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trans-(Aniline-κ*N*)dichlorido(dimethyl sulfoxide-κ*S*)platinum(II)

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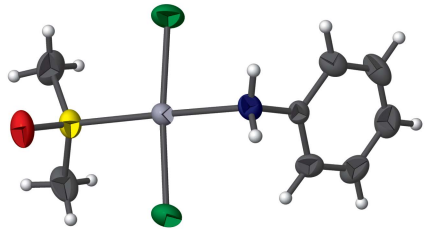
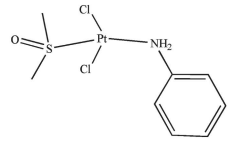
In the title compound, $[PtCl_2(C_6H_7N)(C_2H_6OS)]$, the Pt^{II} ion has an approximately square-planar coordination environment. It binds to the N atom of the aniline ligand and is *trans* to the S atom of the dimethyl sulfoxide. The two Cl^- anions are also in *trans* positions. In the crystal, molecules are linked by N—H···O, C—H···Cl and C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

trans-Platinum(II) complexes attract great attention because such compounds display good cytotoxic activity and have been shown to be able to overcome cisplatin resistance (Sgarbossa *et al.*, 2013; Kalinowska-Lis *et al.*, 2008). It is therefore of interest to synthesize *trans* platinum(II) complexes with different structures.

In the title compound (Fig. 1), the platinum atom is in a slightly distorted square-planar coordination environment, which is defined by the N atom of the aniline ligand, the S atom of dimethyl sulfoxide and the two Cl^- anions that adopt a *trans* arrangement. A slight distortion from planarity is indicated with a dihedral angle of 4.39 (11)° between the Cl2–Pt1–S1 and Cl1–Pt1–N1 planes. The Pt1—N1, 2.081 (3) Å, Pt1—S1, 2.2206 (10) Å, and the two Pt—Cl bond distances Pt1—Cl1 2.2894 (11) Å, and 2.2933 (11) Å are normal and comparable to values reported for related Pt^{II} complexes in the literature (Francisco *et al.*, 2011; Rahman *et al.* 2015; Huo *et al.* 2011).

In the crystal, N1—H1*B*···O1 hydrogen bonds, Table 1, form inversion dimers and enclose $R_2^2(10)$ rings, Fig. 2. The molecules are further linked by N—H···Cl, C—H···Cl and C—H···O hydrogen bonds, generating a three-dimensional framework (Fig. 3).

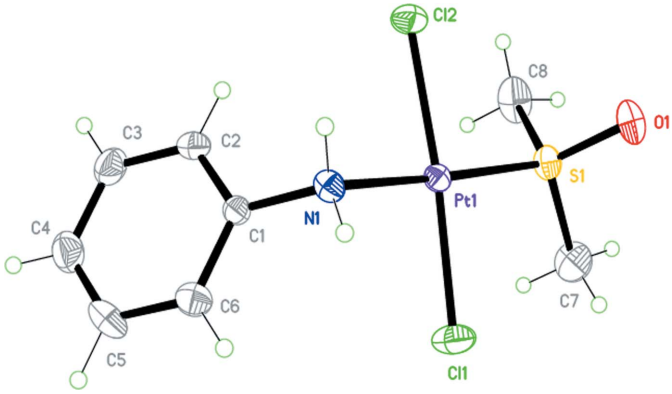


Figure 1
A view of the title compound with 30% probability displacement ellipsoids.

