



Crystal structure and Hirshfeld analysis of *trans*-diiodidobis[(methylsulfanyl)benzene- κ S]-platinum(II)

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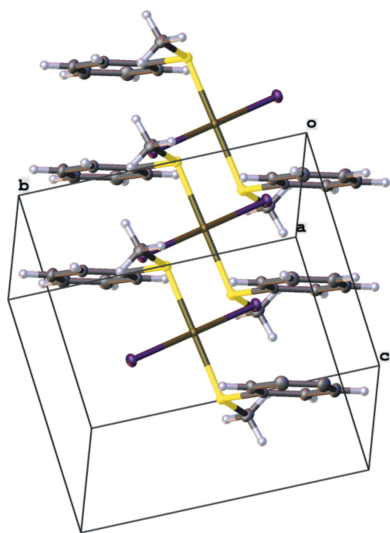
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The title complex, [PtI₂(C₇H₈I₂)₂], represents a further example of a square-planar Pt^{II}-dithioether complex. It crystallizes in the monoclinic space group *P*2₁/*c*. Additional Hirshfeld analyses indicate a C—H... π interaction along the [010] axis to be the most important packing factor.

1. Chemical context

Dithioethers are a quite useful class of ligands for various transition-metal complexes and their coordination chemistry is well documented (Murray & Hartley, 1981). As a result of the soft character of the sulfur center, they preferably bond to soft transition metals like the coinage metals (Cu, Ag, Au), mercury(II), or catalytically active noble metals such as rhodium(I), iridium(I), palladium(II) or platinum(II). Apart from structural aspects (Marangoni *et al.*, 1995) and the investigation of inversion dynamics occurring at the coordinated sulfur atoms (Abel *et al.*, 1984), these complexes have been reported to have several applications in homogeneous catalysis (Masdeu-Bulto *et al.*, 2003; Arrayás & Carretero, 2011). They can form interesting luminescent cluster-like structures (Knorr *et al.*, 2014; Peindy *et al.*, 2007) and even coordination polymers by coordination to Cu^I and Ag^I (Raghuvanshi *et al.*, 2017; Awaleh *et al.*, 2006). Depending on the metal coordination sphere and the remaining ligands, the preparation of dithioether complexes may yield different isomers. In particular, the isomerism of chalcogenoether complexes with palladium and platinum has been intensively investigated (Vigo *et al.*, 2006) and the presence of both *trans*- and *cis*-isomers in solution and the solid state were proven. The clarification of the *trans*-*cis* isomerism is therefore of importance.

In the past, our groups have investigated the coordination of chelating dithioethers such as the vinylic ferrocenyl-dithioether *Z*-[(ArS)(H)C=C(SAr)-Fc] or the silylated compounds (PhSCH₂)₂SiPh₂ and PhSCH₂Si(Me)-Si(Me)-CH₂SPh₂ yielding [Fc-{C(S-*p*-tolyl)=C(S-*p*-tolyl)(H)}PtCl₂], *cis*-[PtCl₂{(PhSCH₂)₂Si₂Me₄}] and *cis*-[PtCl₂{(PhSCH₂)₂-SiPh₂}] and converted them *via* metathesis in the presence of NaI to their corresponding diiodo derivatives (Clement *et al.*, 2007; Knorr *et al.*, 2004; Peindy *et al.*, 2006). We have also shown that the tetrakis(thioether) (PhSCH₂)₄Si can be ligated



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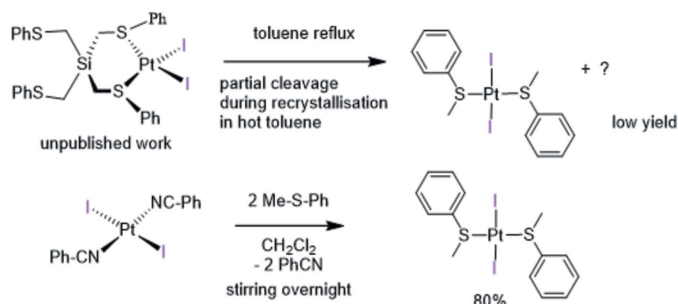
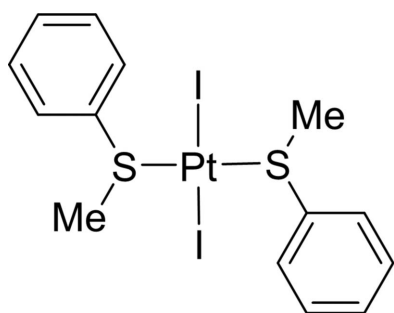


