a result of steric hindrance, the bond angles at the metal sites in each chelate ring of 78·8 (1) (Zn) and 80·4 (1)° (Ni) represent significant departures from the idealized angles. The Zn—O bond distances are uniformly longer than the corresponding Ni—O lengths. The pyrimidine ring is planar and the geometry of the ligand in each compound is consistent with that found in other derivatives containing the orotate(2–) ion (Sabat, Zglinska & Jeżowska-Trzebiatowska, 1980; Mutikainen & Lumme, 1980; Takusagawa & Shimada, 1973; Solbakk, 1971). The dihedral angles between the pyrimidine ring and chelate ring planes are 4·3 and 4·8° in the Zn and Ni compounds, respectively.

For each compound the crystal structure is dominated by an extensive array of hydrogen bonds involving all hydrogen atoms bound to non-carbon atoms except for H2(O9*w*) from the lone lattice water molecule, O(9*w*). Included in this scheme in each is the rather short intramolecular hydrogen bond, O(5*w*)···O(2) of 2·662 (Zn) and 2·659 Å (Ni).

The familiar base stacking patterns found in most pyrimidine structures is also retained in these metal complexes (Bugg, Thomas, Sundaralingham & Rao, 1971). The uracil moieties are stacked parallel with the N(3) atom of one base positioned approximately over the center of an adjacent ring, which is related to the first by an inversion center. Interplanar spacing between these stacked bases is 3·20 Å.

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Complexes of 2,2′-Bipyridine (bpy) and 1,10-Phenanthroline (phen) with Platinum(II). Structures of $[Pt^{II}(bpy)_{1.3}(phen)_{0.7}](NO_3)_2.0{\cdot}3H_2O$ and $[Pt^{II}(bpy)_2](NO_3)_2.H_2O$

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Abstract. (1) $[Pt(C_{10}H_8N_2)_{1.3}(C_{12}H_8N_2)_{0.7}]$-$(NO_3)_2.0{\cdot}3H_2O$, $M_r = 653{\cdot}7$, monoclinic, $C2/c$, $a = 19{\cdot}522$ (4), $b = 15{\cdot}511$ (3), $c = 7{\cdot}078$ (3) Å, $\beta = 101{\cdot}56$ (3)°, $Z = 4$, $V = 2100$ (1) Å^3, $D_m = 2{\cdot}09$, $D_x = 2{\cdot}067$ (1) Mg m^{-3}, $F(000) = 1261{\cdot}6$, Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å), $\mu = 6{\cdot}80$ (3) mm^{-1}, room temperature. $R = 0{\cdot}038$ for 1161 reflexions [$I > 3\sigma(I)$] and 161 variables. (2) Bis(2,2′-bipyridine)platinum(II) dinitrate monohydrate, $[Pt(C_{10}H_8N_2)_2](NO_3)_2.H_2O$, $M_r = 649{\cdot}5$, monoclinic, $C2/c$, $a = 19{\cdot}297$ (5), $b = 15{\cdot}502$ (4), $c = 7{\cdot}093$ (2) Å, $\beta = 101{\cdot}70$ (1)°, $Z = 4$, $V = 2078$ (1) Å^3, $D_x = 2{\cdot}076$ (1) Mg m^{-3}, $F(000) = 1256$, Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å), $\mu = 6{\cdot}88$ (3) mm^{-1}, room temperature. $R = 0{\cdot}045$ for 3653 reflexions [$I > 3\sigma(I)$] and 168 variables. Mean Pt—N distances are 2·013 (6) Å for (1) and 2·026 (3) Å for (2). In both cases the overcrowding of the ligands is relieved by a tetrahedral distortion of PtN_4 [the angle between the planes through PtN_2 is 23·0 (4)° for (1) and 24·0 (3)° for (2)] and by distortion of the ligands [the angle between the best planes through the ligands is 31·8° for (1) and 34·5° for (2)]. The water molecules are in the plane of the bipyridine groups and close to the acid hydrogens, C(3)—O is 3·226 (8) Å for (2).

