Crystal structure of acridine(pyridine-2,6-dicarboxylato-κ^3N,O,O')platinum(II), $Pt(C_7H_3NO_4)(C_{13}H_9N)$

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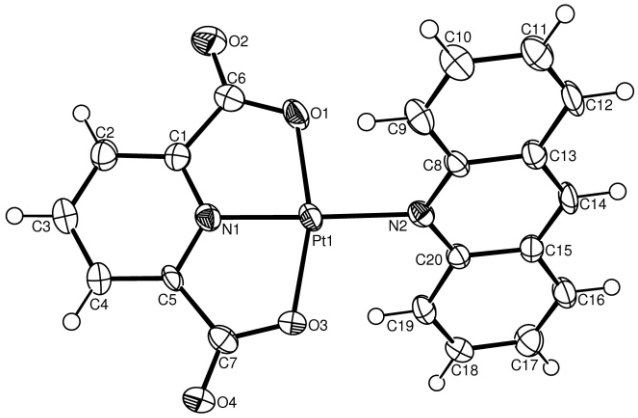
Received May 17, 2011, accepted and available on-line September 2, 2011; CCDC no. 1267/3571



Abstract

$C_{20}H_{12}N_2O_4Pt$, monoclinic, *C*12/*c*1 (no. 15), a = 25.342(2) Å, b = 9.1951(8) Å, c = 13.932(1) Å, β = 94.280(2)°, V = 3237.5 Å^3, Z = 8, $R_{gt}(F)$ = 0.035, $wR_{ref}(F^2)$ = 0.080, T = 200 K.

Source of material

To a solution of K_2PtCl_4 (0.2069 g, 0.498 mmol) in H_2O (20 ml) was added pyridine-2,6-dicarboxylic acid (0.0837 g, 0.501 mmol) and acridine (0.0901 g, 0.503 mmol), and the mixture was refluxed for 3 h. The formed precipitate was separated by filtration, washed with EtOH and ether, and dried at 50 °C to give a yellow powder (0.2534 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a 2-methoxyethanol solution.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with d(C—H) = 0.95 Å and U_{iso}(H) = 1.2 U_{eq}(C). The highest peak (3.23 e Å^{-3}) and the deepest hole (–1.83 e Å^{-3}) in the difference Fourier map are located 1.36 Å and 0.88 Å from the Pt1 atom, respectively.

Discussion

In the title complex, the Pt(II) centre is four-coordinated by one N and two O atoms from the chelating pyridine-2,6-dicarboxylate (dipic) anionic ligand and one N atom of the acridine (acr) ligand in a distorted square-planar environment. The tight chelate angles (∠N1–Pt1–O1 = 81.4(2)° and ∠N1–Pt1–O3 = 81.0(2)°) result in non-linear *trans* arrangement of O1–Pt1–O3 bond with 162.4(2)°, whereas the N1–Pt1–N2 bond is almost linear with ∠N1–Pt1–N2 = 178.5(2)°. The bond lengths d(Pt—O) are nearly equal (2.043(5) Å and 2.046(4)Å), but the bond lengths d(Pt—N) are slightly different. The distance d(Pt1—N1$_{dipic}$) = 1.927(5) Å is somewhat shorter than the distance d(Pt1—N2$_{acr}$) = 2.067(5) Å. The dipic and acr ligands are nearly planar; the dihedral angle between the least-squares planes of the two ligands is 58.47(9)°. In the crystal structure, the complex displays numerous intermolecular π–π interactions between adjacent six-membered rings. For Cg1 (the centroid of ring N2-C20) and Cg1^i (symmetry code i: –x,y,½–z), the centroid-centroid distance is 3.624(3) Å and the dihedral angle between the ring planes is 10°. In addition, there are inter- and intramolecular hydrogen bonds with d(C2–H2···O4) = 3.207(9) Å, d(C14–H14···O1) = 3.324(8) Å, d(C18–H18···O4) = 3.290(9) Å and d(C19–H19···O3) = 3.219(8) Å, forming a three-dimensional network structure.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.10 × 0.15 × 0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	87.00 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	56.58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11506, 3962
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2550
$N(param)_{refined}$:	244
Programs:	SHELXS-97, SHELXL-97 [1], ORTEP-3 [2], PLATON [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	8*f*	0.2393	1.0692	0.5846	0.038
H(3)	8*f*	0.3019	1.0951	0.4707	0.040
H(4)	8*f*	0.2927	0.9638	0.3259	0.034
H(9)	8*f*	0.0392	0.8440	0.3934	0.041
H(10)	8*f*	–0.0451	0.9336	0.3978	0.044
H(11)	8*f*	–0.1188	0.7751	0.3909	0.044
H(12)	8*f*	–0.1065	0.5302	0.3818	0.042
H(14)	8*f*	–0.0455	0.3189	0.3717	0.034
H(16)	8*f*	0.0154	0.1111	0.3520	0.040
H(17)	8*f*	0.0989	0.0293	0.3319	0.045
H(18)	8*f*	0.1705	0.1907	0.3329	0.035
H(19)	8*f*	0.1576	0.4361	0.3559	0.033