Figure 1
Synthesis scheme for *trans*-PtI₂(SMePh)₂ (**1**).

on HgBr₂ in a chelating manner (Peindy *et al.*, 2005). In a similar manner, we also prepared, as shown in Fig. 1, the complex *cis*-[PtI₂{(PhSCH₂)₂Si(CH₂SPh)₂}. When attempting to recrystallize this poorly soluble compound from hot toluene, partial cleavage of the Si—CH₂Ph bond occurred, yielding *trans*-[PtI₂(SMePh)₂] **1**, albeit in a quite low yield of 10%. Alternatively, this air-stable complex could be prepared in a much improved yield of 80% by reaction of bis(benzonitrile)diodoplatinum with 2 equivalents of methyl phenyl sulfide (thioanisole) MeSPh using dichloromethane as solvent. This compound was characterized by NMR spectroscopy in solution and exhibits a singlet resonance for the two magnetically equivalent methyl groups at δ 3.01 ppm, flanked by ¹⁹⁵Pt satellites due to a ³J_{PtH} coupling of 48 Hz. Furthermore, we report herein on the solid-state structure and structural analysis of *trans*-diiodidobis[(methylsulfanyl)benzene- κ S]-platinum(II) (**1**). In addition, the results of a Hirshfeld analysis of the intermolecular interactions are presented.



2. Structural commentary

trans-Diiodidobis[(methylsulfanyl)benzene- κ S]platinum(II) (**1**) crystallizes from dichloromethane in the monoclinic crystal system, space group *P*2₁/*c*. The molecular structure of **1** is

Table 1
Selected geometric parameters (Å, °).

Pt1—I1	2.6121 (2)	S1—C2	1.782 (2)
Pt1—S1	2.3183 (5)	S1—C1	1.800 (2)
I1 ⁱ —Pt1—I1	180.0	S1—Pt1—I1	85.641 (14)
S1—Pt1—I1 ⁱ	94.359 (14)	C2—S1—C1	103.46 (11)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

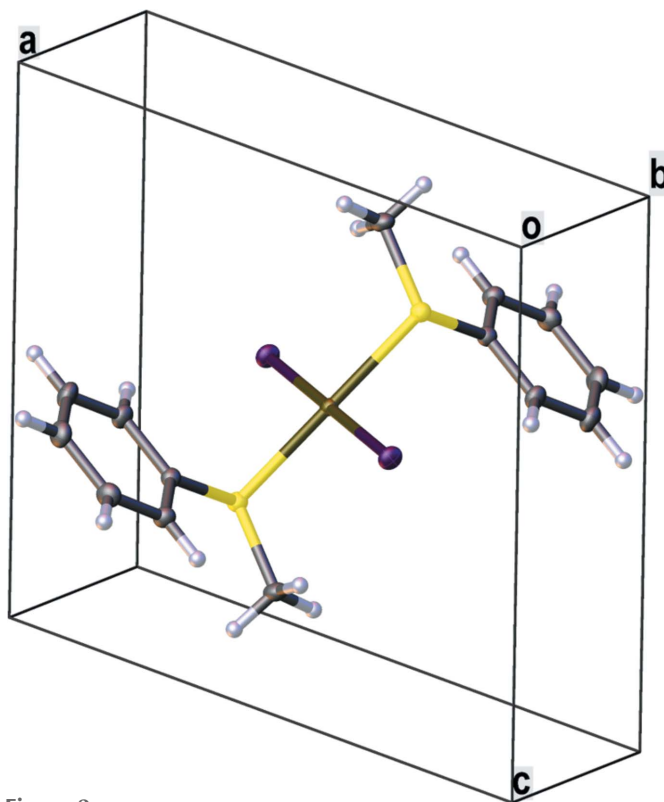


Figure 2
Molecular structure of **1** in the unit cell.

