) | Pt2—I4 | 2.5892 (7) |
| Pt1—I1 | 2.5967 (7) | Pt2—I3 | 2.5981 (7) |
| Pt1—I4 | 2.6600 (7) | Pt2—I2 | 2.6664 (7) |
| P1—Pt1—I2 | 96.20 (3) | P2—Pt2—I4 | 96.25 (4) |
| P1—Pt1—I1 | 90.90 (3) | P2—Pt2—I3 | 91.16 (4) |
| I2—Pt1—I4 | 83.500 (15) | I4—Pt2—I2 | 83.410 (15) |
| I1—Pt1—I4 | 89.342 (17) | I3—Pt2—I2 | 89.298 (18) |

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Financial support (SR/S1/IC-08/2007) from DST, Government of India, is gratefully acknowledged. We thank CSIR (India) for the award of a fellowship (PD & VB) and UGC (New Delhi) for the Special Assistance Programme to our Department. We also thank the Department of Chemistry, IIT Delhi, for providing the X-ray crystallographic facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2435).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2836 [ **doi:10.1107/S1600536807052488** ]

# Di-$\mu$-iodido-bis[iodido(triphenylphosphine-$\kappa P$)platinum(II)]

**A. N. Biswas, V. Bagchi, P. Das and P. Bandyopadhyay**

## Comment

The dimeric halogen bridged complexes of platinum(II) are very important in synthetic organometallic chemistry (Chatt, 1951 & Chatt and Venanzi, 1955). The main application of the halide bridged complexes is in reactions in which the bridged is cleaved to give monomeric complexes (Chatt and Venanzi, 1957 & Chatt *et al.*, 1964). Recently cytotoxicity of some dimeric iodo bridged platinum(II) complexes has been established (Jinchao *et al.*, 2006). Against this background we report here the crystal structure of (I).

The molecular structure of the title compound, (**I**), is shown in Fig. 1, with the atom numbering scheme. The packing arrangement of (**I**) is shown in Fig. 2. The platinum atom is tetracoordinated with a donor set of one triphenylphosphine P atom and three I atoms in an approximately squareplanar geometry. One of the three iodine atoms is a terminal I, and the other two are bridging I for each platinum atom. Selected bond lengths and bond angles are listed in Table 1. The Pt—I bond lengthes *trans* to the triphenylphosphine moieties are longer and this is supposed to be due to the *trans*-influence of the P atom of the triphenylphosphine moiety. On the other hand Pt—P distances are quite close to the reported values (Black *et al.*, 1969) indicating absence of definite correlation between Pt—P distances and the *trans* influence of the ligand in the *trans* position. This, in turn, is indicative of the fact that Pt(II)—P bonds are not simple sigma bonds, but are more complex and therefore affected by the *trans* ligands in a more complex way than Pt(II)—I bonds.

## Experimental

The title compound (I) was synthesized by stirring a mixture of di-µ-chlorido-bis[$\eta^3$-2-methylallylplatinum(II)], triphenylphosphine and iodine in chloroform medium. The pink compound was isolated by chromatographic technique. Crystals suitable for X-ray crystallography was obtained from a mixture of dichloromethane and hexane (1:5 *v*/*v*).

## Refinement

H atoms were included at calculated positions as riding atoms with C–H set to 0.93 Å for aromatic H atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

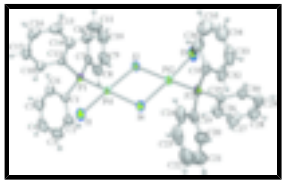

Fig. 1. The asymmetric unit of (**I**), with displacement ellipsoids drawn at the 50% probability level.

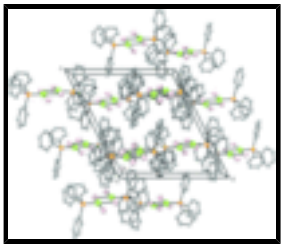

Fig. 2. The molecular arrangement of (**I**) in the *ac* plane. H atoms are omitted for clarity.

**Di-μ-iodido-bis[iodido(triphenylphosphine-κ*P*)platinum(II)]**

*Crystal data*

| | |
|---|---|
| $[Pt_2I_4(C_{18}H_{15}P)_2]$ | $F_{000}$ = 2576 |
| $M_r$ = 1422.32 | $D_x$ = 2.490 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 6689 reflections |
| $a$ = 16.036 (4) Å | θ = 1.4–25.0º |
| $b$ = 15.874 (4) Å | μ = 10.73 mm$^{-1}$ |
| $c$ = 16.882 (4) Å | $T$ = 293 (2) K |
| β = 117.980 (4)º | Needle, pink |
| $V$ = 3794.8 (17) Å$^3$ | 0.41 × 0.26 × 0.12 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 6689 independent reflections |
| Radiation source: fine-focus sealed tube | 6163 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.036 |
| $T$ = 293(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 1.4º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −19→19 |
| $T_{min}$ = 0.048, $T_{max}$ = 0.277 | $k$ = −18→18 |
| 35551 measured reflections | $l$ = −20→20 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.023 | H-atom parameters constrained |
| $wR(F^2)$ = 0.059 | $w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 6.7173P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.09 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 6689 reflections | $\Delta\rho_{max}$ = 0.85 e Å$^{-3}$ |