Introduction. The photochemical properties of transition metal–polypyridine complexes has led to their possible use in the conversion and storage of solar energy. Postulated mechanisms for their reaction with OH^- have been the subject of much, often acrimonious,

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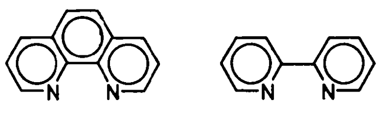
discussion (Gillard, 1975; Serpone, Ponterini, Jamieson, Bolletta & Maestri, 1983; Gillard, 1983; Constable, 1983; Nord, 1985.) The dimensions of 2,2′-bipyridine (bpy), 1,10-phenanthroline (phen) and related ligands are such that a planar arrangement of two of these about a metal atom is only possible if M—N is more than 2·8 Å (Rund, 1968). For complexes with M—N *ca* 2 Å the strain induced by the close approach of hydrogen atoms of opposing ligands may be reduced by a tetrahedral deformation at the metal resulting in the ligands being twisted relative to each other. If the planar MN_4 configuration is retained the ligands can be bowed away from each other or tilted out of the MN_4 plane.



phen bpy

Unlike the $Pt(bpy)_2^{2+}$ complex the mixed-ligand compound does not give good crystals. The only good crystal was unfortunately lost during data collection; the results based on the partial data set are described here although the crystal is probably not typical of the bulk sample. The structures presented here together with that of $[Pt^{II}(phen)_2]^{2+}$ are the first examples of the structure determinations of a complete series $[M(bpy)_2]^{2+}$, $[M(bpy)(phen)]^{2+}$ and $[M(phen)_2]^{2+}$ in which all members have the twist configuration.

Experimental. (2,2′-Bipyridine)(1,10-phenanthroline)-platinum(II) dinitrate, $[Pt(bpy)(phen)](NO_3)_2$, was prepared by boiling a mixture of 300 mg of bipyridine (Fluka, puriss.), 350 mg of $[Pt(phen)Cl_2]$ (Morgan & Burstall, 1934) and 25 ml of water for approximately two hours. The excess of $[Pt(phen)Cl_2]$ was then removed by filtration and the solution was extracted twice with 50 ml of chloroform. The crude product was precipitated by addition of an equal volume of saturated KNO_3 in water and cooling with ice and was collected on a Gooch crucible and washed with 2 ml of ice-cooled water.

The crystals used for the structure determination were grown from an aqueous solution by slow evaporation. Both the crystals obtained by this procedure and a sample purified by dissolving the crude product and isolating the nitrate by adding KNO_3 to the solution gave identical UV spectra.

These UV spectra show essentially a combination of the same type of bands as the spectra of $[Pt(phen)_2]^{2+}$ and $[Pt(bpy)_2]^{2+}$, the most noticeable feature being the splitting of the low-energy band of bpy and the high-energy shift of the CT transitions relative to the $[Pt(phen)_2]^{2+}$ spectrum. The wavelengths of the absorption maxima in nm and the extinction coefficients (given in parentheses) are: 279 (24 000); 309 (17 600); 321·5 (17 900); 347 (5700); 368 (4000). The UV data (Wernberg, 1986, and references therein) for the $[Pt(bpy)_2](ClO_4)_2$ (in $1{\cdot}23 \times 10^{-5}$ mol dm^{-3} aqueous solution) are 321·7 (26 500) and for $[Pt(phen)_2](NO_3)_2$ (in the concentration range $2{\cdot}80 \times 10^{-5}$ to $1{\cdot}31 \times 10^{-4}$ mol dm^{-3}): 276 (29 000); 357 (3400); 373 (6500).

