Inorganic Chemistry
including bioinorganic chemistry

Supporting Information for *Inorg. Chem.*, **1995**, 34(18), 4591-4599, DOI: 10.1021/ic00122a015

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Figure S-1. An ORTEP drawing of the contents of the $[Pt(tpy)Cl]ClO_4$ unit cell, with a unit cell outlined, viewed perpendicular to the *bc* plane.

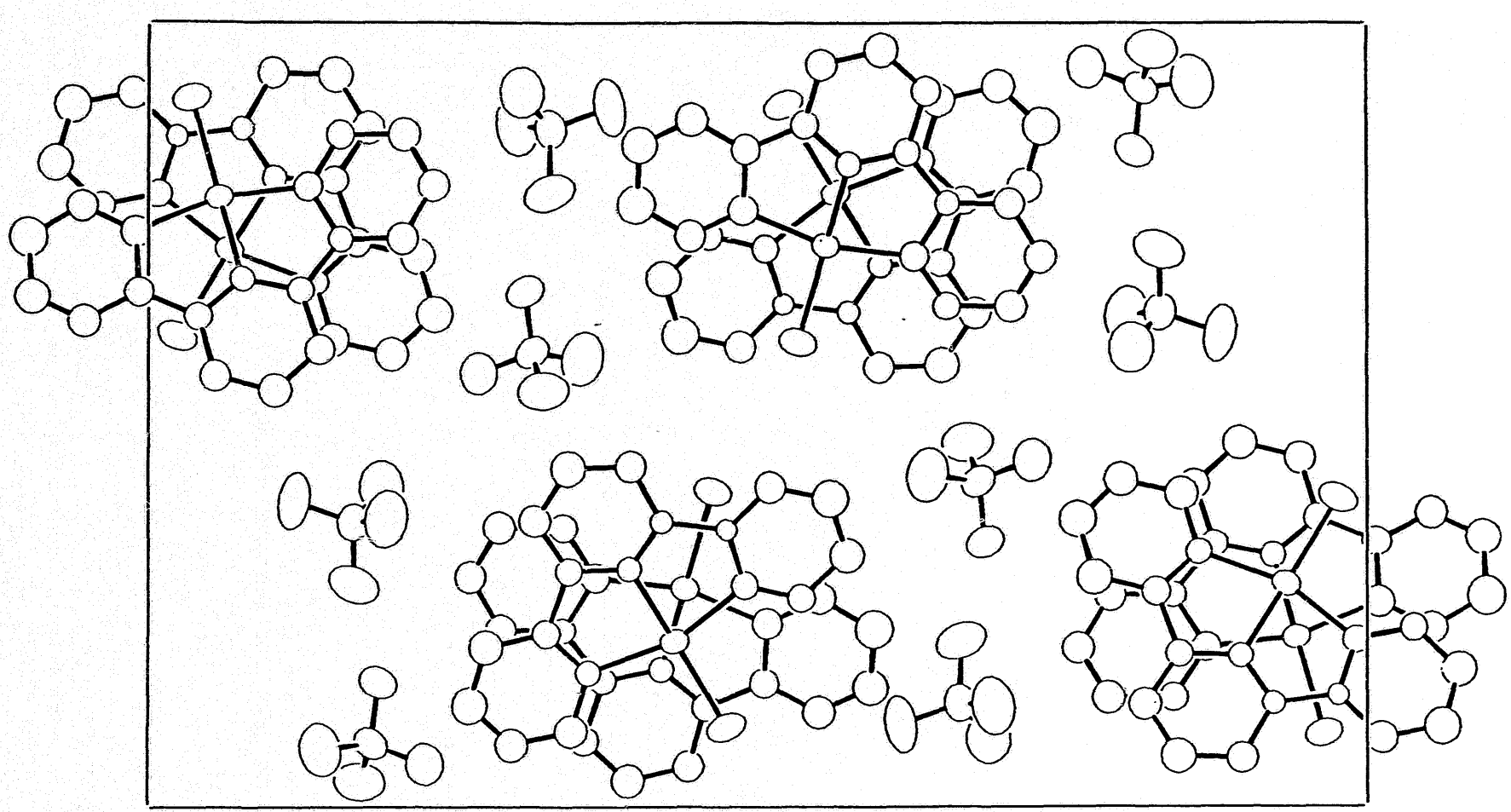

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Figure S-1