presented in Figs. 2 and 3 and selected bond lengths and bond angles are given in Table 1. The asymmetric unit contains half a molecule of **1**, which shows *C*_{2h} symmetry. The distance from the coordinating iodine center I1 to Pt1 is 2.61205 (15) Å, showing a slight elongation with respect to its educt structure

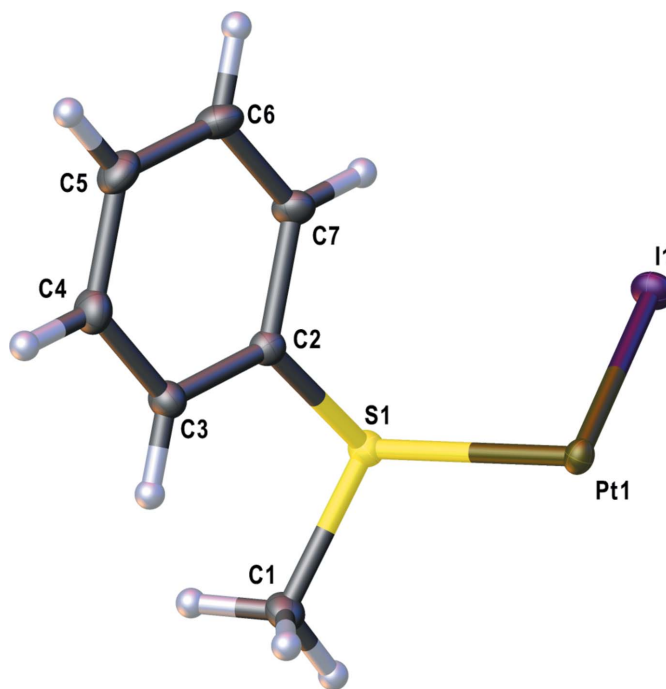


Figure 3
Asymmetric unit of **1** with labeled atoms.

trans-[PtI₂(NCPh)₂] (**2**) (2.6052 (8) Å; Viola *et al.*, 2018). The distance from the coordinating sulfur atom S1 to Pt1 is 2.3183 (5) Å. The S1–Pt1 bond is 0.015 Å longer than in the analogous chlorine compound *trans*-[PtCl₂(SMePh)₂] (**3**) reported by Ahlgrén (CSD LEQSUW; Vigo *et al.*, 2006). This elongation may be explained by the thermodynamic *trans*-effect of the opposite halide ligand. Therefore, similar compounds with iodo ligands such as *trans*-[PtI₂(SMe₂)₂] (**4**) (CSD RAYNOU; Löqvist *et al.*, 1996) and *trans*-[PtI₂(tetrahydrothiophene)₂] (**5**) (CSD SIRPAK; Oskarsson *et al.*, 1990) show S–Pt bond lengths in the same range at 2.310 (2) and 2.310 (1) Å, respectively. Both complexes also have similar bond lengths for the Pt–I bond [2.6039 (8) Å in **4** and 2.606 (1) Å in **5**]. The chelate complexes *cis*-diiodo-[1,2-bis-(phenylsulfanyl)ethane]platinum(II) (CSD ZAJWUC; Marangoni *et al.*, 1995) and *cis*-(1,4-dithiane-*S,S'*)diiodoplatinum(II) (CSD HUFQAA; Johansson & Engelbrecht, 2001) are reported to display Pt–I bond lengths of 2.606 (1) and 2.6035 (5) Å, respectively, and somewhat shorter mean Pt–S bond lengths of 2.265 (2) and 2.2751 (16) Å, respectively.

All further bonds have characteristic dimensions (Allen *et al.*, 1987). The coordination sphere around the platinum center is square-planar. The angles I1–Pt1–I1 and S1–Pt1–

S1 are 180°. However, the angle I1–Pt1–S1 of 85.641 (14)° is somewhat more acute. This slight deviation from the ideal angle of 90° is also reported for the chlorido derivative **3** and the dimethyl sulfide analog **4**, as well as in the tetrahydrothiophene analog **5**. The sulfur center shows a distorted tetrahedral environment with angles C1–S1–Pt1 = 111.00 (8)°, C2–S1–Pt1 = 104.52 (7)° and C2–S1–C1 = 103.46 (11)°.