Synthesis and crystallization

The complex *cis*-$Pt(DMSO)_2Cl_2$ (DMSO = dimethyl sulfoxide) was prepared by a reported method (Kukushkin *et al.*, 1968). A solution of aniline (0.1 mmol, 0.009 g) in methanol (10 ml) was added with stirring to a suspension of *cis*-$Pt(DMSO)_2Cl_2$ (0.1 mmol, 0.042 g) in methanol (10 ml). The solution was refluxed at 338 K with stirring for 2.5 h under a nitrogen atmosphere, cooled slowly and filtered. The filtrate was kept at room temperature and suitable crystals of the title compound were obtained over a period of two weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors acknowledge Shao-dong Li for help with the single-crystal X-ray diffraction data collection.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl2^{i}	0.89	2.78	3.463 (3)	134
N1—H1A···Cl2^{ii}	0.89	2.84	3.425 (3)	125
N1—H1B···O1^{i}	0.89	2.05	2.913 (4)	165
C8—H8A···O1^{iii}	0.96	2.51	3.424 (6)	158
C8—H8C···Cl1^{iv}	0.96	2.77	3.677 (6)	158

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[PtCl_2(C_6H_7N)(C_2H_6OS)]$
M_r	437.24
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	15.1308 (7), 16.6636 (8), 10.0062 (5)
β (°)	100.379 (1)
V (Å^3)	2481.6 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	11.88
Crystal size (mm)	0.30 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.040, 0.051
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13004, 2181, 1967
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.043, 1.09
No. of reflections	2181
No. of parameters	129
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.84

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

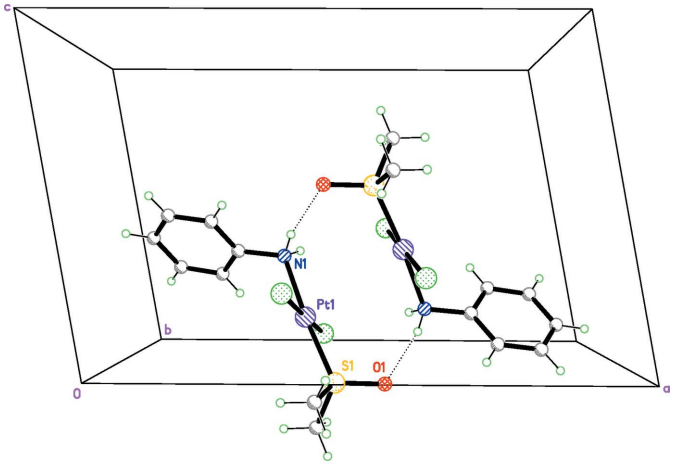


Figure 2
The N—H···O hydrogen-bonding interactions between the amine H-atom donors and dimethyl sulfoxide O-atom acceptors in the title compound.

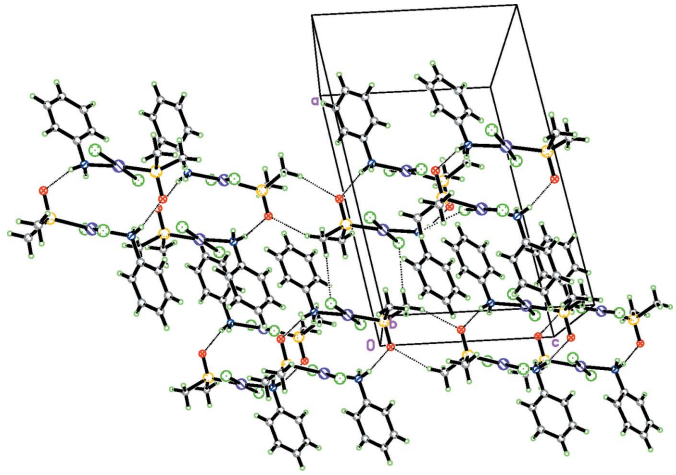


Figure 3
Overall packing of the title compound viewed along the *b*-axis direction.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180387 [https://doi.org/10.1107/S2414314618003875]

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Crystal data

$[PtCl_2(C_6H_7N)(C_2H_6OS)]$
M_r = 437.24
Monoclinic, *C*2/*c*
a = 15.1308 (7) Å
b = 16.6636 (8) Å
c = 10.0062 (5) Å
β = 100.379 (1)°
V = 2481.6 (2) Å^3
Z = 8
F(000) = 1632
D_x = 2.341 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5286 reflections
θ = 2.4–27.3°
μ = 11.88 mm^{-1}
T = 296 K
Block, colorless
0.30 × 0.25 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.040, T_{max} = 0.051
13004 measured reflections
2181 independent reflections
1967 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −17→17
k = −19→19
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.043
S = 1.09
2181 reflections
129 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.020P)^2 + 0.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.39217 (2)	0.34146 (2)	0.14748 (2)	0.02771 (7)