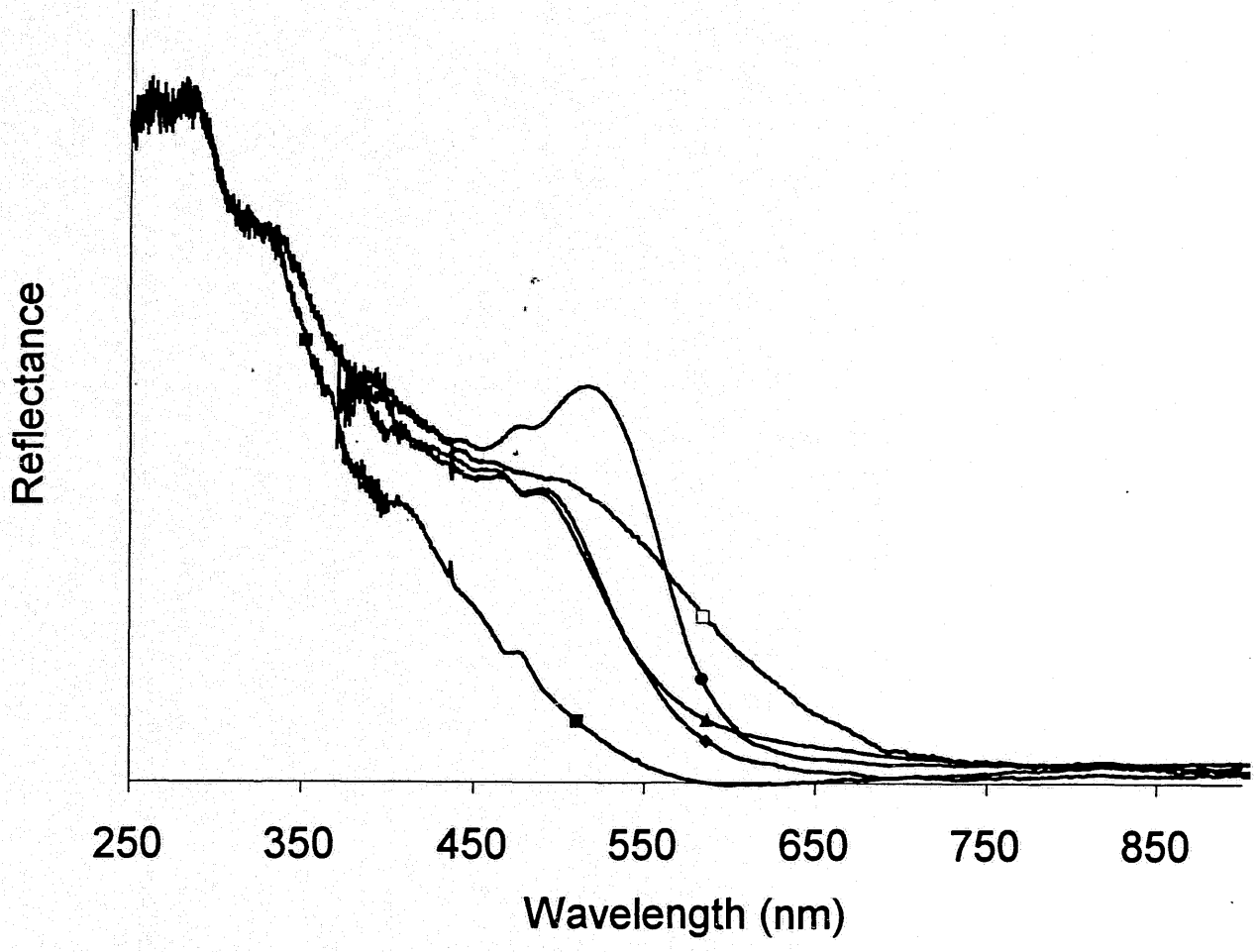

Figure S-2. Reflectance spectra of [Pt(tpy)Cl]X at room temperature, powders diluted with $MgSO_4$ and referenced to pure $MgSO_4$: $X^- = ClO_4^-$, red form (□) and orange form (◆); Cl^- (o); PF_6^- (■); $CF_3SO_3^-$ (▲).

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Supplementary Material

Table S-I. Experimental details for x-ray diffraction study of $[Pt(tpy)Cl]ClO_4$.

