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trans-Chlorido(dimethyl sulfoxide-κS)-(pyridine-2-carboxylato-$\kappa^2 N,O$)-platinum(II)

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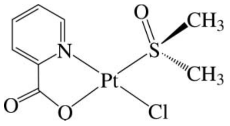
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.013 Å; R factor = 0.027; wR factor = 0.065; data-to-parameter ratio = 13.1.

In the title complex, $[Pt(C_6H_4NO_2)Cl(C_2H_6OS)]$, the Pt^{II} ion is in a distorted square-planar environment defined by the N and O atoms from the chelating pyridine-2-carboxylate (pic) anionic ligand, one S atom of the dimethyl sulfoxide molecule and one Cl ion. The complex is disposed about a crystallographic mirror plane parallel to the *ac* plane passing through all the atoms of the complex except the methyl atoms of the dimethyl sulfoxide. The molecules are stacked in columns along the *b* axis with a Pt⋯Pt distance of 4.9508 (5) Å. Within the column, intermolecular C—H⋯O hydrogen bonds and weak π–π interactions between adjacent pyridine rings are present, the shortest centroid–centroid distance being 5.153 (4) Å.

Related literature

For the crystal structure of the title complex with the monoclinic space group $P2_1/n$, see: Annibale *et al.* (1986). For details of Pt(IV)–pic complexes, see: Griffith *et al.* (2005); Kim *et al.* (2009).



Experimental

Crystal data

$[Pt(C_6H_4NO_2)Cl(C_2H_6OS)]$
M_r = 430.77
Orthorhombic, *Pnma*
a = 19.5900 (15) Å
b = 6.9450 (6) Å
c = 8.1266 (6) Å
V = 1105.64 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 13.11 mm^{-1}
T = 200 K
0.21 × 0.17 × 0.09 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.631, T_{max} = 1.000
6423 measured reflections
1169 independent reflections
1085 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.10
1169 reflections
89 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—O1	2.020 (5)	Pt1—S1	2.202 (2)
Pt1—N1	2.031 (7)	Pt1—Cl1	2.2945 (19)
O1—Pt1—N1	81.0 (2)	O1—Pt1—Cl1	88.98 (16)
O1—Pt1—S1	177.70 (16)	N1—Pt1—Cl1	169.97 (19)
N1—Pt1—S1	101.31 (19)	S1—Pt1—Cl1	88.72 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯O3	0.95	2.16	2.995 (11)	145
C2—H2⋯O1^{i}	0.95	2.35	3.255 (11)	158
C7—H7*A*⋯O2^{ii}	0.98	2.42	3.323 (8)	152
C7—H7*B*⋯Cl1	0.98	2.77	3.355 (7)	119

Symmetry codes: (i) $x, y, z - 1$; (ii) $-x, y - \frac{1}{2}, -z + 2$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

This work was supported by Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2009–0094056).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2243).

References

Annibale, G., Cattalini, L., Canovese, L., Pitteri, B., Tiripicchio, A., Tiripicchio Camellini, M. & Tobe, M. L. (1986). *J. Chem. Soc. Dalton Trans.* pp. 1101–1105.
Bruker (2000). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Griffith, D., Lyssenko, K., Jensen, P., Kruger, P. E. & Marmion, C. J. (2005). *Dalton Trans.* pp. 956–961.
Kim, N.-H., Hwang, I.-C. & Ha, K. (2009). *Acta Cryst.* E**65**, m667.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2010). E**66**, m295 [**doi:10.1107/S1600536810005520**]

trans-Chlorido(dimethyl sulfoxide-*κS*)(pyridine-2-carboxylato-*κ*^{2}*N*,*O*)platinum(II)

K. Ha

Comment

The title complex, [Pt($C_6H_4NO_2$)Cl(C_2H_6OS)], crystallized in the orthorhombic space group *Pnma*, whereas, in the previously reported X-ray structure analysis, the complex crystallized in the monoclinic space group $P2_1/n$ (Annibale *et al.*, 1986). The Pt^{II} ion lies in a distorted square-planar environment defined by the N and O atoms from the chelating pyridine-2-carboxylate (pic) anionic ligand, one S atom of the dimethyl sulfoxide molecule and one Cl ion (Fig. 1). The tight O1—Pt1—N1 chelate angle [81.0 (2)°] results in non-linear trans axes [<O1—Pt1—S1 = 177.70 (16)° and <N1—Pt1—Cl1 = 169.97 (19)°] (Table 1). The complex is disposed about a crystallographic mirror plane parallel to the ac plane passing through all the atoms of the complex at the special positions (x,1/4,z), except the methyl atoms of the dimethyl sulfoxide (Fig. 2). The molecules are stacked in columns along the b axis with a Pt···Pt distance of 4.9508 (5) Å. In the column, intermolecular C—H···O hydrogen bond (Table 2) and weak π-π interactions between adjacent pyridine rings are present, the shortest centroid-centroid distance being 5.153 (4) Å, and the ring planes are parallel and shifted for 3.807 Å. The intramolecular C—H···O and C—H···Cl hydrogen bonds are also observed (Table 2).

