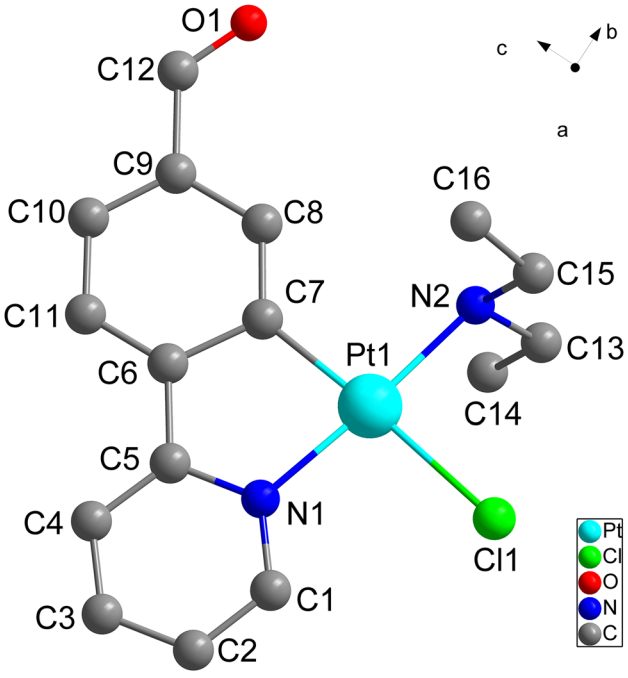
Weixi Xue*

Crystal structure of chlorido-[4-(pyridin-2-yl) benzaldehyde-κ^2*N*,*C*]-(diethylamine-κ^1*N*) platinum(II), $C_{16}H_{18}ClN_2OPt$



https://doi.org/10.1515/ncrs-2024-0033
Received January 22, 2024; accepted March 1, 2024;
published online March 27, 2024

Abstract

$C_{16}H_{18}ClN_2OPt$, monoclinic, $P2_1/c$ (no. 14), a = 7.2964(19) Å, b = 11.010(3) Å, c = 20.283(5) Å, β = 92.582(3)°, V = 1627.7(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0433, w$R_{ref}(F^2)$ = 0.1157, T = 296.15 K.

CCDC no.: 2280555

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.

***Corresponding author: Weixi Xue**, Department of Chemistry, Newcastle University School of Natural and Environmental Sciences, Newcastle upon Tyne, Tyne & Wear, NE1 7RU, UK, E-mail: Xwx10316@outlook.com. https://orcid.org/0009-0006-9231-039X

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.06 × 0.06 × 0.06 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	8.78 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10,927, 2868, 0.063
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 2568
$N(param)_{refined}$:	192
Programs:	Bruker [1], Olex2 [2], Shelx [3, 4]

1 Source of materials

4-(Pyridin-2-yl)benzaldehyde (0.2200 g, 0.0012 mol) and K_2PtCl_4 (1.6602 g, 0.0004 mol) were suspended in 2-ethoxyethanol (100 g). Under nitrogen atmosphere, the suspension liquid was stirred at 80 °C for 12 h, 2-ethoxyethanol was removed by rotary evaporator, added diethylamine (5 g) and methanol (20 g) stirred at 50 °C for 10 h. The title crystals were obtained by slow evaporation from reaction solvent 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 compounds have been deeply studied in various fields and achieved good results, many have even been used in our lives. One-dimensional platinum-based nanostructures electrocatalysis an be effectively used in the field of new energy such as fuel cells due to their excellent oxygen reduction reaction (ORR) [5, 6]. In medicine, pembrolizumab