(A) Crystal Parameters at 296 K

chemical formula	$C_{15}H_{11}N_4Cl_2O_4Pt$
a, Å	7.085(2)
b, Å	17.064(5)
c, Å	26.905(8)
α, °	90
β, °	90.0(1)
γ, °	90
space group(No.)	$P2_1/c$(14)
Z	8
ρ (calc), g cm^{-1}	2.30
Mol. Wt., g mol^{-1}	563.27
V, Å^3	3252.8(17)
μ, cm^{-1}	90.74
$R(F_o^2 > 0)$	0.039 on *F* for 1611 reflections
$R(F_o^2 > 3\sigma(F_o^2))$	0.031 on *F* for 1464 reflections
*w*R	0.005 on F^2 for 1721 reflections
$\Delta\rho_{max}$, eÅ	+1.10
$\Delta\rho_{min}$, eÅ	-1.42

(B) Measurement of Intensity Data

radiation	MoKα
wavelength, Å	0.71073
standards measured	3
at interval	150 minutes
reflections measured	7269 ($2 < 2\theta < 40$)
independent reflections	1721 (*mmm* symmetry)[a]
goodness of fit for merging	1.76 (1714 multiples)
R_{int}	0.027 (247 duplicates)
reflections used in refinement	1721

(C) Treatment of Intensity Data

absorption correction	empirical (CRYM[10] program)
transmission range (relative)	0.785 to 1.252
secondary extinction[b]	$0.008(5)\times10^{-6}$

[a] See **Experimental** section for discussion.

[b] Larson, A.C. *Acta Cryst.* **1967**, *23*, 644.

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Table S-II. Assigned Hydrogen Atom Parameters for Terpyridine Platinum(II) Chloride Perchlorate.

x, y and $z \times 10^4$

Atom	x	y	z	B
H1	1362	952	1401	4.2
H2	1384	953	2280	5.2
H3	391	2043	2700	5.1
H4	−347	3180	2268	4.9
H7	−1276	4282	1749	4.5
H8	−2072	5176	1134	5.4
H9	−2024	4840	307	4.9
H12	−1679	4291	−515	5.2
H13	−1129	3743	−1248	6.0
H14	206	2480	−1295	6.8
H15	745	1792	−552	4.9
H21	3613	4407	1271	5.3
H22	3491	4714	2098	5.4
H23	4330	3845	2695	6.4
H24	5347	2575	2457	5.7
H27	6101	1335	2161	5.1
H28	6972	199	1716	5.8
H29	7058	180	848	4.7
H32	6903	392	−20	4.9
H33	6743	670	−861	6.5
H34	5273	1892	−1099	5.8
H35	4689	2821	−475	4.0

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Table S-III. Anisotropic Displacement Parameters for Terpyridine Platinum(II) Chloride Perchlorate.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt1	233(7)	278(5)	404(6)	3(4)	−2(6)	−17(5)
Pt2	241(7)	310(5)	411(6)	14(4)	−14(6)	32(5)
Cl1	617(53)	383(34)	735(52)	−25(34)	−34(41)	−115(35)
Cl2	476(49)	425(37)	794(52)	−23(32)	157(39)	177(35)
Cl3	1096(73)	498(44)	576(53)	105(44)	−183(55)	−128(43)
Cl4	845(56)	720(48)	505(50)	212(49)	38(51)	30(37)
O1	2099(328)	1424(188)	883(167)	825(215)	612(233)	−131(149)
O2	1357(193)	530(111)	738(137)	256(121)	24(146)	−127(110)
O3	1390(200)	898(121)	726(129)	306(136)	−479(163)	−22(105)
O4	1750(250)	719(130)	1340(238)	−219(137)	−572(195)	−72(140)
O5	1064(199)	1668(180)	523(128)	585(164)	199(144)	216(122)
O6	897(191)	1724(221)	944(194)	−186(179)	−413(158)	143(180)
O7	1752(230)	731(130)	1303(200)	−58(137)	117(175)	−276(137)
O8	1516(219)	1285(174)	1011(187)	378(170)	692(189)	26(166)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S-IV. Complete Distances and Angles for Terpyridine Platinum(II) Chloride Perchlorate.