Experimental

Single crystals of the title complex were unexpectedly obtained by reacting K_2PtCl_4 (0.2000 g, 0.482 mmol) and pyridine-2-carboxylic acid (0.1192 g, 0.968 mmol) in H_2O (10 ml) under reflux for 5 h. Crystals suitable for X-ray analysis were obtained by slow evaporation from a dimethyl sulfoxide solution of the pale yellow reaction product at 80 °C.

Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms [C—H = 0.95 (aromatic) or 0.98 Å (CH_3) and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C)]. The highest peak (2.60 e Å^{-3}) and the deepest hole (-0.79 e Å^{-3}) in the difference Fourier map are located 0.87 and 1.04 Å, respectively, from the atom Pt1.

Figures

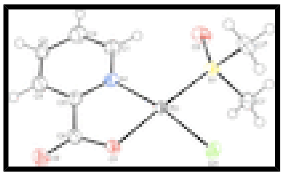


Fig. 1. The structure of the title complex, with displacement ellipsoids drawn at the 50% probability level for non-H atoms [Symmetry code: (a) x, 1/2 - y, z].

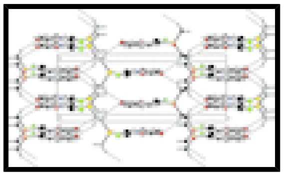


Fig. 2. View of the unit-cell contents of the title complex. Hydrogen-bond interactions are drawn with dashed lines.

trans-Chlorido(dimethyl sulfoxide-κ*S*)(pyridine-2-carboxylato-κ^2*N*,*O*)platinum(II)

Crystal data

$[Pt(C_6H_4NO_2)Cl(C_2H_6OS)]$

$M_r = 430.77$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 19.5900$ (15) Å

$b = 6.9450$ (6) Å

$c = 8.1266$ (6) Å

$V = 1105.64$ (15) Å^3

$Z = 4$

$F(000) = 800$

$D_x = 2.588$ Mg m^{-3}

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3961 reflections

θ = 2.7–26.0°

μ = 13.11 mm^{-1}

$T = 200$ K

Block, colorless

0.21 × 0.17 × 0.09 mm

Data collection

Bruker SMART 1000 CCD diffractometer

Radiation source: fine-focus sealed tube

graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{min} = 0.631$, $T_{max} = 1.000$

6423 measured reflections

1169 independent reflections

1085 reflections with $I > 2\sigma(I)$

$R_{int} = 0.042$

$\theta_{max} = 26.0°$, $\theta_{min} = 2.7°$

$h = -24 \rightarrow 23$

$k = -8 \rightarrow 8$

$l = -7 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.065$

$S = 1.10$

1169 reflections

89 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 1.8204P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 2.60$ e Å^{-3}

$\Delta\rho_{min} = -0.79$ 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.