3. Supramolecular features

While a repetition of the molecular structure of **1** can be seen along the [100] axis and the [001] axis, as shown in Fig. 4, the crystal packing along the [010] axis is defined by C–H··· π interactions of the C2–C7 phenyl ring and H1Bⁱ [symmetry code: (i) $x, \frac{1}{2} - y, -\frac{1}{2} + z$] with a distance between the phenyl ring and H1Bⁱ of 2.5377 (10) Å (Fig. 5). This interaction can also be visualized by a Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) generated by *CrystalExplorer21* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over d_{norm} in the range from –0.0074 to 1.1829 a.u. is shown in Fig. 6, with the close contact between H1Bⁱ and the C2–C7 plane indicated by the red spot. The contributions of the different types of intermolecular interactions for **1** are shown in the two-dimensional fingerprint plots (McKinnon *et al.*, 2007) in Fig. 7. The contribution of the H···H interactions, with a value of 39.8%, has the largest share of the crystal packing of **1**. The remaining hydrogen–heteronuclear interactions have a smaller share with a 15.7% contribution for I···H, a 14.4% contribution for C···H and a 3.6% contribution for S···H.

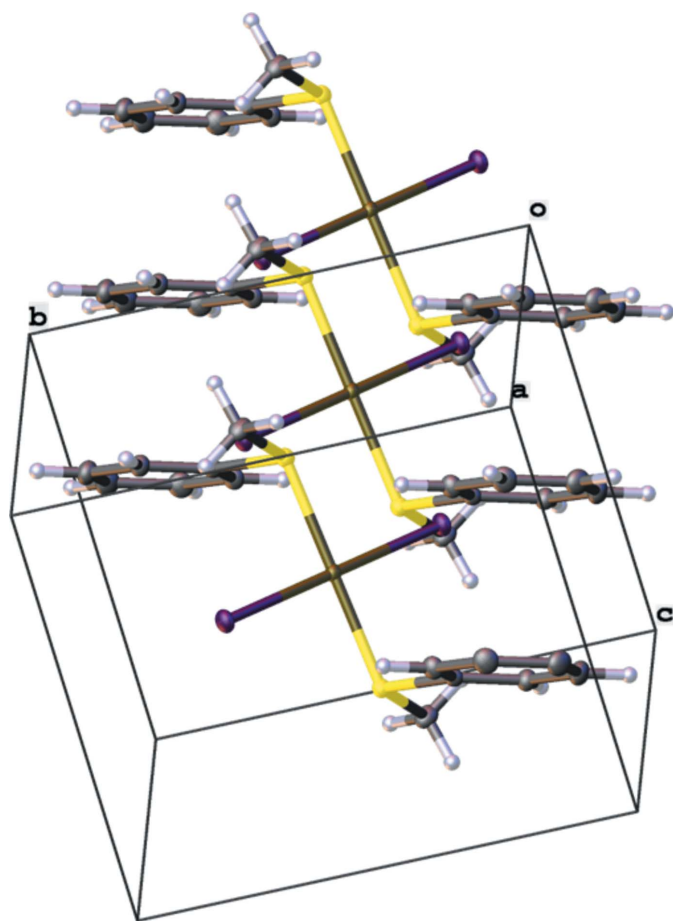


Figure 4
The packing of the solid-state structure of **1** along the [100] axis.