	Distance(Å)		Distance(Å)
Pt1 -Pt2	3.269(1)	N4 -C25	1.31(3)
Pt1 -Cl1	2.302(7)	C21 -C22	1.35(3)
Pt1 -N1	1.976(16)	C22 -C23	1.33(3)
Pt1 -N2	1.952(15)	C23 -C24	1.39(4)
Pt1 -N3	2.003(18)	C24 -C25	1.38(3)
Pt2 -Cl2	2.301(6)	C25 -C26	1.51(3)
Pt2 -N4	2.033(15)	N5 -C26	1.33(3)
Pt2 -N5	1.933(15)	N5 -C30	1.32(2)
Pt2 -N6	2.018(16)	C26 -C27	1.40(3)
Cl3 -O1	1.39(3)	C27 -C28	1.41(3)
Cl3 -O2	1.42(2)	C28 -C29	1.38(3)
Cl3 -O3	1.43(2)	C29 -C30	1.45(3)
Cl3 -O4	1.43(2)	C30 -C31	1.45(3)
Cl4 -O5	1.41(2)	N6 -C31	1.37(3)
Cl4 -O6	1.40(3)	N6 -C35	1.29(3)
Cl4 -O7	1.45(2)	C31 -C32	1.39(3)
Cl4 -O8	1.39(2)	C32 -C33	1.36(3)
N1 -C1	1.36(3)	C33 -C34	1.43(3)
N1 -C5	1.40(3)	C34 -C35	1.40(3)
C1 -C2	1.42(3)	C1 -H1	0.949
C2 -C3	1.33(3)	C2 -H2	0.950
C3 -C4	1.38(3)	C3 -H3	0.955
C4 -C5	1.38(3)	C4 -H4	0.949
C5 -C6	1.46(3)	C7 -H7	0.950
N2 -C6	1.31(3)	C8 -H8	0.951
N2 -C10	1.31(3)	C9 -H9	0.948
C6 -C7	1.45(3)	C12 -H12	0.949
C7 -C8	1.37(3)	C13 -H13	0.951
C8 -C9	1.36(3)	C14 -H14	0.949
C9 -C10	1.44(3)	C15 -H15	0.947
C10 -C11	1.42(3)	C21 -H21	0.946
N3 -C11	1.41(3)	C22 -H22	0.951
N3 -C15	1.31(3)	C23 -H23	0.952
C11 -C12	1.40(3)	C24 -H24	0.952
C12 -C13	1.29(3)	C27 -H27	0.949
C13 -C14	1.39(4)	C28 -H28	0.951
C14 -C15	1.40(3)	C29 -H29	0.948
N4 -C21	1.38(3)	C32 -H32	0.949

Table S-IV. (Cont.)

Distance(Å)		Angle(°)	
C33 –H33	0.950	Cl1 –Pt1 –N1	98.4(5)
C34 –H34	0.954	Cl1 –Pt1 –N2	176.6(5)
C35 –H35	0.949	Cl1 –Pt1 –N3	98.1(5)
		N1 –Pt1 –N2	81.9(6)
		N1 –Pt1 –N3	163.5(7)
		N2 –Pt1 –N3	81.7(7)
		Pt1 –N1 –C1	128.6(14)
		Pt1 –N1 –C5	113.8(12)
		Pt1 –N2 –C6	115.8(13)
		Pt1 –N2 –C10	116.6(13)
		Pt1 –N3 –C11	111.0(13)
		Pt1 –N3 –C15	129.9(15)
		Cl2 –Pt2 –N4	99.3(5)
		Cl2 –Pt2 –N5	178.8(5)
		Cl2 –Pt2 –N6	99.4(5)
		N4 –Pt2 –N5	79.8(6)
		N4 –Pt2 –N6	161.2(6)
		N5 –Pt2 –N6	81.4(6)
		Pt2 –N4 –C21	126.8(13)
		Pt2 –N4 –C25	114.4(13)
		Pt2 –N5 –C26	119.3(13)
		Pt2 –N5 –C30	116.7(12)
		Pt2 –N6 –C31	112.4(12)
		Pt2 –N6 –C35	127.3(14)
		C5 –N1 –C1	117.6(16)
		C2 –C1 –N1	121.9(19)
		C3 –C2 –C1	119.1(21)
		C4 –C3 –C2	120.5(22)
		C5 –C4 –C3	120.8(20)
		C4 –C5 –N1	120.1(17)
		C6 –C5 –N1	111.8(16)
		C6 –C5 –C4	128.1(18)
		C10 –N2 –C6	127.3(17)
		N2 –C6 –C5	116.5(17)
		C7 –C6 –C5	125.6(18)
		C7 –C6 –N2	117.7(18)
		C8 –C7 –C6	116.8(20)
		C9 –C8 –C7	122.6(22)

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Table S-IV. (Cont.)

