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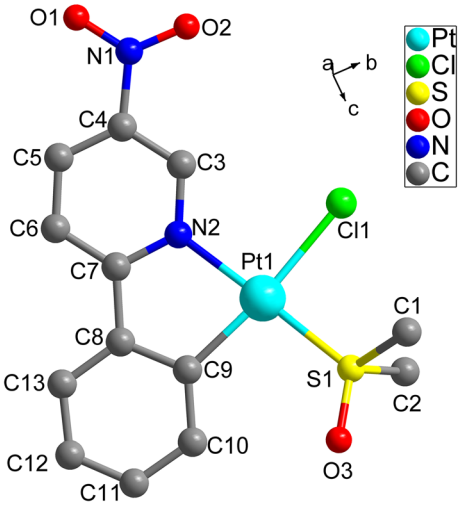
# Crystal structure of chlorido-(5-nitro-2-phenylpyridine-κ²*N*,*C*)-[(methylsulfinyl) methane-κ¹*S*]platinum(II), $C_{13}H_{13}ClN_2O_3PtS$

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**Abstract**

$C_{13}H_{13}ClN_2O_3PtS$, monoclinic, *C*2/*c* (no. 15), *a* = 7.9405(8) Å, *b* = 18.0744(18) Å, *c* = 21.513(2) Å, *β* = 98.781(1)°, *Z* = 8, *V* = 3051.3(5) Å$^3$, $R_{gt}(F)$ = 0.0535, $wR_{ref}(F^2)$ = 0.0233, T = 296 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Orange block |
| Size: | 0.06 × 0.06 × 0.06 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| *μ*: | 9.52 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, *φ* and *ω* |
| $\theta_{max}$, completeness: | 27.0°, >99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 11,267, 3061, 0.046 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2646 |
| $N(param)_{refined}$: | 193 |
| Programs: | Bruker [1], Olex2 [2], SHELX [3, 4] |

## 1 Source of materials

5-nitro-2-phenylpyridine (0. 2402 g, 0.0012 mol) and $K_2PtCl_4$ (1.6602 g, 0.0004 mol) were suspended in 2-ethoxyethanol (90 mL). Under nitrogen atmosphere, the suspension liquid was stirred at 80 °C for 10 h, 2-ethoxyethanol was removed by rotary evaporator, added DMSO (20 mL) stirred at 20 °C for 10 h. The title crystals were obtained by slow evaporation from DMSO at room temperature.

## 2 Experimental details

Absorption corrections were used by using multi-scan program [1]. The structure was solved with SHELX [3, 4]. Hydrogen atoms were placed in their geometrically idealized positions. Hydrogen atoms were constrained to ride on their parent atoms.

## 3 Comment

Platinum complexes have excellent performance in medicine, catalysis, optics, many have even been used in our lives. We successfully synthesized a planar platinum complex and solved its crystal structure. It layed the foundation of exploring application in various fields [5–7].

The title compound is a planar complex with platinum(II) as the central metal. The coordination sites of the

