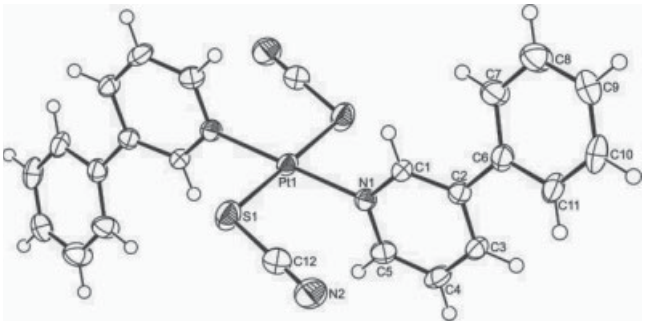
Crystal structure of bis(3-phenylpyridine-κ*N*)bis(thiocyanato-κ*S*)-platinum(II), $C_{24}H_{18}N_4PtS_2$

Kwang Ha*

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

Received December 19, 2012, accepted June 04, 2013, available online June 14, 2013, CCDC no. 1267/3877



Abstract

$C_{24}H_{18}N_4PtS_2$, monoclinic, $P2_1/n$ (no. 14), a = 9.820(1) Å, b = 5.3464(8) Å, c = 21.463(3) Å, β = 102.471(3)°, V = 1100.3 Å^3, Z = 2, $R_{gt}(F)$ = 0.0254, $wR_{ref}(F^2)$ = 0.0578, T = 200 K.

Table 1. Data collection and handling.

Crystal:	yellow sticks, size 0.06×0.09×0.34 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	65.86 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ and ω
$2\theta_{max}$:	52.08°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6373, 2138
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1534
$N(param)_{refined}$:	142
Programs:	SHELX [5], ORTEP-3[6], PLATON [7]

Source of material

To a solution of K_2PtCl_4 (0.205 g, 0.493 mmol) in H_2O (40 ml) were added KSCN (0.505 g, 5.194 mmol) and 3-phenylpyridine (*ppy*; 0.174 g, 1.121 mmol) in EtOH (10 ml) and stirred for 24 h at room temperature. The formed precipitate was separated by filtration, washed with H_2O and EtOH, and dried at 50 °C, to give a pale yellow powder (0.244 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 and U_{iso}(H) = 1.2U_{eq}(C). The highest peak (1.16 e·Å^{-3}) and the deepest hole (–0.90 e·Å^{-3}) in the difference Fourier map are located 0.89 Å and 0.89 Å from the atom Pt1, respectively.

Discussion

Crystal structures of the related Pd(II) complex $[PdCl_2(ppy)_2]$ and Pt(IV) anionic complex (H-*ppy*)$[PtCl_5(ppy)]\cdot H_2O$ have been reported previously [1, 2]. The central Pt(II) ion in the title complex $[Pt(SCN)_2(ppy)_2]$ has a *trans*-S_2N_2 square-planar coordination defined by two N atoms from two 3-phenylpyridine ligands and two S atoms of two SCN^- anions. The Pt atom is located on an inversion center, and therefore the asymmetric unit contains one half of the complex and the PtS_2N_2 moiety is exactly planar. The pyridine ring of the ligand is almost perpendicular to the PtS_2N_2 plane (86.4(1)°). In the crystal structure, the *ppy* ligand is not planar. The pyridine and phenyl rings are twisted by 20.7(2)°. The thiocyanato ligand is almost linear with a S–C–N bond angle of 179.0(5)°, and the S atoms are coordinated to the Pt atom with the nearly tetrahedral Pt–S–C bond angle of 105.4(2)°, characteristic of an S-bonded conformation [3, 4]. The complex molecules are stacked in columns along [010] with d(Pt···Pt) = 5.3464(8) Å (= length of b axis) and successive complexes stack in opposite directions along [001]. In the columns, several intermolecular π-π interactions between the aromatic rings are present. The shortest distance between Cg1 (the centroid of ring N1-C5) and $Cg2^i$ (the centroid of ring C6-C11, symmetry code i: x, y-1, z) is 3.777(3) Å, and the dihedral angle between the ring planes is 20.7(2)°. Moreover, the complex displays intermolecular C–H···N hydrogen bonds with d(C···N) = 3.395(7) Å and 3.402(7) Å.