$[Pt(bpy)_{1.3}(phen)_{0.7}](NO_3)_2.0{\cdot}3H_2O$ crystallizes as pale yellow prisms. The dimensions of the crystal mounted on an Enraf–Nonius CAD-4F were $0{\cdot}16 \times 0{\cdot}07 \times 0{\cdot}07$ mm. D_m by flotation in a mixture of CCl_4 and $CHBr_3$. Graphite-monochromatized Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å), lattice parameters from setting angles for 15 reflexions with $3{\cdot}37 < \theta < 12{\cdot}28°$. 1682 unique reflexions ($-25 \le h \le 27$, $0 \le k \le 20$, $0 \le l \le 9$) with $2{\cdot}0 < \theta < 30°$, 1161 with $I < 3\sigma(I)$. Mixed θ–2θ scan technique, scan width $(1{\cdot}40 + 0{\cdot}35\tan\theta)°$. Standard reflexions $00\bar{4}$, $\bar{4}\bar{2}\bar{2}$ and $\bar{0}82$ for orientation control every 100 reflexions, $00\bar{4}$ for intensity check every 10 800 s of exposure time, overall decay in intensity 5%, correction for decay applied. Data were corrected for absorption; transmission factors ranged from 0·55 to 0·66.

The structure was solved by Patterson and Fourier methods. The absence of data with h and k both even when l is odd, h and k both odd when l is even leads to false mirror planes at $y = \pm 0{\cdot}25$. However, the two overlapping solutions could be distinguished. A difference map showed a peak at $x = 0$, $y = 0{\cdot}75$, $z = 0{\cdot}25$ corresponding to the position of the water molecule later found in the bis(bipyridine) complex. The peak was, however, too low for an O atom and also too close to the phenanthroline. The structure was refined assuming disorder in which $[Pt(bpy)(phen)]^{2+}$ is partially replaced by $[Pt(bpy)_2]^{2+}.H_2O$ and showed the crystal studied to have the composition $[Pt(bpy)_{1.30(2)}(phen)_{0.70(2)}](NO_3)_2.0{\cdot}30(2)H_2O$. Hydrogen atoms were included at calculated positions (C—H = 0·95 Å) except for those of the water molecule. During refinement it was necessary to keep some of the parameters for atoms O(1) and H_2O, which are close to the false mirror plane, at fixed values. The weighting scheme used was $w = 1/\sigma^2(F)$ where $\sigma(F) = [\sigma_{c.s.}(F^2) + 1{\cdot}03F^2]^{1/2} - |F|$ where $\sigma_{c.s.}(F^2)$ is the standard deviation of F^2 from counting statistics. Least-squares refinement on F gave $R = 0{\cdot}038$, $wR = 0{\cdot}044$, $S = 1{\cdot}222$ for 161 variables, $(\Delta/\sigma)_{max} = 0{\cdot}389$, $\Delta\rho$ −0·54 (6) to 0·46 (6) e Å^{-3}. Fractional coordinates are listed in Table 1.*

* Lists of observed and calculated structure factors, anisotropic thermal parameters, coordinates for hydrogen atoms, and detailed descriptions of the size and shape of the crystals have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43208 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates* ($\times 10^5$ *for* Pt, $\times 10^4$ *for* C, N *and* O), *and* U_{eq} *in* Å^2 ($\times 10^4$ *for* Pt, $\times 10^3$ *for* C, N *and* O)

The atoms are numbered such that *e.g.* C(14) is atom 4 of ring 1.