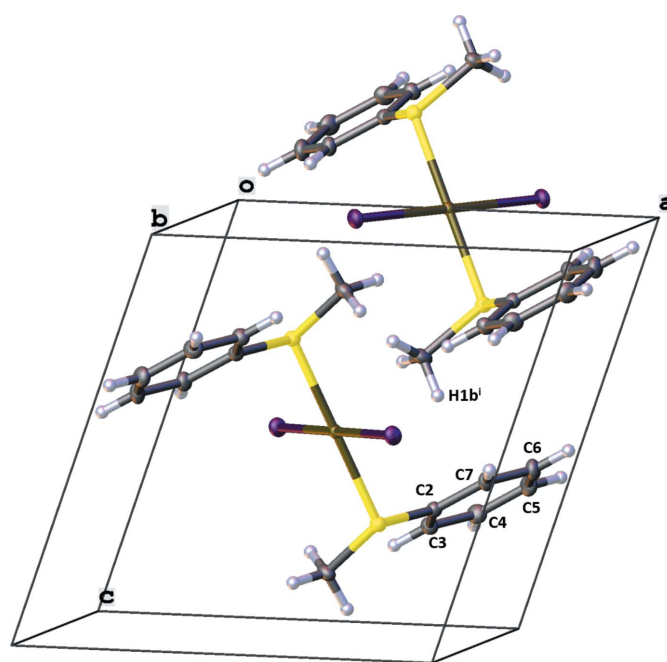


Figure 5
The packing of the solid-state structure of **1** along the [010] axis [symmetry code: (i) $x, \frac{1}{2} - y, -\frac{1}{2} + z$].

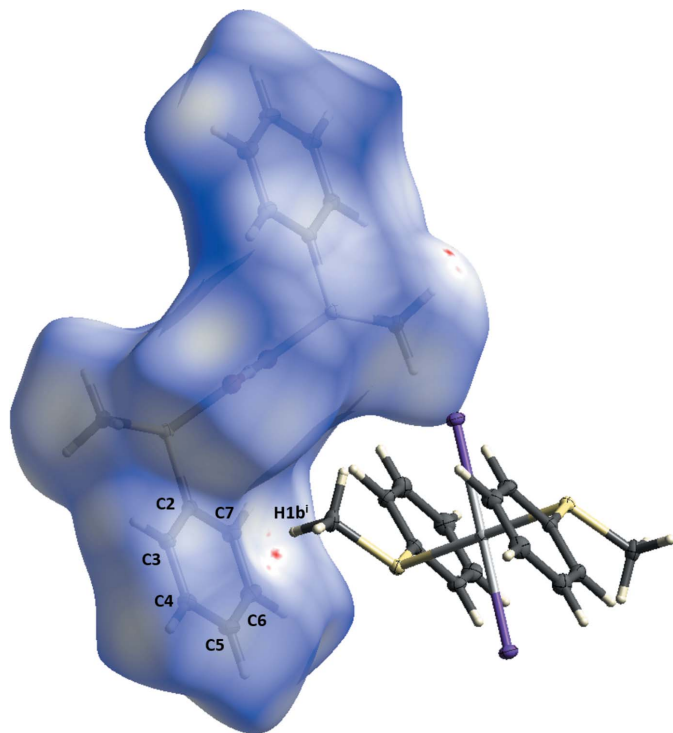


Figure 6
Hirshfeld surface analysis of **1** showing close contacts in the crystal. The π -interaction between hydrogen atom H1b' and the phenyl ring C2–C7 is indicated by the red spot [symmetry code: (i) $x, \frac{1}{2} - y, -\frac{1}{2} + z$].

The heteronuclear I \cdots H and C \cdots H interactions appear as spikes.