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.2448	0.3261	0.0503	0.031
H(3)	4*e*	0.4380	0.0680	0.2228	0.035
H(4)	4*e*	0.2665	–0.2358	0.2153	0.039
H(5)	4*e*	0.0895	–0.2586	0.1249	0.038
H(7)	4*e*	0.4377	0.4943	0.0448	0.048
H(8)	4*e*	0.6018	0.8124	0.0510	0.054
H(9)	4*e*	0.7373	0.9323	0.1489	0.047
H(10)	4*e*	0.7024	0.7405	0.2421	0.051
H(11)	4*e*	0.5362	0.4295	0.2364	0.041

* 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)	2*a*	0	0	0	0.0265(2)	0.0286(1)	0.0209(1)	–0.0043(1)	0.00010(9)	0.0005(1)
S(1)	4*e*	–0.1587(1)	0.2408(3)	0.03968(6)	0.0373(8)	0.0517(8)	0.0301(7)	0.0068(7)	0.0001(5)	–0.0054(6)
N(1)	4*e*	0.1528(4)	0.0307(7)	0.0791(2)	0.025(2)	0.032(2)	0.021(2)	–0.005(2)	0.002(2)	–0.002(2)
N(2)	4*e*	–0.0238(5)	0.3692(9)	0.1653(2)	0.050(3)	0.060(3)	0.035(3)	–0.005(3)	0.008(2)	–0.009(2)
C(1)	4*e*	0.2509(5)	0.2097(9)	0.0843(2)	0.024(3)	0.031(3)	0.021(2)	0.001(2)	0.003(2)	0.003(2)
C(2)	4*e*	0.3598(5)	0.2318(8)	0.1365(2)	0.025(3)	0.027(2)	0.024(2)	0.003(2)	0.006(2)	–0.002(2)
C(3)	4*e*	0.3645(5)	0.0600(8)	0.1859(2)	0.029(3)	0.037(3)	0.019(2)	0.003(2)	0.001(2)	0.000(2)
C(4)	4*e*	0.2637(5)	–0.1202(9)	0.1814(2)	0.039(3)	0.034(3)	0.024(3)	0.006(3)	0.004(2)	0.009(2)
C(5)	4*e*	0.1590(5)	–0.1330(9)	0.1279(2)	0.034(3)	0.030(3)	0.034(3)	0.000(2)	0.009(2)	0.007(2)
C(6)	4*e*	0.4673(5)	0.4302(9)	0.1402(2)	0.025(3)	0.038(3)	0.026(3)	0.003(2)	0.002(2)	–0.005(2)
C(7)	4*e*	0.4903(6)	0.5451(9)	0.0853(2)	0.038(3)	0.056(4)	0.026(3)	–0.016(3)	0.009(2)	–0.010(2)
C(8)	4*e*	0.5891(6)	0.733(1)	0.0889(2)	0.047(4)	0.054(3)	0.037(3)	–0.016(3)	0.014(3)	–0.009(3)
C(9)	4*e*	0.6688(5)	0.805(1)	0.1467(2)	0.027(3)	0.039(3)	0.052(3)	–0.006(2)	0.006(2)	–0.005(3)
C(10)	4*e*	0.6481(5)	0.691(1)	0.2017(2)	0.030(3)	0.045(3)	0.043(3)	0.000(3)	–0.013(2)	–0.009(3)
C(11)	4*e*	0.5490(5)	0.5066(9)	0.1982(2)	0.030(3)	0.037(3)	0.030(3)	0.001(3)	–0.007(2)	0.004(3)
C(12)	4*e*	–0.0774(5)	0.3163(9)	0.1143(2)	0.039(3)	0.034(3)	0.035(3)	0.000(2)	0.010(2)	0.001(2)

Acknowledgments. 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 (2009-0094055).

References

1. Ha, K.: Crystal structure of dichlorobis(3-phenylpyridine-κ*N*)palladium(II), $PdCl_2(C_{11}H_9N)_2$. Z. Kristallogr. NCS **226** (2011) 507-508.
2. Ha, K.: Crystal structure of 3-phenylpyridinium pentachloro(3-phenylpyridine-κ*N*)platinate(IV) hydrate, $[C_{11}H_{10}N][PtCl_5(C_{11}H_9N)]\cdot H_2O$. Z. Kristallogr. NCS **227** (2012) 12-14.
3. Sun, Y.-M.; Dong, F.-Y.; Dou. J.-M.; Li, D.-C.; Gao, X.-K.; Wang, D.-Q.: Synthesis and crystal structure of *catena*-poly[aqua(*cis*-*syn*-*cis*-dicyclohexyl-18-crown-6) tetra(thiocyanato)barium(II) platinum(II)]: $[BaPt(NCS)_4(C_{20}H_{36}O_6)(H_2O)]_n$. J. Chem. Crystallogr. **36** (2006) 315-319.
4. Ha, K.: Crystal structure of bis(1,10-phenanthrolinium) hexakis-(thiocyanato-κ*S*)platinate(IV), $(C_{12}H_9N_2)_2[Pt(SCN)_6]$. Z. Kristallogr. NCS **225** (2010) 699-700.
5. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.
6. Farrugia, L. J.: ORTEP-3 for Windows - a version of ORTEP-III with a Graphical User Interface (GUI). J. Appl. Crystallogr. **30** (1997) 565.
7. Spek, A. L.: Single-crystal structure validation with the program PLATON. J. Appl. Crystallogr. **36** (2003) 7-13.