Platinum-Ruthenium Dinuclear Complex Bridged by Bis(terpyridyl)xanthene

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Supporting Information

1. X-ray structure of [**2**]$(PF_6)_2 \cdot 6CH_3CN$

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Supporting Information

X-ray Structure of $[(PtCl)_2(btpyxa)]$ $(PF_6)_2 \cdot 6CH_3CN$ ($[2](PF_6)_2 \cdot 6CH_3CN$).

Yellow crystals of $[\mathbf{2}](PF_6)_2 \cdot 6CH_3CN$ were obtained by vapor diffusion of diethyl ether into an acetonitrile solution of the complex. Crystal data of $[\mathbf{2}](PF_6)_2 \cdot 6CH_3CN$ are summarized in Table S1.

Data for $[\mathbf{2}](PF_6)_2 \cdot 6CH_3CN$ were collected on a Rigaku/MSC Mercury CCD difractometer using graphite-monochromated Mo Kα radiation (λ = 0.71070 Å) at 173 K, and processed using Crystal Clear. [1] The structure was solved by heavy-atom Patterson methods (Dirdif 94 Patty)[2] and refined by full-matrix least square refinement on F^2. All non-hydrogen atoms except for C19 in terpyridyl moiety were refined anisotopically. All hydrogen atoms were located on the calculated positions and not refined. All calculations were performed using the teXsan crystallographic software package.[3]

REFERENCE
(1) Crystal Clear: Software Package, Rigaku and Molecular Structure Corporation, 1999.
(2) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
(3) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation, 1985 & 1999.

Table S1. Crystallographic data for complex [**2**]$(PF_6)_2 \cdot 6CH_3CN$

	[**2**]$(PF_6)_2 \cdot 6CH_3CN$
formula	$C_{53}H_{48}Cl_2F_{12}N_6OP_2Pt_2 \cdot 6CH_3CN$
formula weight	1782.33
color	yellow
crystal size/mm^3	0.40 × 0.30 × 0.10
crystal system	triclinic
space group	*P*-1
a/ Å	13.841(7)
b/ Å	14.377(7)
c/ Å	19.442(10)
α/deg	95.226(7)
β/deg	100.167(5)
γ/deg	110.974(7)
V/ Å^3	3505(3)
Z	2
T/K	-173
D_{calc}/g cm^{-3}	1.689
radiation	MoKα (λ = 0.71070)
μ/cm^{-1}	41.75
F(000)	1752.00
$2\theta_{max}$/deg	55.0
no. of reflections (all, $2\theta < 54.97^o$)	15186
no. of variables	860
reflection/parameter ratio	17.66
GOF	1.52
R1[a] [$I > 2\sigma(I)$]	0.065
R[b] (all data)	0.112
R_w[c] (all data)	0.155

[a] $R1 = \Sigma||F_o^2|-|F_c^2||/\Sigma|F_o^2|$. [b] $R = \Sigma(F_o^2-F_c^2)/\Sigma F_o^2$. [c] $Rw = [(\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2)]^{1/2}$.

Table 2. Selected Bond Lengths (Å) and Bond Angles (deg) of [**2**]$(PF_6)_2 \cdot 6CH_3CN$*

Pt1 – Cl1	2.298(2)	Pt1 – N1	2.017(6)
Pt1 – N2	1.949(6)	Pt1 – N3	2.021(7)
Pt2 – Cl2	2.297(2)	Pt2 – N4	2.019(6)
Pt2 – N5	1.942(6)	Pt2 – N6	2.026(7)
Cl1 – Pt1 – N1	98.8(2)	N1 – Pt1 – N2	80.9(3)
Cl1 – Pt1 – N3	99.3(2)	N2 – Pt1 – N3	81.0(3)
Cl2 – Pt2 – N4	99.5(2)	N4 – Pt2 – N5	80.8(2)
Cl2 – Pt2 – N6	98.8(2)	N5 – Pt2 – N6	80.9(2)

*Intramolecular distance: Pt1···Pt2, 4.38 Å. Intermolecular distance: Pt1···Pt1, 4.20 Å, Pt2···Pt2, 4.39 Å.

Figure S1. ORTEP drawing of the cationic part of [**2**]$(PF_6)_2 \cdot 6CH_3CN$ with 50% thermal ellipsoids except for C19 atom. Hydrogen atoms are omitted for clarify.

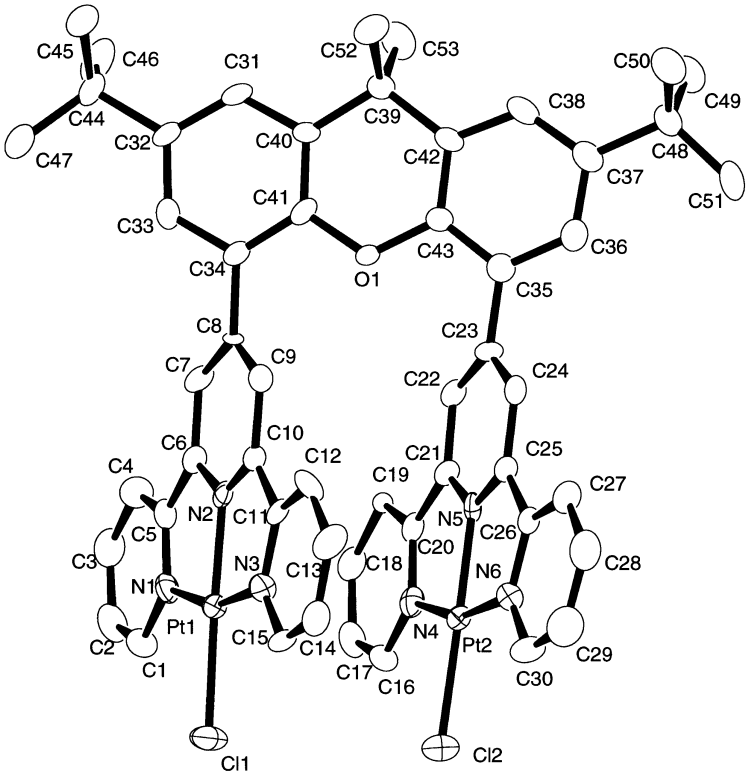

Figure S2. Crystal packing of [**2**]$(PF_6)_2 \cdot 6CH_3CN$. The PF_6^- ions and CH_3CN molecules are omitted for clarify.