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Complex (1)				
Pt	0	30643 (3)	25000	374 (3)
N(11)	672 (4)	4063 (6)	3186 (11)	34 (4)
C(12)	367 (4)	4883 (7)	2902 (13)	36 (5)
C(13)	723 (5)	5627 (6)	3369 (13)	38 (5)
C(14)	1445 (5)	5572 (7)	4275 (15)	47 (5)
C(15)	1733 (5)	4770 (8)	4647 (15)	50 (6)
C(16)	1348 (5)	4024 (7)	4113 (14)	47 (5)
C(17)*	354 (9)	6396 (9)	2850 (26)	55 (10)
N(21)	649 (4)	2067 (5)	2447 (11)	41 (4)
C(22)	371 (6)	1281 (7)	2421 (17)	46 (6)
C(23)	725 (7)	548 (8)	2194 (20)	60 (7)
C(24)	1420 (7)	613 (7)	1920 (18)	62 (7)
C(25)	1708 (7)	1394 (8)	1898 (19)	61 (8)
C(26)	1317 (6)	2121 (7)	2139 (16)	53 (6)
N	−1792 (7)	8148 (8)	2734 (17)	73 (7)
O(1)	−1760 (8)	7400	2551 (23)	167 (13)
O(2)	−1198 (8)	8496 (10)	3118 (26)	141 (13)
O(3)	−2284 (5)	8635 (6)	2508 (17)	87 (7)
H_2O*	0	7500	2500	62 (18)
Complex (2)				
Pt	0	31414 (1)	25000	313 (1)
N(11)	675 (2)	4142 (2)	3244 (6)	32 (2)
C(12)	382 (2)	4950 (3)	2959 (7)	30 (2)
C(13)	766 (3)	5691 (3)	3477 (8)	37 (2)
C(14)	1471 (3)	5612 (4)	4399 (8)	40 (2)
C(15)	1759 (3)	4806 (4)	4817 (8)	42 (3)
C(16)	1343 (3)	4077 (3)	4229 (8)	40 (3)
N(21)	674 (2)	2139 (3)	2478 (7)	35 (2)
C(22)	370 (3)	1344 (3)	2393 (9)	38 (2)
C(23)	737 (3)	613 (3)	2044 (10)	48 (3)
C(24)	1428 (3)	693 (4)	1816 (11)	54 (3)
C(25)	1724 (3)	1490 (4)	1857 (11)	50 (3)
C(26)	1341 (3)	2197 (4)	2182 (10)	44 (3)
N	−1696 (3)	8234 (3)	2809 (9)	49 (3)
O(1)	−1687 (3)	7440 (3)	2633 (10)	82 (4)
O(2)	−1128 (3)	8628 (3)	3144 (10)	73 (3)
O(3)	−2253 (3)	8636 (4)	2643 (10)	79 (4)
H_2O	0	7533 (5)	2500	91 (6)

* Occupation factor 0·70 (2) for C(17), 0·30 (2) for H_2O.

$[Pt(bpy)_2](NO_3)_2.H_2O$ (2) crystallizes as pale yellow prisms terminated by {001} and bounded by {110}, {100} and in some cases {010}. A crystal of dimensions 0·27 × 0·25 × 0·30 mm was mounted on a Picker FACS-1 diffractometer. Cell dimensions were determined from the setting angles of 28 reflexions with $11{\cdot}2 < \theta < 18{\cdot}3°$. Intensities were measured out to $2\theta_{max} = 70°$ using an ω–2θ scan and Nb-filtered Mo $K\alpha$ radiation, scan width $(2{\cdot}0 + 0{\cdot}692\tan\theta)°$, step length 0·04°, 1 second per step. Reflexions with $-31 \le h \le 30$, $0 \le k \le 25$, $0 \le l \le 11$ were measured giving 4583 independent reflexions of which 3653 had $I > 3\sigma(I)$. Reflexions $19\bar{1}$ and 621 were monitored every 60 reflexions, overall decay in intensity of 3%. Reflexions were integrated using Nelmes' (1975) method. Data were corrected for absorption, transmission factors ranged from 0·19 to 0·32. The structure was solved by Patterson and Fourier methods; the hydrogen atoms were located on a difference synthesis, coordinates of the water hydrogen atoms were refined but the other hydrogens were kept fixed at positions calculated assuming C—H = 0·95 Å. All non-hydrogen atoms were refined anisotropically. An isotropic extinction factor was refined giving $g = 1{\cdot}0\ (1) \times 10^{-4}$ which corresponds to a minimum value of I/I_{corr} of 0·90. The weighting scheme was as for (1). Final $R(F) = 0{\cdot}045$, $wR = 0{\cdot}054$, $S = 1{\cdot}583$, $(\Delta/\sigma)_{max} = 0{\cdot}10$, $\Delta\rho = -2{\cdot}5\ (1)$ to $2{\cdot}4\ (1)$ e Å^{-3} close to Pt, the next highest peak is 0·69 e Å^{-3}. Fractional coordinates are listed in Table 1.