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

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pt1 | 0.68613 (2) | 0.39794 (2) | 0.33000 (2) | 0.03261 (9) |
| Cl1 | 0.7653 (2) | 0.51377 (7) | 0.28952 (6) | 0.0654 (4) |
| S1 | 0.60251 (15) | 0.45712 (6) | 0.41050 (5) | 0.0402 (3) |
| O1 | 0.8944 (7) | 0.3322 (3) | 0.05315 (19) | 0.0979 (16) |
| O2 | 0.8893 (5) | 0.4362 (3) | 0.10061 (17) | 0.0712 (12) |
| O3 | 0.5033 (5) | 0.4186 (2) | 0.45274 (18) | 0.0649 (11) |
| N1 | 0.8746 (5) | 0.3696 (3) | 0.09840 (19) | 0.0563 (12) |
| N2 | 0.7516 (4) | 0.34077 (19) | 0.25412 (14) | 0.0321 (8) |
| C1 | 0.4835 (8) | 0.5364 (3) | 0.3840 (3) | 0.0694 (16) |
| H1A | 0.552846 | 0.569172 | 0.363607 | 0.104* |
| H1B | 0.447534 | 0.561119 | 0.419226 | 0.104* |
| H1C | 0.385285 | 0.521953 | 0.354793 | 0.104* |
| C2 | 0.7811 (6) | 0.4968 (3) | 0.4571 (2) | 0.0703 (17) |
| H2A | 0.853956 | 0.458292 | 0.476662 | 0.105* |
| H2B | 0.744057 | 0.527270 | 0.489033 | 0.105* |
| H2C | 0.842579 | 0.526495 | 0.431193 | 0.105* |
| C3 | 0.7988 (6) | 0.3730 (3) | 0.2029 (2) | 0.0385 (10) |
| H3 | 0.810300 | 0.424172 | 0.201302 | 0.046* |
| C4 | 0.8298 (5) | 0.3305 (3) | 0.1535 (2) | 0.0390 (11) |
| C5 | 0.8168 (6) | 0.2553 (3) | 0.1544 (2) | 0.0484 (12) |
| H5 | 0.838568 | 0.227160 | 0.120290 | 0.058* |
| C6 | 0.7710 (6) | 0.2223 (3) | 0.2065 (2) | 0.0453 (12) |
| H6 | 0.763996 | 0.170985 | 0.208722 | 0.054* |
| C7 | 0.7349 (5) | 0.2660 (2) | 0.25636 (19) | 0.0349 (10) |
| C8 | 0.6807 (5) | 0.2390 (2) | 0.31379 (19) | 0.0335 (9) |
| C9 | 0.6510 (5) | 0.2935 (2) | 0.35805 (18) | 0.0333 (9) |
| C10 | 0.6036 (7) | 0.2680 (3) | 0.4144 (2) | 0.0493 (12) |
| H10 | 0.582526 | 0.301863 | 0.444796 | 0.059* |
| C11 | 0.5879 (7) | 0.1930 (3) | 0.4253 (2) | 0.0572 (14) |
| H11 | 0.560355 | 0.177403 | 0.463691 | 0.069* |
| C12 | 0.6116 (7) | 0.1418 (3) | 0.3813 (2) | 0.0530 (13) |
| H12 | 0.596358 | 0.091846 | 0.389098 | 0.064* |
| C13 | 0.6583 (6) | 0.1639 (3) | 0.3250 (2) | 0.0469 (12) |
| H13 | 0.674779 | 0.129036 | 0.294674 | 0.056* |

compound was occupied by carbon, nitrogen, sulfur and chlorine atoms respectively. The carbon and nitrogen atoms are derived from the bidentate ligand 5-nitro-2-phenylpyridine, the sulfur atom is derived from DMSO. The distances of Pt–C9 bonds are 2.013(4) Å, the distances of Pt–N2 bonds are 2.064(3) Å, the distances of Pt1–S1 bonds are 2.2215(10) Å, the distances of Pt1–Cl1 bonds are 2.3882(12) Å. In addition, the C9–Pt1–N2 angle is 80.27(14)°, the C9–Pt1–S1 angle is 98.39(11)°, the N2–Pt1–S1 angle is 177.10(9)°, the C9–Pt1–Cl1 angle is 170.78(12)°, the N2–Pt1–Cl1 angle is 92.20(10)°, the S1–Pt1–Cl1 angle is 89.36(4)°. All bond lengths and bond angles fall within the normal range [8–10].

In the columns, several p-p interactions between adjacent aromatic rings are present. The shortest distance between Cg2 (the centroid of ring N2–C3–C7) and Cg2$^{i}$ (ring N2–C3–C7; symmetry code i: 2–*x*,*y*,1/2–*z*) is 3.681(2) Å, and the dihedral angle between the ring planes is –10.8. The shortest distance between Cg2 (the centroid of ring N2–C3–C7) and Cg3$^{ii}$ (ring C8–C13; symmetry code *ii*: 1–*x*,*y*,1/2–*z*) is 3.745(3) Å, and the dihedral angle between the ring planes is –3.6176° [11–13].

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