| | |
|---|---|
| 397 parameters | $\Delta\rho_{min} = -0.70$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C7 | 0.4954 (3) | −0.0138 (3) | 0.1966 (3) | 0.0358 (11) |
| C25 | −0.0345 (3) | −0.3163 (3) | 0.1088 (3) | 0.0401 (11) |
| C13 | 0.5214 (3) | 0.0905 (3) | 0.3493 (3) | 0.0333 (10) |
| C19 | −0.0385 (4) | −0.1714 (3) | 0.2082 (4) | 0.0520 (14) |
| C1 | 0.4272 (3) | 0.1514 (3) | 0.1632 (3) | 0.0356 (11) |
| C2 | 0.3426 (4) | 0.1903 (4) | 0.1075 (4) | 0.0501 (13) |
| H2 | 0.2872 | 0.1737 | 0.1080 | 0.060* |
| C14 | 0.5590 (4) | 0.1701 (3) | 0.3723 (3) | 0.0452 (12) |
| H14 | 0.5408 | 0.2121 | 0.3290 | 0.054* |
| C18 | 0.5461 (4) | 0.0302 (4) | 0.4155 (4) | 0.0522 (14) |
| H18 | 0.5188 | −0.0231 | 0.4011 | 0.063* |
| C6 | 0.5078 (4) | 0.1776 (4) | 0.1598 (4) | 0.0477 (13) |
| H6 | 0.5653 | 0.1518 | 0.1967 | 0.057* |
| C31 | 0.0757 (4) | −0.3099 (4) | 0.3057 (4) | 0.0504 (14) |
| C8 | 0.4557 (4) | −0.0283 (3) | 0.1055 (4) | 0.0494 (13) |
| H8 | 0.4021 | 0.0015 | 0.0664 | 0.059* |
| C26 | −0.0529 (5) | −0.2902 (4) | 0.0234 (4) | 0.0572 (15) |
| H26 | −0.0233 | −0.2425 | 0.0164 | 0.069* |
| C30 | −0.0774 (4) | −0.3872 (3) | 0.1179 (4) | 0.0502 (13) |
| H30 | −0.0658 | −0.4050 | 0.1746 | 0.060* |
| C12 | 0.5733 (4) | −0.0612 (4) | 0.2536 (4) | 0.0609 (16) |
| H12 | 0.6006 | −0.0531 | 0.3153 | 0.073* |
| C3 | 0.3409 (5) | 0.2546 (4) | 0.0508 (4) | 0.0679 (18) |
| H3 | 0.2841 | 0.2811 | 0.0136 | 0.082* |
| C17 | 0.6110 (5) | 0.0485 (4) | 0.5030 (4) | 0.0621 (16) |
| H17 | 0.6282 | 0.0074 | 0.5472 | 0.075* |
| C32 | 0.0074 (5) | −0.3298 (4) | 0.3322 (4) | 0.0621 (17) |
| H32 | −0.0543 | −0.3107 | 0.2984 | 0.075* |
| C36 | 0.1678 (5) | −0.3348 (4) | 0.3594 (4) | 0.0664 (17) |
| H36 | 0.2144 | −0.3207 | 0.3438 | 0.080* |