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	8*f*	0.13387(1)	0.71131(3)	0.40281(2)	0.0192(1)	0.0256(2)	0.0322(2)	–0.0031(1)	0.0052(1)	0.0020(1)
O(1)	8*f*	0.1163(2)	0.7861(5)	0.5348(3)	0.029(3)	0.034(3)	0.040(3)	–0.007(2)	0.013(2)	0.005(2)
O(2)	8*f*	0.1470(2)	0.9444(6)	0.6476(4)	0.054(4)	0.049(3)	0.038(3)	–0.005(3)	0.018(3)	–0.005(3)
O(3)	8*f*	0.1709(2)	0.6774(5)	0.2792(3)	0.028(3)	0.032(3)	0.028(3)	–0.002(2)	0.009(2)	–0.007(2)
O(4)	8*f*	0.2390(2)	0.7618(5)	0.2034(3)	0.035(3)	0.039(3)	0.031(3)	–0.002(2)	0.014(2)	–0.004(2)
N(1)	8*f*	0.1929(2)	0.8419(6)	0.4269(4)	0.021(3)	0.023(3)	0.035(3)	0.002(2)	0.005(3)	0.001(3)
C(1)	8*f*	0.1953(3)	0.9159(7)	0.5092(5)	0.027(4)	0.020(3)	0.026(4)	0.001(3)	0.001(3)	0.004(3)
C(2)	8*f*	0.2364(3)	1.0139(7)	0.5268(5)	0.030(4)	0.033(4)	0.032(4)	–0.005(3)	–0.001(3)	–0.001(3)
C(3)	8*f*	0.2731(3)	1.0298(8)	0.4589(5)	0.027(4)	0.033(4)	0.040(5)	–0.008(3)	0.000(3)	0.006(3)
C(4)	8*f*	0.2681(3)	0.9509(7)	0.3735(5)	0.026(4)	0.027(4)	0.031(4)	–0.006(3)	–0.001(3)	0.004(3)
C(5)	8*f*	0.2273(2)	0.8546(7)	0.3596(4)	0.010(3)	0.025(3)	0.029(4)	–0.001(3)	0.004(3)	0.001(3)
C(6)	8*f*	0.1502(3)	0.8827(8)	0.5711(5)	0.030(4)	0.032(4)	0.030(4)	0.003(3)	0.006(3)	0.002(3)
C(7)	8*f*	0.2128(3)	0.7591(7)	0.2729(5)	0.021(4)	0.034(4)	0.026(4)	0.003(3)	0.003(3)	0.006(3)
N(2)	8*f*	0.0696(2)	0.5742(6)	0.3796(3)	0.023(3)	0.028(3)	0.020(3)	0.000(2)	0.003(2)	0.005(2)
C(8)	8*f*	0.0198(2)	0.6276(8)	0.3830(4)	0.019(4)	0.032(4)	0.020(4)	–0.003(3)	0.004(3)	0.003(3)
C(9)	8*f*	0.0102(3)	0.7783(8)	0.3904(5)	0.027(4)	0.035(4)	0.041(4)	–0.005(4)	0.008(3)	0.011(4)
C(10)	8*f*	–0.0398(3)	0.8316(8)	0.3932(5)	0.030(4)	0.039(5)	0.042(5)	0.002(3)	0.006(3)	0.008(3)
C(11)	8*f*	–0.0841(3)	0.7368(8)	0.3893(5)	0.021(4)	0.046(5)	0.041(5)	0.003(3)	0.000(3)	0.002(4)
C(12)	8*f*	–0.0767(3)	0.5931(9)	0.3832(5)	0.016(4)	0.053(5)	0.035(4)	–0.013(3)	0.001(3)	0.000(4)
C(13)	8*f*	–0.0252(3)	0.5320(7)	0.3789(5)	0.021(4)	0.034(4)	0.025(4)	–0.004(3)	0.000(3)	0.001(3)
C(14)	8*f*	–0.0163(3)	0.3839(8)	0.3719(5)	0.023(4)	0.032(4)	0.031(4)	–0.016(3)	0.005(3)	0.004(3)
C(15)	8*f*	0.0338(3)	0.3289(7)	0.3653(4)	0.028(4)	0.034(4)	0.017(3)	–0.010(3)	0.001(3)	0.001(3)
C(16)	8*f*	0.0439(3)	0.1786(7)	0.3525(5)	0.025(4)	0.033(4)	0.042(5)	–0.008(3)	0.006(3)	0.001(3)
C(17)	8*f*	0.0931(3)	0.1303(8)	0.3408(5)	0.040(5)	0.028(4)	0.045(5)	–0.003(4)	0.005(4)	0.002(4)
C(18)	8*f*	0.1361(3)	0.2265(8)	0.3417(5)	0.025(4)	0.034(4)	0.030(4)	0.003(3)	0.007(3)	0.001(3)
C(19)	8*f*	0.1283(3)	0.3717(8)	0.3552(4)	0.019(4)	0.035(4)	0.029(4)	–0.004(3)	0.000(3)	0.003(3)
C(20)	8*f*	0.0770(3)	0.4287(7)	0.3681(4)	0.022(4)	0.023(4)	0.025(4)	–0.002(3)	0.004(3)	0.001(3)

Acknowledgment. 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 (grant no. 2010-0029626).

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