Cl1	0.36154 (9)	0.21751 (7)	0.22668 (12)	0.0532 (3)
Cl2	0.41711 (8)	0.47049 (7)	0.08370 (11)	0.0452 (3)
S1	0.42812 (7)	0.29389 (7)	−0.04301 (10)	0.0355 (3)
O1	0.52497 (18)	0.2944 (2)	−0.0457 (3)	0.0470 (8)
N1	0.3694 (2)	0.3897 (2)	0.3300 (3)	0.0318 (8)
H1A	0.400822	0.434933	0.344778	0.038*
H1B	0.391932	0.355693	0.396038	0.038*
C1	0.2775 (2)	0.4074 (2)	0.3444 (4)	0.0283 (9)
C2	0.2311 (3)	0.4691 (3)	0.2705 (4)	0.0404 (10)
H2	0.257308	0.497612	0.207829	0.048*
C3	0.1460 (3)	0.4882 (3)	0.2904 (5)	0.0501 (12)
H3	0.114762	0.530426	0.242771	0.060*
C4	0.1068 (3)	0.4437 (3)	0.3822 (5)	0.0543 (14)
H4	0.049190	0.456414	0.395805	0.065*
C5	0.1521 (3)	0.3820 (3)	0.4519 (5)	0.0508 (13)
H5	0.125046	0.351931	0.511744	0.061*
C6	0.2378 (3)	0.3637 (3)	0.4343 (4)	0.0421 (11)
H6	0.269067	0.321907	0.483229	0.050*
C7	0.3881 (4)	0.1953 (3)	−0.0826 (5)	0.0609 (15)
H7A	0.417547	0.158835	−0.014625	0.091*
H7B	0.400683	0.180089	−0.169763	0.091*
H7C	0.324459	0.193677	−0.084796	0.091*
C8	0.3738 (4)	0.3477 (3)	−0.1877 (5)	0.0612 (16)
H8A	0.387880	0.323519	−0.268400	0.092*
H8B	0.394203	0.402408	−0.181841	0.092*
H8C	0.310016	0.346455	−0.191259	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02819 (10)	0.02928 (11)	0.02603 (10)	−0.00066 (7)	0.00590 (6)	0.00100 (7)
Cl1	0.0786 (9)	0.0331 (6)	0.0493 (7)	−0.0117 (6)	0.0152 (6)	0.0038 (5)
Cl2	0.0558 (7)	0.0359 (6)	0.0468 (6)	−0.0025 (5)	0.0168 (5)	0.0111 (5)
S1	0.0331 (6)	0.0451 (7)	0.0280 (5)	0.0024 (5)	0.0048 (4)	−0.0054 (5)
O1	0.0327 (16)	0.071 (2)	0.0384 (17)	0.0042 (16)	0.0093 (13)	−0.0105 (16)
N1	0.0323 (18)	0.036 (2)	0.0274 (17)	−0.0041 (16)	0.0058 (14)	−0.0025 (16)
C1	0.031 (2)	0.027 (2)	0.028 (2)	−0.0034 (17)	0.0082 (17)	−0.0044 (17)
C2	0.042 (3)	0.030 (2)	0.051 (3)	−0.006 (2)	0.012 (2)	0.003 (2)
C3	0.042 (3)	0.041 (3)	0.068 (3)	0.010 (2)	0.010 (2)	0.001 (3)
C4	0.042 (3)	0.058 (4)	0.067 (3)	−0.001 (3)	0.020 (3)	−0.010 (3)
C5	0.043 (3)	0.070 (4)	0.043 (3)	−0.014 (3)	0.018 (2)	0.004 (3)
C6	0.046 (3)	0.043 (3)	0.038 (3)	−0.002 (2)	0.009 (2)	0.006 (2)
C7	0.074 (4)	0.052 (3)	0.058 (3)	−0.008 (3)	0.016 (3)	−0.025 (3)
C8	0.059 (3)	0.093 (5)	0.030 (3)	0.020 (3)	0.005 (2)	0.008 (3)