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	$U_{\rm iso}$*/$U_{\rm eq}$
Pt1	0.087714 (15)	0.2500	1.04929 (4)	0.01771 (13)
Cl1	0.14026 (11)	0.2500	1.3016 (2)	0.0265 (5)
S1	0.18928 (11)	0.2500	0.9332 (2)	0.0209 (4)
O1	−0.0036 (3)	0.2500	1.1647 (7)	0.0243 (13)
O2	−0.1160 (3)	0.2500	1.1182 (8)	0.0311 (14)
O3	0.1947 (3)	0.2500	0.7524 (8)	0.0353 (15)
N1	0.0258 (3)	0.2500	0.8489 (8)	0.0204 (15)
C1	0.0441 (5)	0.2500	0.6884 (10)	0.029 (2)
H1	0.0911	0.2500	0.6596	0.035*
C2	−0.0051 (5)	0.2500	0.5652 (11)	0.035 (2)
H2	0.0085	0.2500	0.4530	0.042*
C3	−0.0726 (4)	0.2500	0.6045 (12)	0.0274 (19)
H3	−0.1066	0.2500	0.5211	0.033*
C4	−0.0903 (4)	0.2500	0.7672 (12)	0.028 (2)
H4	−0.1372	0.2500	0.7968	0.034*
C5	−0.0410 (4)	0.2500	0.8904 (11)	0.0205 (17)
C6	−0.0570 (4)	0.2500	1.0681 (10)	0.0217 (18)
C7	0.2372 (3)	0.0507 (9)	1.0071 (8)	0.0300 (14)
H7A	0.2145	−0.0694	0.9755	0.045*
H7B	0.2405	0.0577	1.1273	0.045*
H7C	0.2832	0.0539	0.9593	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.0175 (2)	0.02225 (19)	0.0134 (2)	0.000	0.00107 (12)	0.000
Cl1	0.0231 (11)	0.0425 (12)	0.0138 (10)	0.000	−0.0040 (8)	0.000
S1	0.0195 (11)	0.0258 (10)	0.0174 (10)	0.000	0.0024 (8)	0.000
O1	0.018 (3)	0.044 (3)	0.011 (3)	0.000	0.003 (2)	0.000
O2	0.024 (3)	0.047 (4)	0.022 (3)	0.000	0.003 (3)	0.000
O3	0.036 (4)	0.055 (4)	0.015 (3)	0.000	0.016 (3)	0.000
N1	0.023 (4)	0.019 (3)	0.019 (4)	0.000	0.000 (3)	0.000

C1	0.028 (5)	0.049 (5)	0.009 (4)	0.000	0.003 (3)	0.000
C2	0.037 (6)	0.047 (6)	0.020 (5)	0.000	−0.001 (4)	0.000
C3	0.021 (5)	0.038 (5)	0.023 (5)	0.000	−0.006 (4)	0.000
C4	0.023 (5)	0.033 (5)	0.028 (5)	0.000	0.001 (4)	0.000
C5	0.023 (4)	0.013 (3)	0.025 (4)	0.000	−0.002 (4)	0.000
C6	0.019 (4)	0.024 (4)	0.022 (5)	0.000	0.002 (3)	0.000
C7	0.023 (3)	0.029 (3)	0.038 (4)	0.007 (3)	0.005 (3)	0.005 (3)

Geometric parameters (Å, °)

Pt1—O1	2.020 (5)	C1—H1	0.9500
Pt1—N1	2.031 (7)	C2—C3	1.361 (13)
Pt1—S1	2.202 (2)	C2—H2	0.9500
Pt1—Cl1	2.2945 (19)	C3—C4	1.367 (14)
S1—O3	1.473 (6)	C3—H3	0.9500
S1—C7^{i}	1.778 (6)	C4—C5	1.390 (13)
S1—C7	1.778 (6)	C4—H4	0.9500
O1—C6	1.308 (10)	C5—C6	1.477 (12)
O2—C6	1.225 (11)	C7—H7A	0.9800
N1—C5	1.352 (10)	C7—H7B	0.9800
N1—C1	1.352 (11)	C7—H7C	0.9800
C1—C2	1.390 (13)		
O1—Pt1—N1	81.0 (2)	C3—C2—H2	119.8
O1—Pt1—S1	177.70 (16)	C1—C2—H2	119.8
N1—Pt1—S1	101.31 (19)	C2—C3—C4	118.2 (8)
O1—Pt1—Cl1	88.98 (16)	C2—C3—H3	120.9
N1—Pt1—Cl1	169.97 (19)	C4—C3—H3	120.9
S1—Pt1—Cl1	88.72 (7)	C3—C4—C5	121.4 (8)
O3—S1—C7^{i}	107.4 (3)	C3—C4—H4	119.3
O3—S1—C7	107.4 (3)	C5—C4—H4	119.3
C7^{i}—S1—C7	102.3 (5)	N1—C5—C4	119.5 (8)
O3—S1—Pt1	119.5 (3)	N1—C5—C6	116.7 (7)
C7^{i}—S1—Pt1	109.4 (2)	C4—C5—C6	123.8 (8)
C7—S1—Pt1	109.4 (2)	O2—C6—O1	123.7 (8)
C6—O1—Pt1	115.4 (5)	O2—C6—C5	121.7 (8)
C5—N1—C1	119.8 (7)	O1—C6—C5	114.7 (7)
C5—N1—Pt1	112.2 (6)	S1—C7—H7A	109.5
C1—N1—Pt1	127.9 (6)	S1—C7—H7B	109.5
N1—C1—C2	120.7 (8)	H7A—C7—H7B	109.5
N1—C1—H1	119.6	S1—C7—H7C	109.5
C2—C1—H1	119.6	H7A—C7—H7C	109.5
C3—C2—C1	120.3 (9)	H7B—C7—H7C	109.5
N1—Pt1—S1—O3	0.0	N1—C1—C2—C3	0.000 (2)
Cl1—Pt1—S1—O3	180.0	C1—C2—C3—C4	0.000 (2)
N1—Pt1—S1—C7^{i}	124.3 (3)	C2—C3—C4—C5	0.000 (2)
Cl1—Pt1—S1—C7^{i}	−55.7 (3)	C1—N1—C5—C4	0.000 (2)
N1—Pt1—S1—C7	−124.3 (3)	Pt1—N1—C5—C4	180.000 (2)