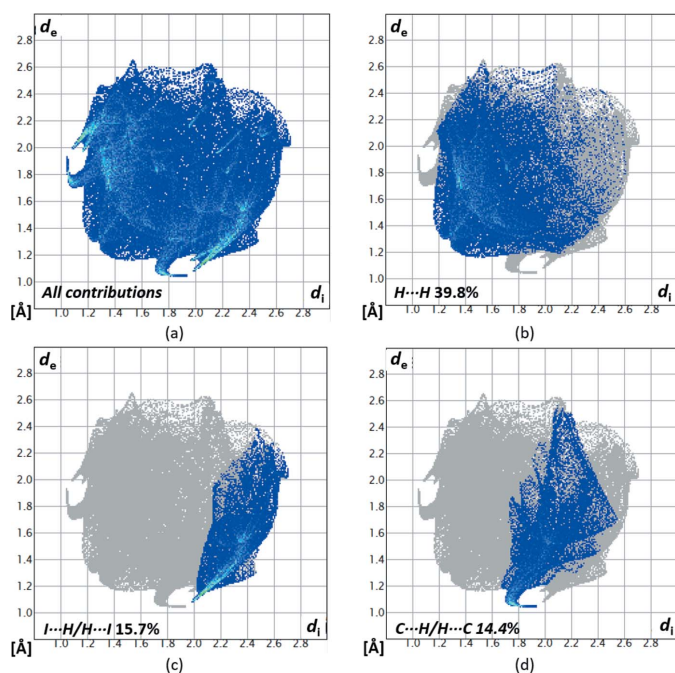


Figure 7
Two-dimensional fingerprint plots for compound **1**, showing (a) all contributions, and (b)–(d) delineated into the contributions of atoms within specific interacting pairs (blue areas).

4. Database survey

By a search in the Cambridge Crystallographic Database (WebCSD, November 2022; Groom *et al.*, 2016), various structures of dihalide transition-metal complexes with the same ligand motif as **1** were found. To compare the most similar structures, only dihalide transition metal complexes with the bis[(methylsulfanyl)benzene] ligand and its oxidized derivative are focused on now. The already compared structure *trans*-dichloro-bis[methyl(phenyl)sulfanyl]platinum (LEQSUW; Vigo *et al.*, 2006) has been published, as well as its palladium derivative with (SARWEP; Oilunkaniemi *et al.*, 2006) and without (LEQSOQ; Vigo *et al.*, 2006) inserted benzene. In addition, *cis*-dichlorobis(methylphenylsulfoxide)-palladium has been published independently by two different research groups [JISWUD (Antolini *et al.*, 1991) and JISWUD01 (Gama de Almeida *et al.*, 1992)]. Further examples of Pt₂ thioether complexes are *cis*-diiodo-(1,4,7-trithia-cyclononane-*S,S'*)platinum(II) (ACUXAX; Grant *et al.*, 2001), diiodo-(2,9-dimethyl-1,10-phenanthroline)(dimethylsulfide)-platinum(II) (BERTIC; Fanizzi *et al.*, 2004), and diiodo-(5-phenyl-1-thia-5-phosphacyclo-octane-*P,S*)platinum(II) (KEJHEM; Toto *et al.*, 1990).

Similar complexes were also structurally characterized by our research groups and include *cis*-[PtBr₂{(PhSCH₂)₂SiPh₂}] (ECOAG; Knorr *et al.*, 2004) and *cis*-[PtI₂{(PhSCH₂)₂SiPh₂}]·DCM (ECOIO, Knorr *et al.*, 2004), which were determined in order to investigate the *trans*-influence of different halide ligands on the Pt–S bond. Further examples of dithioether complexes stemming from our laboratories are *cis*-[PtCl₂{(PhSCH₂)₂Si₂Me₄}] (MEDYOK; Peindy *et al.*, 2006) and *cis*-[PtI₂{(PhSCH₂)₂Si₂Me₄}]·DCM (MEDZIF; Peindy *et al.*, 2006).

5. Synthesis and crystallization

trans-Diiodobis[(methylsulfanyl)benzene]platinum (**1**) was synthesized by adding methylphenyl sulfide (37 mg, 0.30 mmol, 1.50 eq.) dissolved in 0.5 mL of dichloromethane *via* a microsyringe to a solution of bis(benzonitrile)diiodo-platinum (65 mg, 0.10 mmol, 1.00 eq.) in dichloromethane (3 mL) and stirring overnight at room temperature. *trans*-Diiodobis[(methylsulfanyl)benzene]platinum (**1**, 557 mg, 0.80 mmol, 80%) was isolated as red crystals after layering with heptane.

Calculated for C₁₄H₁₆I₂PtS₂ (697.30 g mol^{−1}): C, 24.11; H, 2.32; S, 9.20. Found: C, 23.92; H, 2.21; S, 9.05%.

¹H NMR (400MHz, CDCl₃): δ = 3.01 (*s*, ³J_{PtH} = 48 Hz, 6H; CH₃), 7.05–7.73 (*m*, 10H; phenyl) ppm.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C–H = 0.95–1.00 Å) and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂ and CH hydrogen atoms and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃ hydrogen atoms.

