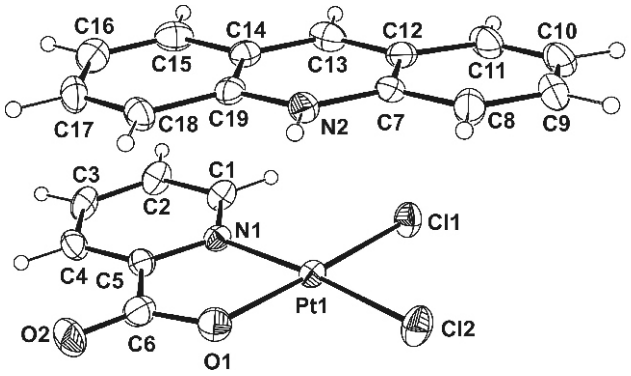
Crystal structure of acridinium dichloro(pyridine-2-carboxylato-k^2*N*,*O*)platinate(II), $[C_{13}H_{10}N][PtCl_2(C_6H_4NO_2)]$

Kwang Ha*

Chonnam National University, School of Applied Chemical Engineering, Research Institute of Catalysis, Gwangju 500-757, Republic of Korea

Received February 28, 2011, accepted and available on-line May 20, 2011; CCDC no. 1267/3419



Abstract

$C_{19}H_{14}Cl_2N_2O_2Pt$, monoclinic, *C*12/*c*1 (no. 15), *a* = 26.276(5) Å, *b* = 8.056(1) Å, *c* = 19.944(3) Å, β = 121.309(3)°, *V* = 3606.8 Å^3, *Z* = 8, $R_{gt}(F)$ = 0.037, $wR_{ref}(F^2)$ = 0.086, *T* = 200 K.

Source of material

To a suspension of acridine (0.1792 g, 1.000 mmol) and pyridine-2-carboxylic acid (0.1231 g, 1.000 mmol) in H_2O (20 ml) was added K_2PtCl_4 (0.4156 g, 1.001 mmol), and the mixture was stirred at room temperature for 3 h. The formed precipitate was separated by filtration, washed with H_2O, EtOH and ether, and dried at 50 °C, to give a yellow powder (0.4513 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a CH_3CN solution.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with *d*(C—H) = 0.95 Å, *d*(N—H) = 0.88 Å and U_{iso}(H) = 1.2U_{eq}(C, N). The highest peak (1.46 e·Å^{-3}) and the deepest hole (–2.10 e·Å^{-3}) in the difference Fourier map are located 0.96 Å and 0.95 Å from the atoms N1 and Pt1, respectively.

Discussion

The crystal structure of the title compound consists of an acridinium cation and an anionic Pt(II) complex. In the complex, the Pt(II) ion has a distorted square-planar environment defined by the N and O atoms from the chelating pyridine-2-carboxylate anionic ligand and two Cl^- anions. The tight N1–Pt1–O1 chelate angle of 81.6(2)° results in non-linear *trans* arrangements (∠Cl1–Pt1–O1 = 176.6(2)° and ∠Cl2–Pt1–N1 = 172.4(2)°). Because the two Pt—Cl bond lengths are almost equal (2.286(2) Å and 2.292(2) Å), the different *trans* effects of the O and N atoms cannot be observed reliably. The Pt—O bond (2.035(5) Å) is slightly longer than the Pt—N bond (2.002(6) Å). In the crystal structure, the ions are linked by intermolecular N–H···O hydrogen bonding with *d*(N···O) = 2.792(9) Å. The acridinium and the complex are located approximately parallel: the dihedral angle between the cation and pyridyl ring planes is 5.2(4)°. There are also numerous intermolecular π-π interactions between adjacent six-membered rings. For Cg1 (the centroid of ring N2-C19) and Cg2^i (ring C14-C19; symmetry code i: –*x*,1–*y*,–*z*), the centroid-centroid distance is 3.811(5) Å and the dihedral angle between the ring planes is 1.9(4)°.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.09 × 0.15 × 0.16 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	80.93 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	56.58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12849, 4428
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2827
$N(param)_{refined}$:	235
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(1)	8*f*	0.2304	0.7466	0.2921	0.048
H(2)	8*f*	0.2145	0.6672	0.3922	0.053
H(3)	8*f*	0.1334	0.7755	0.3950	0.054
H(4)	8*f*	0.0659	0.9466	0.2929	0.051
H(2A)	8*f*	0.0250	0.7751	–0.0593	0.047
H(8)	8*f*	0.0699	0.7830	–0.1378	0.059
H(9)	8*f*	0.1533	0.7245	–0.1428	0.067
H(10)	8*f*	0.2325	0.5770	–0.0441	0.069
H(11)	8*f*	0.2320	0.4884	0.0659	0.061
H(13)	8*f*	0.1740	0.4590	0.1349	0.052
H(15)	8*f*	0.1170	0.4465	0.2031	0.058
H(16)	8*f*	0.0344	0.5287	0.2079	0.058
H(17)	8*f*	–0.0377	0.7001	0.1111	0.054
H(18)	8*f*	–0.0324	0.7881	0.0045	0.049