| | | | | |
|---|---|---|---|---|
| C16 | 0.6499 (4) | 0.1270 (4) | 0.5247 (4) | 0.0576 (16) |
| H16 | 0.6939 | 0.1394 | 0.5835 | 0.069* |
| C15 | 0.6239 (4) | 0.1871 (4) | 0.4599 (4) | 0.0586 (16) |
| H15 | 0.6505 | 0.2406 | 0.4751 | 0.070* |
| C5 | 0.5042 (5) | 0.2406 (4) | 0.1032 (4) | 0.0585 (16) |
| H5 | 0.5592 | 0.2572 | 0.1021 | 0.070* |
| C4 | 0.4216 (6) | 0.2795 (4) | 0.0487 (4) | 0.0635 (18) |
| H4 | 0.4198 | 0.3224 | 0.0105 | 0.076* |
| C29 | −0.1384 (4) | −0.4329 (4) | 0.0426 (5) | 0.0671 (18) |
| H29 | −0.1669 | −0.4815 | 0.0492 | 0.081* |
| C9 | 0.4946 (5) | −0.0863 (4) | 0.0720 (5) | 0.0632 (17) |
| H9 | 0.4683 | −0.0945 | 0.0104 | 0.076* |
| C20 | −0.0143 (5) | −0.1257 (4) | 0.2860 (5) | 0.0679 (18) |
| H20 | 0.0429 | −0.1359 | 0.3368 | 0.081* |
| C27 | −0.1150 (5) | −0.3354 (5) | −0.0509 (4) | 0.0715 (19) |
| H27 | −0.1286 | −0.3171 | −0.1080 | 0.086* |
| C28 | −0.1567 (5) | −0.4069 (4) | −0.0409 (4) | 0.0685 (18) |
| H28 | −0.1976 | −0.4377 | −0.0911 | 0.082* |
| C10 | 0.5714 (5) | −0.1317 (4) | 0.1288 (6) | 0.074 (2) |
| H10 | 0.5976 | −0.1711 | 0.1061 | 0.088* |
| C21 | −0.0755 (7) | −0.0649 (4) | 0.2878 (6) | 0.082 (2) |
| H21 | −0.0583 | −0.0334 | 0.3397 | 0.099* |
| C22 | −0.1594 (7) | −0.0509 (5) | 0.2153 (8) | 0.104 (3) |
| H22 | −0.2011 | −0.0115 | 0.2178 | 0.125* |
| C33 | 0.0311 (6) | −0.3775 (5) | 0.4082 (5) | 0.081 (2) |
| H33 | −0.0149 | −0.3922 | 0.4245 | 0.098* |
| C34 | 0.1221 (7) | −0.4031 (5) | 0.4593 (5) | 0.094 (3) |
| H34 | 0.1381 | −0.4359 | 0.5100 | 0.113* |
| C35 | 0.1905 (6) | −0.3803 (6) | 0.4359 (5) | 0.098 (3) |
| H35 | 0.2529 | −0.3960 | 0.4724 | 0.118* |
| C11 | 0.6099 (5) | −0.1195 (5) | 0.2191 (5) | 0.082 (2) |
| H11 | 0.6618 | −0.1514 | 0.2577 | 0.099* |
| C24 | −0.1237 (5) | −0.1534 (4) | 0.1342 (5) | 0.075 (2) |
| H24 | −0.1413 | −0.1817 | 0.0804 | 0.090* |
| C23 | −0.1826 (6) | −0.0936 (6) | 0.1400 (7) | 0.108 (3) |
| H23 | −0.2402 | −0.0826 | 0.0899 | 0.130* |
| Pt1 | 0.303078 (12) | 0.014176 (11) | 0.230490 (12) | 0.03130 (6) |
| Pt2 | 0.167402 (13) | −0.199608 (12) | 0.193463 (14) | 0.03806 (6) |
| I2 | 0.32173 (2) | −0.140087 (19) | 0.19114 (2) | 0.04119 (9) |
| I4 | 0.14558 (2) | −0.04414 (2) | 0.22637 (3) | 0.04403 (9) |
| I1 | 0.27457 (3) | 0.15825 (2) | 0.28661 (3) | 0.05148 (10) |
| I3 | 0.20461 (3) | −0.34792 (2) | 0.15292 (4) | 0.07113 (14) |
| P1 | 0.43647 (8) | 0.06234 (7) | 0.23499 (8) | 0.0307 (2) |
| P2 | 0.04244 (9) | −0.25019 (8) | 0.20388 (9) | 0.0402 (3) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.036 (3) | 0.030 (2) | 0.047 (3) | −0.003 (2) | 0.024 (2) | 0.001 (2) |
| C25 | 0.036 (3) | 0.038 (3) | 0.046 (3) | −0.006 (2) | 0.019 (2) | −0.006 (2) |
| C13 | 0.025 (2) | 0.040 (3) | 0.035 (2) | 0.0006 (19) | 0.014 (2) | 0.001 (2) |
| C19 | 0.052 (3) | 0.041 (3) | 0.077 (4) | −0.015 (3) | 0.042 (3) | −0.013 (3) |
| C1 | 0.040 (3) | 0.032 (2) | 0.033 (2) | −0.001 (2) | 0.016 (2) | 0.001 (2) |
| C2 | 0.047 (3) | 0.050 (3) | 0.049 (3) | 0.003 (3) | 0.020 (3) | 0.007 (3) |
| C14 | 0.047 (3) | 0.044 (3) | 0.040 (3) | −0.006 (2) | 0.017 (2) | 0.002 (2) |
| C18 | 0.056 (4) | 0.048 (3) | 0.046 (3) | −0.004 (3) | 0.019 (3) | 0.008 (3) |