Geometric parameters (Å, º)

Pt1—N1	2.081 (3)	C3—C4	1.393 (7)
Pt1—S1	2.2206 (10)	C3—H3	0.9300
Pt1—Cl1	2.2894 (11)	C4—C5	1.358 (7)
Pt1—Cl2	2.2933 (11)	C4—H4	0.9300
S1—O1	1.470 (3)	C5—C6	1.374 (6)
S1—C7	1.770 (5)	C5—H5	0.9300
S1—C8	1.775 (5)	C6—H6	0.9300
N1—C1	1.453 (5)	C7—H7A	0.9600
N1—H1A	0.8899	C7—H7B	0.9600
N1—H1B	0.8900	C7—H7C	0.9600
C1—C6	1.377 (6)	C8—H8A	0.9600
C1—C2	1.382 (6)	C8—H8B	0.9600
C2—C3	1.376 (6)	C8—H8C	0.9600
C2—H2	0.9300		
N1—Pt1—S1	175.23 (9)	C2—C3—C4	119.6 (5)
N1—Pt1—Cl1	88.19 (10)	C2—C3—H3	120.2
S1—Pt1—Cl1	94.09 (4)	C4—C3—H3	120.2
N1—Pt1—Cl2	86.79 (10)	C5—C4—C3	120.4 (4)
S1—Pt1—Cl2	91.01 (4)	C5—C4—H4	119.8
Cl1—Pt1—Cl2	174.81 (4)	C3—C4—H4	119.8
O1—S1—C7	107.7 (2)	C4—C5—C6	120.2 (5)
O1—S1—C8	107.4 (2)	C4—C5—H5	119.9
C7—S1—C8	101.4 (3)	C6—C5—H5	119.9
O1—S1—Pt1	114.36 (12)	C5—C6—C1	120.0 (4)
C7—S1—Pt1	113.35 (18)	C5—C6—H6	120.0
C8—S1—Pt1	111.77 (18)	C1—C6—H6	120.0
C1—N1—Pt1	118.6 (2)	S1—C7—H7A	109.5
C1—N1—H1A	107.7	S1—C7—H7B	109.5
Pt1—N1—H1A	107.7	H7A—C7—H7B	109.5
C1—N1—H1B	107.6	S1—C7—H7C	109.5
Pt1—N1—H1B	107.7	H7A—C7—H7C	109.5
H1A—N1—H1B	107.1	H7B—C7—H7C	109.5
C6—C1—C2	120.3 (4)	S1—C8—H8A	109.5
C6—C1—N1	119.6 (4)	S1—C8—H8B	109.5
C2—C1—N1	120.1 (4)	H8A—C8—H8B	109.5
C3—C2—C1	119.5 (4)	S1—C8—H8C	109.5
C3—C2—H2	120.2	H8A—C8—H8C	109.5
C1—C2—H2	120.2	H8B—C8—H8C	109.5
Pt1—N1—C1—C6	112.7 (4)	C2—C3—C4—C5	0.0 (8)
Pt1—N1—C1—C2	−68.9 (4)	C3—C4—C5—C6	1.2 (8)
C6—C1—C2—C3	1.8 (6)	C4—C5—C6—C1	−0.9 (7)
N1—C1—C2—C3	−176.5 (4)	C2—C1—C6—C5	−0.6 (7)
C1—C2—C3—C4	−1.5 (7)	N1—C1—C6—C5	177.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl2^{i}	0.89	2.78	3.463 (3)	134
N1—H1*A*···Cl2^{ii}	0.89	2.84	3.425 (3)	125
N1—H1*B*···O1^{i}	0.89	2.05	2.913 (4)	165
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C8—H8*C*···Cl1^{iv}	0.96	2.77	3.677 (6)	158

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