Cl1—Pt1—S1—C7	55.7 (3)	C1—N1—C5—C6	180.000 (2)
N1—Pt1—O1—C6	0.000 (2)	Pt1—N1—C5—C6	0.000 (2)
Cl1—Pt1—O1—C6	180.000 (2)	C3—C4—C5—N1	0.000 (2)
O1—Pt1—N1—C5	0.000 (1)	C3—C4—C5—C6	180.000 (2)
S1—Pt1—N1—C5	180.000 (1)	Pt1—O1—C6—O2	180.000 (2)
Cl1—Pt1—N1—C5	0.000 (4)	Pt1—O1—C6—C5	0.000 (2)
O1—Pt1—N1—C1	180.000 (1)	N1—C5—C6—O2	180.000 (2)
S1—Pt1—N1—C1	0.000 (1)	C4—C5—C6—O2	0.000 (2)
Cl1—Pt1—N1—C1	180.000 (3)	N1—C5—C6—O1	0.000 (2)
C5—N1—C1—C2	0.000 (2)	C4—C5—C6—O1	180.000 (2)
Pt1—N1—C1—C2	180.000 (1)		

Symmetry codes: (i) x, $-y+1/2$, z.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O3	0.95	2.16	2.995 (11)	145.
C2—H2···O1^{ii}	0.95	2.35	3.255 (11)	158.
C7—H7A···O2^{iii}	0.98	2.42	3.323 (8)	152.
C7—H7B···Cl1	0.98	2.77	3.355 (7)	119.

Symmetry codes: (ii) x, y, $z-1$; (iii) $-x$, $y-1/2$, $-z+2$.

Fig. 1

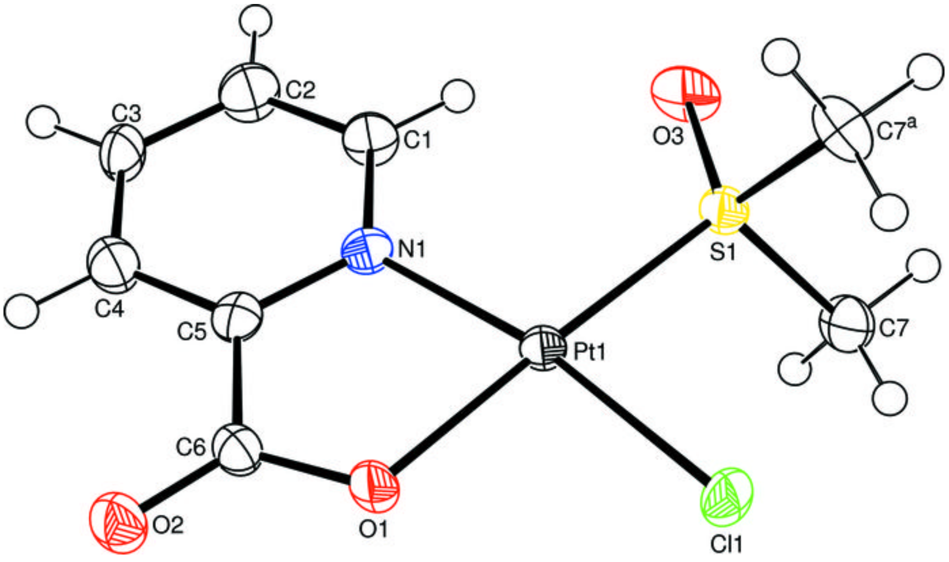


Fig. 2