| C6 | 0.052 (3) | 0.052 (3) | 0.042 (3) | −0.012 (3) | 0.024 (3) | 0.002 (2) |
| C31 | 0.053 (3) | 0.048 (3) | 0.049 (3) | −0.020 (3) | 0.023 (3) | −0.009 (3) |
| C8 | 0.057 (3) | 0.046 (3) | 0.052 (3) | 0.002 (3) | 0.031 (3) | 0.000 (3) |
| C26 | 0.071 (4) | 0.051 (3) | 0.058 (4) | −0.009 (3) | 0.037 (3) | 0.000 (3) |
| C30 | 0.052 (3) | 0.044 (3) | 0.054 (3) | −0.012 (3) | 0.024 (3) | −0.003 (3) |
| C12 | 0.049 (3) | 0.068 (4) | 0.058 (4) | 0.014 (3) | 0.018 (3) | −0.009 (3) |
| C3 | 0.078 (5) | 0.057 (4) | 0.051 (4) | 0.018 (3) | 0.014 (3) | 0.011 (3) |
| C17 | 0.062 (4) | 0.073 (4) | 0.044 (3) | 0.010 (3) | 0.019 (3) | 0.016 (3) |
| C32 | 0.065 (4) | 0.072 (4) | 0.054 (4) | −0.032 (3) | 0.032 (3) | −0.013 (3) |
| C36 | 0.056 (4) | 0.077 (5) | 0.056 (4) | −0.012 (3) | 0.018 (3) | −0.005 (3) |
| C16 | 0.044 (3) | 0.085 (5) | 0.036 (3) | 0.000 (3) | 0.012 (3) | −0.006 (3) |
| C15 | 0.063 (4) | 0.061 (4) | 0.048 (3) | −0.021 (3) | 0.023 (3) | −0.015 (3) |
| C5 | 0.072 (4) | 0.060 (4) | 0.047 (3) | −0.023 (3) | 0.032 (3) | −0.003 (3) |
| C4 | 0.105 (6) | 0.043 (3) | 0.046 (3) | −0.015 (4) | 0.039 (4) | 0.001 (3) |
| C29 | 0.058 (4) | 0.052 (4) | 0.079 (5) | −0.017 (3) | 0.021 (4) | −0.012 (3) |
| C9 | 0.085 (5) | 0.054 (4) | 0.062 (4) | 0.000 (3) | 0.044 (4) | −0.008 (3) |
| C20 | 0.078 (5) | 0.060 (4) | 0.091 (5) | −0.024 (3) | 0.061 (4) | −0.019 (4) |
| C27 | 0.081 (5) | 0.089 (5) | 0.044 (3) | −0.003 (4) | 0.029 (3) | −0.008 (3) |
| C28 | 0.068 (4) | 0.069 (4) | 0.055 (4) | −0.010 (4) | 0.018 (3) | −0.018 (3) |
| C10 | 0.077 (5) | 0.060 (4) | 0.106 (6) | 0.009 (4) | 0.061 (5) | −0.015 (4) |
| C21 | 0.109 (7) | 0.056 (4) | 0.130 (7) | −0.027 (4) | 0.097 (6) | −0.033 (4) |
| C22 | 0.100 (7) | 0.065 (5) | 0.183 (11) | 0.005 (5) | 0.095 (8) | −0.016 (6) |
| C33 | 0.114 (7) | 0.080 (5) | 0.059 (4) | −0.052 (5) | 0.049 (5) | −0.023 (4) |
| C34 | 0.118 (7) | 0.090 (6) | 0.047 (4) | −0.039 (5) | 0.016 (5) | −0.003 (4) |
| C35 | 0.090 (6) | 0.113 (7) | 0.059 (5) | −0.013 (5) | 0.006 (4) | 0.005 (5) |
| C11 | 0.073 (5) | 0.080 (5) | 0.083 (5) | 0.038 (4) | 0.029 (4) | −0.006 (4) |
| C24 | 0.064 (4) | 0.061 (4) | 0.094 (5) | 0.015 (3) | 0.032 (4) | −0.009 (4) |
| C23 | 0.087 (6) | 0.084 (6) | 0.144 (9) | 0.029 (5) | 0.047 (6) | −0.012 (6) |
| Pt1 | 0.02656 (10) | 0.02947 (10) | 0.03885 (11) | −0.00243 (7) | 0.01617 (8) | −0.00024 (7) |
| Pt2 | 0.03339 (11) | 0.03118 (11) | 0.05433 (13) | −0.00463 (8) | 0.02450 (10) | −0.00138 (8) |
| I2 | 0.03562 (18) | 0.03096 (16) | 0.0641 (2) | −0.00209 (13) | 0.02933 (17) | −0.00143 (14) |
| I4 | 0.03608 (18) | 0.03389 (17) | 0.0713 (2) | −0.00430 (13) | 0.03281 (17) | −0.00441 (15) |
| I1 | 0.0483 (2) | 0.03940 (19) | 0.0768 (3) | −0.00636 (15) | 0.0377 (2) | −0.01506 (17) |
| I3 | 0.0653 (3) | 0.0387 (2) | 0.1323 (4) | −0.00821 (18) | 0.0654 (3) | −0.0169 (2) |
| P1 | 0.0267 (6) | 0.0299 (6) | 0.0356 (6) | −0.0025 (5) | 0.0147 (5) | 0.0001 (5) |
| P2 | 0.0378 (7) | 0.0372 (7) | 0.0510 (8) | −0.0108 (6) | 0.0254 (6) | −0.0056 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C7—C8 | 1.380 (7) | C36—C35 | 1.372 (10) |
| C7—C12 | 1.388 (8) | C36—H36 | 0.9300 |