Table 2
Experimental details.

Crystal data	
Chemical formula	[PtI ₂ (C ₇ H ₈ I) ₂]
<i>M</i> _r	697.28
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.5796 (3), 9.5104 (3), 9.7960 (3)
β (°)	107.645 (1)
<i>V</i> (Å ³)	850.48 (5)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	12.11
Crystal size (mm)	0.31 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.263, 0.498
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	27554, 4125, 4033
<i>R</i> _{int}	0.038
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.833
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.021, 0.053, 1.17
No. of reflections	4125
No. of parameters	89
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	2.26, -1.80

Computer programs: *APEX2* and *SAINT* V8.38A (Bruker, 2018), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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Crystal structure and Hirshfeld analysis of *trans*-diiodidobis[(methylsulfanyl)benzene- κ S]platinum(II)

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Computing details

Data collection: *APEX2* (Bruker, 2018); cell refinement: *S SAINT V8.38A* (Bruker, 2018); data reduction: *S SAINT V8.38A* (Bruker, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2019/2* (Sheldrick, 2015b); molecular graphics: *Olex2 1.5* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

trans-Diiodidobis[(methylsulfanyl)benzene- κ S]platinum(II)

Crystal data

[PtI₂(C₇H₈I)₂]

$M_r = 697.28$

Monoclinic, $P2_1/c$

$a = 9.5796$ (3) Å

$b = 9.5104$ (3) Å

$c = 9.7960$ (3) Å

$\beta = 107.645$ (1)°

$V = 850.48$ (5) Å³

$Z = 2$

$F(000) = 632$

$D_x = 2.723$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9775 reflections

$\theta = 3.1$ – 36.3 °

$\mu = 12.11$ mm⁻¹

$T = 100$ K

Prism, red

$0.31 \times 0.25 \times 0.20$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: microfocus sealed X-ray tube,

Incoatec I μ s

HELIOS mirror optics monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω and ϕ scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.263$, $T_{\max} = 0.498$

27554 measured reflections

4125 independent reflections

4033 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 36.3$ °, $\theta_{\min} = 2.2$ °

$h = -15 \rightarrow 15$

$k = -15 \rightarrow 15$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.053$

$S = 1.17$

4125 reflections

89 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2 + 1.6484P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 2.26$ e Å⁻³

$\Delta\rho_{\min} = -1.79$ e Å⁻³

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.500000	0.500000	0.500000	0.01069 (3)
I1	0.67448 (2)	0.70668 (2)	0.48539 (2)	0.01650 (4)
S1	0.66656 (6)	0.45396 (6)	0.72234 (6)	0.01359 (8)
C3	0.7382 (3)	0.1669 (2)	0.7476 (2)	0.0159 (3)
H3	0.668801	0.154647	0.798352	0.019*
C7	0.8623 (2)	0.3176 (2)	0.6213 (3)	0.0168 (4)
H7	0.876638	0.407868	0.586351	0.020*
C2	0.7595 (2)	0.2989 (2)	0.6957 (2)	0.0134 (3)
C1	0.5743 (3)	0.3994 (3)	0.8486 (2)	0.0188 (4)
H1A	0.518020	0.478370	0.868893	0.028*
H1B	0.646855	0.368646	0.937513	0.028*
H1C	0.507882	0.321330	0.807968	0.028*
C4	0.8199 (3)	0.0527 (3)	0.7244 (3)	0.0200 (4)
H4	0.806058	-0.037609	0.759612	0.024*
C5	0.9216 (3)	0.0705 (3)	0.6501 (3)	0.0216 (4)
H5	0.976478	-0.007512	0.633993	0.026*
C6	0.9426 (3)	0.2037 (3)	0.5991 (3)	0.0209 (4)
H6	1.012472	0.216130	0.549005	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01172 (5)	0.00914 (5)	0.01237 (5)	0.00010 (3)	0.00539 (3)	0.00002 (3)
I1	0.01712 (6)	0.01357 (6)	0.02033 (7)	-0.00397 (4)	0.00794 (5)	0.00006 (4)
S1	0.0149 (2)	0.0124 (2)	0.01360 (19)	-0.00016 (15)	0.00455 (16)	-0.00055 (15)
C3	0.0176 (8)	0.0150 (8)	0.0162 (8)	0.0008 (7)	0.0067 (7)	0.0012 (7)
C7	0.0142 (8)	0.0170 (9)	0.0205 (9)	-0.0018 (7)	0.0073 (7)	-0.0004 (7)
C2	0.0135 (8)	0.0132 (8)	0.0134 (8)	-0.0002 (6)	0.0039 (6)	-0.0010 (6)
C1	0.0226 (10)	0.0214 (10)	0.0147 (8)	0.0047 (8)	0.0092 (7)	0.0018 (7)
C4	0.0229 (10)	0.0164 (9)	0.0206 (10)	0.0038 (7)	0.0063 (8)	0.0029 (7)
C5	0.0194 (10)	0.0210 (10)	0.0244 (11)	0.0073 (8)	0.0065 (8)	-0.0001 (8)
C6	0.0149 (9)	0.0243 (11)	0.0257 (11)	0.0010 (8)	0.0094 (8)	-0.0012 (8)