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.74376 (4)	0.65376 (2)	0.36935 (2)	0.02980 (16)
Cl1	0.8282 (3)	0.6232 (2)	0.25627 (10)	0.0477 (5)
O1	0.5171 (13)	0.9677 (6)	0.5810 (3)	0.081 (2)
N1	0.8114 (7)	0.4821 (5)	0.3980 (3)	0.0308 (13)
N2	0.6623 (10)	0.8304 (5)	0.3459 (3)	0.0377 (16)
C1	0.8693 (11)	0.3940 (8)	0.3583 (4)	0.0402 (19)
H1	0.882036	0.411564	0.313871	0.048*
C2	0.9106 (11)	0.2790 (7)	0.3806 (5)	0.048 (2)
H2	0.952034	0.219857	0.352064	0.058*
C3	0.8890 (10)	0.2535 (8)	0.4464 (5)	0.051 (2)
H3	0.914455	0.176185	0.462932	0.062*
C4	0.8302 (11)	0.3423 (6)	0.4870 (5)	0.042 (2)
H4	0.817411	0.325529	0.531462	0.050*
C5	0.7891 (10)	0.4568 (6)	0.4632 (3)	0.0326 (16)
C6	0.7233 (10)	0.5583 (6)	0.5014 (4)	0.0319 (16)
C7	0.6899 (10)	0.6696 (6)	0.4633 (4)	0.0265 (16)
C8	0.6298 (9)	0.7678 (7)	0.4988 (3)	0.0332 (16)
H8	0.606757	0.840881	0.476980	0.040*
C9	0.6022 (9)	0.7610 (8)	0.5672 (3)	0.0354 (17)
C10	0.6326 (13)	0.6547 (7)	0.6009 (4)	0.046 (2)
H10	0.611917	0.650088	0.645732	0.055*
C11	0.6954 (11)	0.5528 (7)	0.5671 (3)	0.0351 (17)
H11	0.718116	0.480732	0.589875	0.042*
C12	0.5435 (13)	0.8689 (9)	0.6039 (4)	0.049 (2)
H12	0.525366	0.859135	0.648640	0.059*
C13	0.5057 (15)	0.8306 (8)	0.2933 (4)	0.059 (3)
H13A	0.466094	0.913665	0.285375	0.071*
H13B	0.550881	0.799187	0.252397	0.071*
C14	0.3443 (13)	0.7563 (13)	0.3122 (5)	0.084 (3)
H14A	0.243297	0.770409	0.281169	0.126*
H14B	0.309812	0.779169	0.355596	0.126*
H14C	0.376430	0.671773	0.311929	0.126*
C15	0.8142 (16)	0.9096 (9)	0.3254 (5)	0.065 (3)
H15A	0.765606	0.987944	0.311425	0.078*
H15B	0.873351	0.873039	0.288437	0.078*
C16	0.9504 (16)	0.9263 (9)	0.3814 (6)	0.078 (3)
H16A	1.041210	0.984315	0.369420	0.117*
H16B	1.008665	0.850037	0.391787	0.117*
H16C	0.889185	0.955264	0.419306	0.117*

plus pemetrexed and cisplatin or carboplatin complexes can effectively treat nonsquamous non-small-cell lung cancer, and can effectively improve the 5-year survival rate to 19.4 % [7]. Organic light-emitting diodes (OLEDs) optical device containing platinum complex as emissive layer can emit three primary colors of light efficiently, which occupied the mainstream position in various optical devices today [8]. The synthesis of Pt(II)complex is complicated and the product is not easy to purify. We synthesized the target complex by a one-pot reaction and the crystal was obtained by slow volatilization.

The title compound is a planar complex with platinum(II) as the central metal. The coordination sites of the compound was occupied by carbon, nitrogen and chlorine atoms respectively. The carbon atom is derived from the bidentate ligand 4-(pyridin-2-yl)benzaldehyde, the nitrogen atoms are derived from 4-(pyridin-2-yl)benzaldehyde and diethylamine, the chlorine atom is derived from K_2PtCl_4.