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|---|---|---|---|
| C7—P1 | 1.829 (5) | C16—C15 | 1.361 (9) |
| C25—C30 | 1.365 (7) | C16—H16 | 0.9300 |
| C25—C26 | 1.391 (8) | C15—H15 | 0.9300 |
| C25—P2 | 1.828 (5) | C5—C4 | 1.355 (9) |
| C13—C14 | 1.376 (7) | C5—H5 | 0.9300 |
| C13—C18 | 1.381 (7) | C4—H4 | 0.9300 |
| C13—P1 | 1.820 (5) | C29—C28 | 1.361 (9) |
| C19—C24 | 1.382 (9) | C29—H29 | 0.9300 |
| C19—C20 | 1.386 (8) | C9—C10 | 1.359 (9) |
| C19—P2 | 1.828 (6) | C9—H9 | 0.9300 |
| C1—C2 | 1.382 (7) | C20—C21 | 1.387 (10) |
| C1—C6 | 1.383 (7) | C20—H20 | 0.9300 |
| C1—P1 | 1.823 (5) | C27—C28 | 1.367 (10) |
| C2—C3 | 1.391 (8) | C27—H27 | 0.9300 |
| C2—H2 | 0.9300 | C28—H28 | 0.9300 |
| C14—C15 | 1.379 (8) | C10—C11 | 1.363 (10) |
| C14—H14 | 0.9300 | C10—H10 | 0.9300 |
| C18—C17 | 1.382 (8) | C21—C22 | 1.347 (12) |
| C18—H18 | 0.9300 | C21—H21 | 0.9300 |
| C6—C5 | 1.367 (8) | C22—C23 | 1.329 (13) |
| C6—H6 | 0.9300 | C22—H22 | 0.9300 |
| C31—C36 | 1.378 (9) | C33—C34 | 1.363 (12) |
| C31—C32 | 1.400 (8) | C33—H33 | 0.9300 |
| C31—P2 | 1.811 (6) | C34—C35 | 1.376 (12) |
| C8—C9 | 1.374 (8) | C34—H34 | 0.9300 |
| C8—H8 | 0.9300 | C35—H35 | 0.9300 |
| C26—C27 | 1.381 (9) | C11—H11 | 0.9300 |
| C26—H26 | 0.9300 | C24—C23 | 1.375 (10) |
| C30—C29 | 1.391 (8) | C24—H24 | 0.9300 |
| C30—H30 | 0.9300 | C23—H23 | 0.9300 |
| C12—C11 | 1.365 (8) | Pt1—P1 | 2.2391 (13) |
| C12—H12 | 0.9300 | Pt1—I2 | 2.5910 (7) |
| C3—C4 | 1.368 (10) | Pt1—I1 | 2.5967 (7) |
| C3—H3 | 0.9300 | Pt1—I4 | 2.6600 (7) |
| C17—C16 | 1.364 (9) | Pt2—P2 | 2.2409 (13) |
| C17—H17 | 0.9300 | Pt2—I4 | 2.5892 (7) |
| C32—C33 | 1.382 (9) | Pt2—I3 | 2.5981 (7) |
| C32—H32 | 0.9300 | Pt2—I2 | 2.6664 (7) |
| C8—C7—C12 | 118.5 (5) | C28—C29—H29 | 119.8 |
| C8—C7—P1 | 117.4 (4) | C30—C29—H29 | 119.8 |
| C12—C7—P1 | 124.0 (4) | C10—C9—C8 | 120.1 (6) |
| C30—C25—C26 | 119.2 (5) | C10—C9—H9 | 119.9 |
| C30—C25—P2 | 122.9 (4) | C8—C9—H9 | 119.9 |
| C26—C25—P2 | 117.8 (4) | C19—C20—C21 | 119.9 (8) |
| C14—C13—C18 | 119.2 (5) | C19—C20—H20 | 120.0 |
| C14—C13—P1 | 122.4 (4) | C21—C20—H20 | 120.0 |
| C18—C13—P1 | 118.4 (4) | C28—C27—C26 | 120.3 (6) |
| C24—C19—C20 | 117.8 (6) | C28—C27—H27 | 119.8 |
| C24—C19—P2 | 121.7 (5) | C26—C27—H27 | 119.8 |