Geometric parameters (\AA , $^\circ$)

Pt1—I1	2.6121 (1)	C7—C2	1.403 (3)
Pt1—I1 ⁱ	2.6120 (1)	C7—C6	1.383 (3)
Pt1—S1 ⁱ	2.3183 (5)	C1—H1A	0.9800
Pt1—S1	2.3183 (5)	C1—H1B	0.9800

S1—C2	1.782 (2)	C1—H1C	0.9800
S1—C1	1.800 (2)	C4—H4	0.9500
C3—H3	0.9500	C4—C5	1.392 (4)
C3—C2	1.393 (3)	C5—H5	0.9500
C3—C4	1.397 (3)	C5—C6	1.398 (4)
C7—H7	0.9500	C6—H6	0.9500
I1 ⁱ —Pt1—I1	180.0	C7—C2—S1	115.60 (17)
S1 ⁱ —Pt1—I1	94.358 (14)	S1—C1—H1A	109.5
S1—Pt1—I1 ⁱ	94.359 (14)	S1—C1—H1B	109.5
S1—Pt1—I1	85.641 (14)	S1—C1—H1C	109.5
S1 ⁱ —Pt1—I1 ⁱ	85.643 (14)	H1A—C1—H1B	109.5
S1—Pt1—S1 ⁱ	180.0	H1A—C1—H1C	109.5
C2—S1—Pt1	104.52 (7)	H1B—C1—H1C	109.5
C2—S1—C1	103.46 (11)	C3—C4—H4	119.8
C1—S1—Pt1	111.00 (8)	C5—C4—C3	120.4 (2)
C2—C3—H3	120.3	C5—C4—H4	119.8
C2—C3—C4	119.3 (2)	C4—C5—H5	120.1
C4—C3—H3	120.3	C4—C5—C6	119.7 (2)
C2—C7—H7	120.2	C6—C5—H5	120.1
C6—C7—H7	120.2	C7—C6—C5	120.4 (2)
C6—C7—C2	119.6 (2)	C7—C6—H6	119.8
C3—C2—S1	123.88 (17)	C5—C6—H6	119.8
C3—C2—C7	120.5 (2)		
Pt1—S1—C2—C3	-107.26 (19)	C1—S1—C2—C7	-168.90 (18)
Pt1—S1—C2—C7	74.82 (17)	C4—C3—C2—S1	-178.09 (18)
C3—C4—C5—C6	0.4 (4)	C4—C3—C2—C7	-0.3 (3)
C2—C3—C4—C5	0.0 (4)	C4—C5—C6—C7	-0.5 (4)
C2—C7—C6—C5	0.2 (4)	C6—C7—C2—S1	178.21 (19)
C1—S1—C2—C3	9.0 (2)	C6—C7—C2—C3	0.2 (3)

Symmetry code: (i) $-x+1, -y+1, -z+1$.