* e-mail: hakwang@chonnam.ac.kr

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*	0.16636(1)	0.97934(3)	0.14687(2)	0.0332(2)	0.0331(2)	0.0323(2)	–0.0021(1)	0.0176(1)	0.0013(1)
Cl(1)	8*f*	0.25548(9)	0.8535(2)	0.1856(1)	0.038(1)	0.058(1)	0.049(1)	0.0054(9)	0.026(1)	0.007(1)
Cl(2)	8*f*	0.16119(9)	1.0930(3)	0.0382(1)	0.052(1)	0.064(1)	0.044(1)	0.003(1)	0.029(1)	0.015(1)
O(1)	8*f*	0.0876(2)	1.0874(6)	0.1185(3)	0.046(4)	0.045(3)	0.049(4)	0.013(3)	0.026(3)	0.015(3)
O(2)	8*f*	0.0239(3)	1.1127(6)	0.1594(4)	0.051(4)	0.057(3)	0.090(5)	0.028(3)	0.045(4)	0.021(3)
N(1)	8*f*	0.1604(3)	0.8941(6)	0.2369(3)	0.031(4)	0.033(3)	0.029(4)	–0.006(3)	0.013(3)	–0.003(3)
C(1)	8*f*	0.1970(3)	0.7896(9)	0.2930(4)	0.034(5)	0.045(4)	0.034(5)	–0.001(4)	0.014(4)	0.008(4)
C(2)	8*f*	0.1878(4)	0.7417(9)	0.3526(5)	0.044(5)	0.058(5)	0.027(5)	–0.001(4)	0.015(4)	0.012(4)
C(3)	8*f*	0.1396(4)	0.804(1)	0.3535(5)	0.053(6)	0.061(5)	0.028(5)	–0.014(4)	0.026(5)	–0.003(4)
C(4)	8*f*	0.1003(4)	0.9062(9)	0.2941(5)	0.043(5)	0.045(4)	0.046(6)	–0.002(4)	0.027(5)	–0.012(4)
C(5)	8*f*	0.1113(3)	0.9499(8)	0.2365(5)	0.046(5)	0.035(4)	0.035(5)	–0.002(3)	0.026(4)	–0.004(3)
C(6)	8*f*	0.0707(4)	1.0579(9)	0.1684(5)	0.046(6)	0.040(4)	0.054(6)	–0.001(4)	0.028(5)	0.005(4)
N(2)	8*f*	0.0536(3)	0.7148(6)	–0.0220(4)	0.034(4)	0.034(3)	0.053(5)	0.003(3)	0.025(4)	–0.001(3)
C(7)	8*f*	0.1006(3)	0.6742(8)	–0.0292(5)	0.042(5)	0.025(3)	0.059(6)	0.000(3)	0.034(5)	–0.005(4)
C(8)	8*f*	0.1024(4)	0.7249(9)	–0.0960(5)	0.060(6)	0.045(4)	0.062(6)	0.011(4)	0.045(6)	0.012(4)
C(9)	8*f*	0.1513(4)	0.689(1)	–0.0988(6)	0.076(7)	0.048(5)	0.071(7)	0.006(5)	0.057(7)	–0.003(5)
C(10)	8*f*	0.1991(4)	0.601(1)	–0.0394(6)	0.052(6)	0.048(5)	0.091(8)	0.002(4)	0.050(6)	–0.015(5)
C(11)	8*f*	0.1989(4)	0.5471(9)	0.0254(6)	0.038(5)	0.046(5)	0.071(7)	0.004(4)	0.030(5)	–0.011(4)
C(12)	8*f*	0.1482(3)	0.5808(8)	0.0312(5)	0.035(5)	0.028(4)	0.063(6)	–0.003(3)	0.028(5)	–0.006(4)
C(13)	8*f*	0.1435(3)	0.5258(8)	0.0951(5)	0.032(5)	0.038(4)	0.045(5)	0.005(3)	0.010(4)	–0.005(4)
C(14)	8*f*	0.0941(3)	0.5694(8)	0.0996(5)	0.038(5)	0.031(4)	0.037(5)	–0.006(3)	0.017(4)	–0.005(3)
C(15)	8*f*	0.0876(4)	0.5156(9)	0.1631(5)	0.056(6)	0.040(4)	0.037(5)	–0.004(4)	0.016(4)	–0.003(4)
C(16)	8*f*	0.0388(4)	0.564(1)	0.1658(5)	0.054(6)	0.056(5)	0.039(5)	–0.013(4)	0.026(5)	–0.009(4)
C(17)	8*f*	–0.0048(4)	0.6665(9)	0.1069(5)	0.034(5)	0.057(5)	0.050(6)	–0.001(4)	0.026(5)	–0.005(4)
C(18)	8*f*	–0.0022(3)	0.7197(9)	0.0438(5)	0.031(5)	0.044(4)	0.048(6)	0.000(3)	0.020(4)	–0.011(4)
C(19)	8*f*	0.0482(3)	0.6679(8)	0.0393(5)	0.033(5)	0.033(4)	0.033(5)	–0.009(3)	0.015(4)	–0.007(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).

References

1. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.
2. Farrugia, L. J.: ORTEP-3 for Windows - a version of ORTEP-III with a Graphical User Interface (GUI) J. Appl. Crystallogr. **30** (1997) 565.
3. Spek, A. L.: Single-crystal structure validation with the program PLATON. J. Appl. Crystallogr. **36** (2003) 7-13.