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|---|---|---|---|
| C20—C19—P2 | 120.5 (5) | C29—C28—C27 | 119.9 (6) |
| C2—C1—C6 | 118.5 (5) | C29—C28—H28 | 120.0 |
| C2—C1—P1 | 123.1 (4) | C27—C28—H28 | 120.0 |
| C6—C1—P1 | 118.3 (4) | C9—C10—C11 | 119.9 (6) |
| C1—C2—C3 | 119.4 (6) | C9—C10—H10 | 120.1 |
| C1—C2—H2 | 120.3 | C11—C10—H10 | 120.1 |
| C3—C2—H2 | 120.3 | C22—C21—C20 | 120.6 (8) |
| C13—C14—C15 | 119.6 (5) | C22—C21—H21 | 119.7 |
| C13—C14—H14 | 120.2 | C20—C21—H21 | 119.7 |
| C15—C14—H14 | 120.2 | C23—C22—C21 | 119.8 (8) |
| C13—C18—C17 | 120.3 (6) | C23—C22—H22 | 120.1 |
| C13—C18—H18 | 119.8 | C21—C22—H22 | 120.1 |
| C17—C18—H18 | 119.8 | C34—C33—C32 | 119.8 (7) |
| C5—C6—C1 | 120.9 (6) | C34—C33—H33 | 120.1 |
| C5—C6—H6 | 119.5 | C32—C33—H33 | 120.1 |
| C1—C6—H6 | 119.5 | C33—C34—C35 | 120.1 (8) |
| C36—C31—C32 | 118.9 (6) | C33—C34—H34 | 120.0 |
| C36—C31—P2 | 121.4 (5) | C35—C34—H34 | 120.0 |
| C32—C31—P2 | 119.6 (5) | C36—C35—C34 | 120.9 (8) |
| C9—C8—C7 | 120.6 (6) | C36—C35—H35 | 119.6 |
| C9—C8—H8 | 119.7 | C34—C35—H35 | 119.6 |
| C7—C8—H8 | 119.7 | C10—C11—C12 | 120.9 (6) |
| C27—C26—C25 | 119.9 (6) | C10—C11—H11 | 119.5 |
| C27—C26—H26 | 120.1 | C12—C11—H11 | 119.5 |
| C25—C26—H26 | 120.1 | C23—C24—C19 | 119.9 (8) |
| C25—C30—C29 | 120.2 (6) | C23—C24—H24 | 120.0 |
| C25—C30—H30 | 119.9 | C19—C24—H24 | 120.0 |
| C29—C30—H30 | 119.9 | C22—C23—C24 | 121.8 (9) |
| C11—C12—C7 | 120.0 (6) | C22—C23—H23 | 119.1 |
| C11—C12—H12 | 120.0 | C24—C23—H23 | 119.1 |
| C7—C12—H12 | 120.0 | P1—Pt1—I2 | 96.20 (3) |
| C4—C3—C2 | 121.1 (6) | P1—Pt1—I1 | 90.90 (3) |
| C4—C3—H3 | 119.5 | I2—Pt1—I1 | 170.796 (13) |
| C2—C3—H3 | 119.5 | P1—Pt1—I4 | 179.44 (3) |
| C16—C17—C18 | 120.0 (6) | I2—Pt1—I4 | 83.500 (15) |
| C16—C17—H17 | 120.0 | I1—Pt1—I4 | 89.342 (17) |
| C18—C17—H17 | 120.0 | P2—Pt2—I4 | 96.25 (4) |
| C33—C32—C31 | 120.3 (7) | P2—Pt2—I3 | 91.16 (4) |
| C33—C32—H32 | 119.9 | I4—Pt2—I3 | 172.337 (14) |
| C31—C32—H32 | 119.9 | P2—Pt2—I2 | 176.76 (4) |
| C35—C36—C31 | 119.9 (7) | I4—Pt2—I2 | 83.410 (15) |
| C35—C36—H36 | 120.0 | I3—Pt2—I2 | 89.298 (18) |
| C31—C36—H36 | 120.0 | Pt1—I2—Pt2 | 96.405 (15) |
| C15—C16—C17 | 119.7 (5) | Pt2—I4—Pt1 | 96.605 (16) |
| C15—C16—H16 | 120.2 | C13—P1—C1 | 107.6 (2) |
| C17—C16—H16 | 120.2 | C13—P1—C7 | 106.5 (2) |
| C16—C15—C14 | 121.2 (6) | C1—P1—C7 | 99.8 (2) |
| C16—C15—H15 | 119.4 | C13—P1—Pt1 | 110.34 (15) |
| C14—C15—H15 | 119.4 | C1—P1—Pt1 | 117.65 (16) |

