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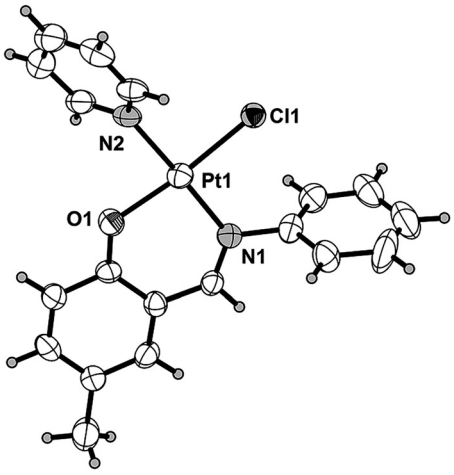
Crystal structure of chlorido-(4-methyl-2-((phenylimino)methyl)phenolato-κ^2*N,O*)-(pyridine-κ^1*N*)platinum(II), $C_{19}H_{17}ClN_2OPt$



https://doi.org/10.1515/ncrs-2021-0301
Received July 24, 2021; accepted August 29, 2021;
published online September 8, 2021

Abstract

$C_{10}H_8BrN_3$, orthorhombic, $P\bar{1}$ (no. 2), a = 12.114(7) Å, b = 12.254(8) Å, c = 13.186(8) Å, α = 71.659(10)°, β = 84.744(10)°, γ = 89.725(10)°, V = 1850(2) Å^3, Z = 4, $R_{gt}(F)$ = 0.0511, $wR_{ref}(F^2)$ = 0.1644, T = 293 K.

CCDC no.: 2106192

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.55 × 0.40 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	7.74 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.6°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13,405, 8311, 0.042
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5880
$N(param)_{refined}$:	435
Programs:	Bruker [1], SHELX [2], Diamond [3]

One of the two crystallographically independent tile complexes 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.

Source of materials

The complex was synthesized in quantitate yield from our previously reported method [4]. Block-shaped yellow crystals of the title complex were grown by slow evaporation from their CH_2Cl_2 solution.

Experimental details

The hydrogen atoms were placed in calculated positions and refined using a riding mode. Some non-fitting reflections were removed manually. The structural model is not affected by this procedure.

Comment

Platinum metal-based complexes (cisplatin, carboplatin, and oxaliplatin) draw immense attention owing to their anticancer potentials. The interest in Pt-based complexes growing worldwide interest due to their ease of synthesis,