The distances of Pt1–Cl1 bonds are 2.4250(19) Å, the distances of Pt–N1 bonds are 2.032(6) Å, the distances of Pt1–N2 bonds are 2.082(6) Å, The distances of Pt1–C7 bonds are 1.971(7) Å, in addition, the C9–Pt1–N2 angle is 80.27(14)°. the N1–Pt1–Cl1 angle is 94.15(16)°, the N1–Pt1–N2 angle is 175.8(2)°, the N2–Pt1–Cl1 angle is 89.78(18)°, the C7–Pt1–Cl1 angle is 175.6(2)°, the C7–Pt1–N1 angle is 82.1(2)°, the C7–Pt1–N2 angle is 94.1(3)°. All bond lengths and bond angles fall within the normal range [9].

In the columns, two π···π interactions between adjacent aromatic rings are present. All the π···π interactions in the range of 3.647(4)–3.897(4) Å, all the dihedral angles are 0.6(4)° [10]. Also the crystal packing is consolidated by weak hydrogen bond interactions. The hydrogen bond is C8–H8···O1, the distance of C8–H8 bond is 0.93 Å, the distance of H8···O1 bond is 2.56 Å, the angle of C8–H8···O1 is 170° [11].

Author contributions: The author has accepted responsibility for the entire content of this submitted manuscript and approved submission.
Research funding: None declared.
Competing interests: The author declares no conflicts of interest regarding this article.

References

1. Bruker. *Apex2, Saint and Sadabs*; Bruker AXS Inc.: Madison, Wisconsin, USA, 2009.
2. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, *42*, 339–341.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Isabel U., Sheldrick G. M. An introduction to experimental phasing of macromolecules illustrated by SHELX; new autotracing features. *Acta Crystallogr.* 2018, *D74*, 106–116.
5. Huiting N., Chenfeng X., Lei H., Shahid Z., Thandavarayan M., Wei G., Bo Y., Bao Yu X. Rational design and synthesis of one-dimensional platinum-based nanostructures for oxygen-reduction electrocatalysis. *Chin. J. Catal.* 2022, *43*, 1459–1472.
6. Erkin N., Sander R., Yurii P. I., Matija G., Luka P., Can Ruüstü Y., Peter W., Giorgio D., Nejc H., Ivar K. Sustainable CO_2-derived nanoscale carbon support to a platinum catalyst for oxygen reduction reaction. *ACS Appl. Nano Mater.* 2023, *6*, 5772–5780.
7. Marina C. G., Shirish G., Giovanna S., Enriqueta F., Emilio E., Manuel D., Maximilian J. H., Steven F. P., Helge G. B., Nir P., Francesco G., Ross R. J.,

Martin R., Rina H., Edward B. G., Takayasu K., Jhanelle E. G., Paul S., Erin J., Catherine M. P., Delvys R. Pembrolizumab plus pemetrexed and platinum in nonsquamous non-small-cell lung cancer: 5-Year outcomes from the phase 3 KEYNOTE-189 study. *J. Clin. Oncol.* 2023, *41*, 1992–1998.

8. Gloria H., Xuemin G., Céline L., Zhen Z., Jasmin S., Jasmin M. B., Stefan B. A brief history of OLEDs-emitter development and industry milestones. *Adv. Mater.* 2021, *33*, 2005630.
9. Felix W., Sergej S., Joshua Immanuel K., Thomas S. Synthesis and photophysical properties of monometallic $C^{\wedge}C^{*}$ platinum(II) formamidinate complexes using Sterically demanding ligands. *Angew. Chem. Int. Ed.* 2023, *62*, e202301225.
10. Dai Z., Kai T., Ziyan F., Aiping X. Crystal structure of 2-(5-phenyl-1-(quinolin-2-yl)-4,5-dihydro-1*H*-pyrazol-3-yl)phenol $C_{24}H_{19}N_3O$. *Z. Kristallogr. N. Cryst. Struct.* 2023, *238*, 1153–1155.
11. Miao-Chang L., Xiao-Bo H., Deng-Ze W. The crystal structure of 6-(benzofuran-2-yl)-2-oxo-4,5-diphenyl-3,4-dihydro-2*H*-pyran-3-carbonitrile, $C_{26}H_{17}NO_3$. *Z. Kristallogr. N. Cryst. Struct.* 2024, *239*, 255–256.