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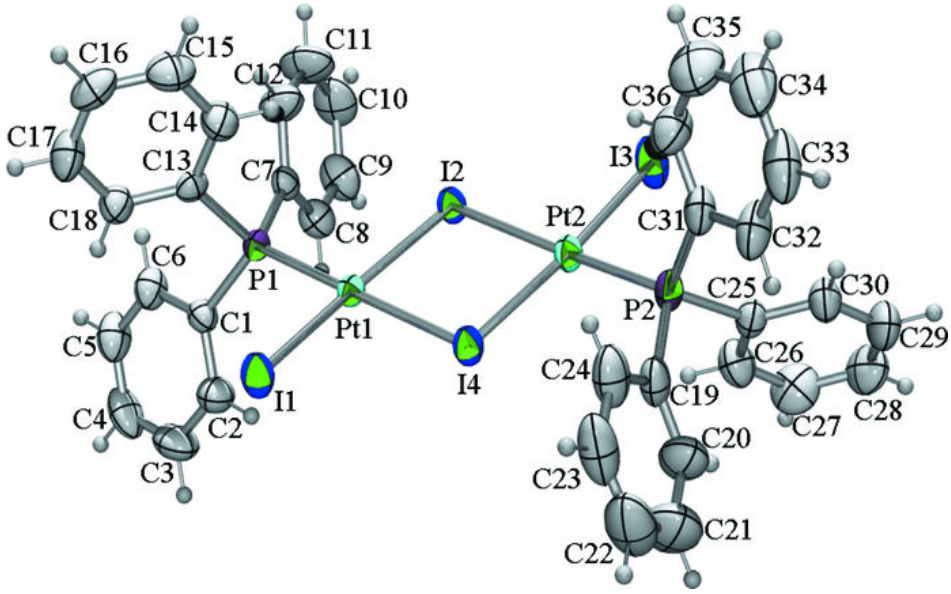
|---|---|---|---|
| C4—C5—C6 | 121.0 (6) | C7—P1—Pt1 | 113.98 (15) |
| C4—C5—H5 | 119.5 | C31—P2—C25 | 108.1 (2) |
| C6—C5—H5 | 119.5 | C31—P2—C19 | 102.6 (3) |
| C5—C4—C3 | 119.1 (6) | C25—P2—C19 | 103.2 (3) |
| C5—C4—H4 | 120.5 | C31—P2—Pt2 | 112.71 (19) |
| C3—C4—H4 | 120.5 | C25—P2—Pt2 | 113.36 (17) |
| C28—C29—C30 | 120.3 (6) | C19—P2—Pt2 | 115.85 (17) |
| C6—C1—C2—C3 | −0.6 (8) | P2—Pt2—I4—Pt1 | 174.64 (4) |
| P1—C1—C2—C3 | −176.1 (4) | I2—Pt2—I4—Pt1 | −2.114 (12) |
| C18—C13—C14—C15 | 3.1 (8) | I2—Pt1—I4—Pt2 | 2.176 (13) |
| P1—C13—C14—C15 | −179.3 (4) | I1—Pt1—I4—Pt2 | −172.027 (14) |
| C14—C13—C18—C17 | −2.9 (8) | C14—C13—P1—C1 | 7.3 (5) |
| P1—C13—C18—C17 | 179.4 (5) | C18—C13—P1—C1 | −175.1 (4) |
| C2—C1—C6—C5 | 0.3 (8) | C14—C13—P1—C7 | 113.6 (4) |
| P1—C1—C6—C5 | 176.0 (4) | C18—C13—P1—C7 | −68.8 (4) |
| C12—C7—C8—C9 | −2.2 (8) | C14—C13—P1—Pt1 | −122.3 (4) |
| P1—C7—C8—C9 | −178.2 (5) | C18—C13—P1—Pt1 | 55.4 (4) |
| C30—C25—C26—C27 | 0.9 (9) | C2—C1—P1—C13 | −124.7 (4) |
| P2—C25—C26—C27 | −176.1 (5) | C6—C1—P1—C13 | 59.8 (4) |
| C26—C25—C30—C29 | 0.3 (9) | C2—C1—P1—C7 | 124.4 (5) |
| P2—C25—C30—C29 | 177.2 (5) | C6—C1—P1—C7 | −51.1 (4) |
| C8—C7—C12—C11 | 1.1 (9) | C2—C1—P1—Pt1 | 0.6 (5) |
| P1—C7—C12—C11 | 176.8 (6) | C6—C1—P1—Pt1 | −174.9 (3) |
| C1—C2—C3—C4 | 0.5 (9) | C8—C7—P1—C13 | −163.5 (4) |
| C13—C18—C17—C16 | 1.1 (9) | C12—C7—P1—C13 | 20.7 (5) |
| C36—C31—C32—C33 | −3.6 (9) | C8—C7—P1—C1 | −51.8 (4) |
| P2—C31—C32—C33 | 178.0 (5) | C12—C7—P1—C1 | 132.5 (5) |
| C32—C31—C36—C35 | 1.9 (10) | C8—C7—P1—Pt1 | 74.6 (4) |
| P2—C31—C36—C35 | −179.7 (6) | C12—C7—P1—Pt1 | −101.2 (5) |
| C18—C17—C16—C15 | 0.4 (10) | I2—Pt1—P1—C13 | −111.86 (17) |
| C17—C16—C15—C14 | −0.2 (10) | I1—Pt1—P1—C13 | 62.29 (17) |
| C13—C14—C15—C16 | −1.6 (9) | I2—Pt1—P1—C1 | 124.25 (18) |
| C1—C6—C5—C4 | 0.0 (9) | I1—Pt1—P1—C1 | −61.61 (18) |
| C6—C5—C4—C3 | −0.1 (9) | I2—Pt1—P1—C7 | 7.88 (18) |
| C2—C3—C4—C5 | −0.1 (9) | I1—Pt1—P1—C7 | −177.97 (18) |
| C25—C30—C29—C28 | −0.7 (10) | C36—C31—P2—C25 | 113.6 (5) |
| C7—C8—C9—C10 | 1.8 (9) | C32—C31—P2—C25 | −68.0 (5) |
| C24—C19—C20—C21 | 0.7 (9) | C36—C31—P2—C19 | −137.8 (5) |
| P2—C19—C20—C21 | 178.6 (5) | C32—C31—P2—C19 | 40.6 (5) |
| C25—C26—C27—C28 | −1.7 (10) | C36—C31—P2—Pt2 | −12.5 (6) |
| C30—C29—C28—C27 | −0.1 (11) | C32—C31—P2—Pt2 | 165.9 (4) |
| C26—C27—C28—C29 | 1.3 (11) | C30—C25—P2—C31 | 16.1 (5) |
| C8—C9—C10—C11 | −0.1 (11) | C26—C25—P2—C31 | −167.0 (4) |
| C19—C20—C21—C22 | 1.5 (10) | C30—C25—P2—C19 | −92.1 (5) |
| C20—C21—C22—C23 | −2.5 (13) | C26—C25—P2—C19 | 84.8 (5) |
| C31—C32—C33—C34 | 2.2 (10) | C30—C25—P2—Pt2 | 141.8 (4) |
| C32—C33—C34—C35 | 0.9 (12) | C26—C25—P2—Pt2 | −41.3 (5) |
| C31—C36—C35—C34 | 1.2 (12) | C24—C19—P2—C31 | −134.2 (5) |
| C33—C34—C35—C36 | −2.6 (13) | C20—C19—P2—C31 | 48.0 (5) |