	Angle(°)		Angle(°)
C10 -C9 -C8	118.8(20)	O2 -Cl3 -O1	112.3(14)
C9 -C10 -N2	116.4(18)	O3 -Cl3 -O1	111.7(14)
C11 -C10 -N2	115.2(18)	O4 -Cl3 -O1	105.8(14)
C11 -C10 -C9	128.3(19)	O3 -Cl3 -O2	111.0(12)
C15 -N3 -C11	119.1(18)	O4 -Cl3 -O2	107.9(13)
N3 -C11 -C10	115.4(18)	O4 -Cl3 -O3	107.8(12)
C12 -C11 -C10	126.8(20)	O6 -Cl4 -O5	109.5(14)
C12 -C11 -N3	117.8(19)	O7 -Cl4 -O5	112.4(13)
C13 -C12 -C11	122.4(22)	O8 -Cl4 -O5	110.0(13)
C14 -C13 -C12	120.4(23)	O7 -Cl4 -O6	108.2(14)
C15 -C14 -C13	117.9(22)	O8 -Cl4 -O6	109.1(14)
C14 -C15 -N3	122.3(20)	O8 -Cl4 -O7	107.6(14)
C25 -N4 -C21	118.7(17)	H1 -C1 -N1	119.1
C22 -C21 -N4	118.8(20)	H1 -C1 -C2	119.0
C23 -C22 -C21	122.8(22)	H2 -C2 -C1	120.5
C24 -C23 -C22	118.9(23)	H2 -C2 -C3	120.4
C25 -C24 -C23	117.3(22)	H3 -C3 -C2	119.9
C24 -C25 -N4	123.3(19)	H3 -C3 -C4	119.6
C26 -C25 -N4	115.1(17)	H4 -C4 -C3	119.8
C26 -C25 -C24	121.5(19)	H4 -C4 -C5	119.5
C30 -N5 -C26	123.9(16)	H7 -C7 -C6	121.7
N5 -C26 -C25	111.3(17)	H7 -C7 -C8	121.5
C27 -C26 -C25	127.8(18)	H8 -C8 -C7	118.8
C27 -C26 -N5	120.9(18)	H8 -C8 -C9	118.6
C28 -C27 -C26	116.3(20)	H9 -C9 -C8	120.6
C29 -C28 -C27	123.2(22)	H9 -C9 -C10	120.7
C30 -C29 -C28	116.2(20)	H12 -C12 -C11	118.7
C29 -C30 -N5	119.4(17)	H12 -C12 -C13	118.9
C31 -C30 -N5	115.3(16)	H13 -C13 -C12	119.5
C31 -C30 -C29	125.3(17)	H13 -C13 -C14	120.1
C35 -N6 -C31	120.3(17)	H14 -C14 -C13	120.8
N6 -C31 -C30	114.1(16)	H14 -C14 -C15	121.3
C32 -C31 -C30	126.8(18)	H15 -C15 -N3	119.0
C32 -C31 -N6	119.0(18)	H15 -C15 -C14	118.7
C33 -C32 -C31	122.6(21)	H21 -C21 -N4	120.7
C34 -C33 -C32	116.7(22)	H21 -C21 -C22	120.4
C35 -C34 -C33	118.1(21)	H22 -C22 -C21	118.6
C34 -C35 -N6	123.0(19)	H22 -C22 -C23	118.6

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Table S-IV. (Cont.)

	Angle(°)
H23 -C23 -C22	120.5
H23 -C23 -C24	120.6
H24 -C24 -C23	121.3
H24 -C24 -C25	121.5
H27 -C27 -C26	121.7
H27 -C27 -C28	122.1
H28 -C28 -C27	118.2
H28 -C28 -C29	118.6
H29 -C29 -C28	121.9
H29 -C29 -C30	121.9
H32 -C32 -C31	118.8
H32 -C32 -C33	118.6
H33 -C33 -C32	121.7
H33 -C33 -C34	121.6
H34 -C34 -C33	121.1
H34 -C34 -C35	120.8
H35 -C35 -N6	118.4
H35 -C35 -C34	118.5