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

Atom	x	y	z	U_{iso}*/U_{eq}
Pt1	0.18009 (3)	0.03568 (3)	0.19872 (3)	0.03592 (13)
Pt2	0.68252 (3)	0.33125 (3)	0.19834 (3)	0.03727 (13)
Cl1	0.1784 (2)	−0.1114 (3)	0.1260 (3)	0.0605 (8)
Cl2	0.6815 (2)	0.5276 (2)	0.1190 (3)	0.0655 (8)
N1	0.0221 (7)	0.0089 (7)	0.2603 (7)	0.0377 (17)
N2	0.3379 (7)	0.0727 (8)	0.1339 (7)	0.044 (2)
N3	0.5231 (7)	0.3216 (7)	0.2591 (7)	0.0383 (18)
N4	0.8425 (7)	0.3338 (7)	0.1330 (7)	0.044 (2)
O1	0.2002 (5)	0.1639 (7)	0.2583 (7)	0.055 (2)
O2	0.7023 (6)	0.1616 (6)	0.2605 (6)	0.0460 (17)
C1	0.1246 (8)	0.2057 (9)	0.3107 (8)	0.041 (2)
C2	0.0142 (8)	0.1610 (8)	0.3430 (8)	0.038 (2)
C3	−0.0624 (9)	0.2186 (9)	0.3918 (9)	0.047 (2)
H3	−0.1352	0.1901	0.4083	0.056*
C4	−0.0347 (9)	0.3181 (9)	0.4173 (9)	0.047 (2)
C5	0.0748 (10)	0.3574 (11)	0.3896 (10)	0.059 (3)
H5	0.0968	0.4210	0.4075	0.070*
C6	0.1511 (9)	0.3073 (10)	0.3377 (10)	0.051 (3)
H6	0.2224	0.3394	0.3189	0.061*
C7	−0.0295 (8)	0.0678 (8)	0.3133 (8)	0.039 (2)
H7	−0.1039	0.0481	0.3352	0.047*
C8	−0.0496 (8)	−0.0800 (8)	0.2439 (10)	0.045 (2)
C9	−0.0956 (9)	−0.0643 (11)	0.1505 (11)	0.055 (3)
H9	−0.0782	0.0042	0.0955	0.066*
C10	−0.1643 (11)	−0.1397 (12)	0.1311 (13)	0.066 (4)
H10	−0.1923	−0.1263	0.0650	0.079*
C11	−0.1918 (13)	−0.2434 (15)	0.2204 (17)	0.089 (6)
H11	−0.2404	−0.2981	0.2127	0.106*
C12	−0.1478 (14)	−0.2616 (14)	0.3145 (18)	0.104 (6)
H12	−0.1648	−0.3295	0.3704	0.125*
C13	−0.0761 (11)	−0.1785 (9)	0.3287 (10)	0.057 (3)
H13	−0.0472	−0.1899	0.3941	0.068*
C14	−0.1162 (12)	0.3737 (13)	0.4744 (16)	0.092 (6)
H14A	−0.1250	0.3299	0.5492	0.137*
H14B	−0.1862	0.3770	0.4449	0.137*
H14C	−0.0903	0.4502	0.4660	0.137*
C15	0.3699 (9)	0.1831 (11)	0.0767 (9)	0.053 (3)
H15	0.3157	0.2385	0.0673	0.063*
C16	0.4750 (11)	0.2192 (11)	0.0318 (11)	0.062 (3)
H16	0.4933	0.2953	−0.0077	0.074*
C17	0.5541 (10)	0.1302 (17)	0.0509 (13)	0.083 (5)
H17	0.6273	0.1480	0.0221	0.099*
C18	0.5244 (9)	0.0173 (12)	0.1117 (10)	0.059 (3)
H18	0.5769	−0.0398	0.1255	0.071*
C19	0.4198 (9)	−0.0059 (10)	0.1490 (8)	0.046 (2)
H19	0.4002	−0.0816	0.1886	0.056*
C20	0.6213 (8)	0.0837 (8)	0.3105 (7)	0.036 (2)
C21	0.5102 (7)	0.1110 (7)	0.3312 (7)	0.0316 (18)
C22	0.4337 (8)	0.0211 (10)	0.3808 (9)	0.050 (3)
H22	0.3612	0.0392	0.3978	0.059*
C23	0.4591 (9)	−0.0885 (12)	0.4046 (10)	0.058 (3)
C24	0.5723 (9)	−0.1174 (10)	0.3859 (9)	0.052 (3)
H24	0.5927	−0.1940	0.4060	0.062*
C25	0.6505 (9)	−0.0315 (9)	0.3381 (9)	0.048 (3)
H25	0.7235	−0.0503	0.3240	0.057*
C26	0.4711 (8)	0.2236 (8)	0.3078 (8)	0.037 (2)
H26	0.3968	0.2290	0.3305	0.044*
C27	0.4550 (9)	0.4239 (10)	0.2484 (11)	0.053 (3)
C28	0.4387 (17)	0.4658 (13)	0.3326 (16)	0.100 (6)
H28	0.4726	0.4329	0.3952	0.120*
C29	0.3717 (18)	0.5569 (15)	0.3225 (18)	0.112 (6)
H29	0.3622	0.5886	0.3781	0.135*
C30	0.3179 (18)	0.6029 (16)	0.2331 (19)	0.112 (6)
H30	0.2704	0.6639	0.2282	0.134*
C31	0.3351 (14)	0.5581 (13)	0.1516 (15)	0.088 (5)
H31	0.3002	0.5900	0.0893	0.106*
C32	0.4021 (9)	0.4678 (11)	0.1590 (11)	0.061 (3)
H32	0.4116	0.4364	0.1032	0.073*
C33	0.3727 (10)	−0.1838 (9)	0.4537 (11)	0.058 (3)
H33A	0.3303	−0.1695	0.5132	0.088*
H33B	0.4088	−0.2561	0.4782	0.088*
H33C	0.3242	−0.1863	0.4007	0.088*
C34	0.8717 (9)	0.2678 (11)	0.0737 (11)	0.060 (3)
H34	0.8171	0.2211	0.0620	0.072*
C35	0.9775 (10)	0.2635 (11)	0.0279 (12)	0.073 (4)
H35	0.9937	0.2153	−0.0132	0.088*
C36	1.0565 (11)	0.3303 (13)	0.0439 (12)	0.077 (4)
H36	1.1284	0.3290	0.0131	0.092*
C37	1.0331 (10)	0.4000 (12)	0.1046 (11)	0.066 (4)
H37	1.0877	0.4476	0.1147	0.079*
C38	0.9214 (9)	0.3987 (10)	0.1529 (10)	0.064 (4)
H38	0.9040	0.4427	0.1979	0.077*

stability, favorable therapeutic indices, lower toxicity, etc. [4]. The chemistry of platinum complexes has been extensively studied owing to their antitumor/anticancer properties [5–13] and as a sensor [14, 15].

The asymmetric unit of the title structure contains two Pt-complexes. Each Pt is coordinated by nitrogen and oxygen atom to form a six-member ring and exhibited a square planar environment because the angles of OPtCl and N1PtN2 were ca. 180° respectively. The crystal structures is assembled by collaborative π–π interactions (3.345 Å between pyridine and benzene ring) and CH···π bonds (3.110 Å) to form a linear chain along the c-axis.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This research was financially supported by the Scientific Research Foundation for Talents, Sichuan University of Science & Engineering, Taif University Researches Supporting Project number (TURSP-2020/01), Taif University, Taif, Saudi Arabia. Inner Mongolia University funding under the title Academic Backbone (No.10000-21311201/092).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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