| | | | |
|---|---|---|---|
| C9—C10—C11—C12 | −1.0 (12) | C24—C19—P2—C25 | −21.9 (6) |
| C7—C12—C11—C10 | 0.5 (12) | C20—C19—P2—C25 | 160.3 (5) |
| C20—C19—C24—C23 | −1.9 (11) | C24—C19—P2—Pt2 | 102.6 (5) |
| P2—C19—C24—C23 | −179.8 (7) | C20—C19—P2—Pt2 | −75.2 (5) |
| C21—C22—C23—C24 | 1.3 (15) | I4—Pt2—P2—C31 | −106.6 (2) |
| C19—C24—C23—C22 | 1.0 (14) | I3—Pt2—P2—C31 | 75.3 (2) |
| P1—Pt1—I2—Pt2 | 177.41 (3) | I4—Pt2—P2—C25 | 130.19 (19) |
| I4—Pt1—I2—Pt2 | −2.112 (12) | I3—Pt2—P2—C25 | −47.87 (19) |
| I4—Pt2—I2—Pt1 | 2.170 (13) | I4—Pt2—P2—C19 | 11.1 (2) |
| I3—Pt2—I2—Pt1 | 179.809 (16) | I3—Pt2—P2—C19 | −166.9 (2) |

**Fig. 1**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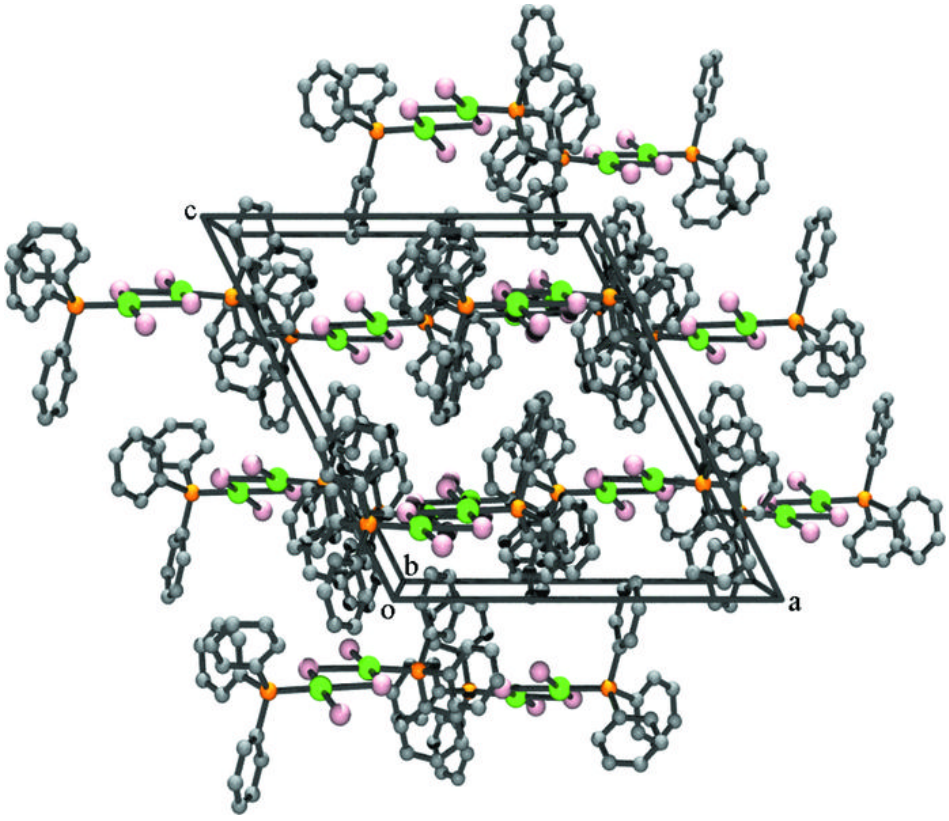
**Fig. 2**