Computations were carried out on a VAX 11/780 with the following programs: *DATAP* and *DSORTH* (State University of New York, Buffalo) – data processing; modified *ORFLS* (Busing, Martin & Levy, 1962) – least-squares refinement; *ORTEP* (Johnson, 1965) – drawings. Scattering curves: *International Tables for X-ray Crystallography* (1974) for Pt; Cromer & Mann (1968) for O, N and C; Stewart, Davidson & Simpson (1965) for H; anomalous-dispersion corrections for Pt from Cromer & Liberman (1970).

Discussion. The two crystal structures, Fig. 1, are almost identical, the water molecule in (2) replacing the vinylene bridge of the phenanthroline in (1). (1) is actually a mixed crystal containing 30 (2)% of $[Pt(bpy)_2](NO_3)_2.H_2O$. In both compounds the complex cations are on twofold axes, the ligands being twisted so that there is a tetrahedral distortion from planarity. Distances and angles are given in Table 2. The mean Pt—N distances are 2·013 (6) for (1) and 2·026 (3) Å for (2); *cf.* 2·033 (6) Å in $[Pt(phen)_2]Cl_2.3H_2O$. The

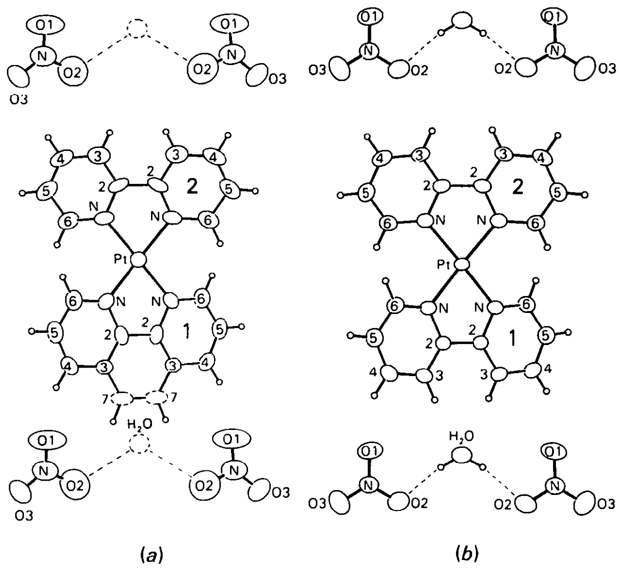


Fig. 1. Perspective drawings of (*a*) $[Pt^{II}(bpy)_{1.3}(phen)_{0.7}]$-$(NO_3)_2.0{\cdot}3H_2O$ and (*b*) $[Pt^{II}(bpy)_2](NO_3)_2.H_2O$. The disordered carbon atoms and water molecule of (*a*) are drawn with broken lines.

Table 2. *Bond distances* (Å) *and angles* (°)

	$[Pt(bpy)(phen)]^{2+}$ Ring 1	Ring 2	$[Pt(bpy)_2]^{2+}$ Ring 1	Ring 2
Pt—N	2·025 (10)	2·005 (8)	2·025 (4)	2·028 (5)
N—C(2)	1·401 (13)	1·333 (12)	1·373 (6)	1·361 (7)
C(2)—C(2′)	1·431 (17)	1·475 (22)	1·486 (9)	1·465 (11)
C(2)—C(3)	1·355 (13)	1·358 (16)	1·375 (6)	1·386 (7)
C(3)—C(4)	1·428 (13)	1·412 (18)	1·390 (7)	1·381 (9)
C(4)—C(5)	1·370 (15)	1·337 (17)	1·376 (8)	1·358 (9)
C(5)—C(6)	1·391 (15)	1·391 (14)	1·400 (8)	1·369 (9)
C(6)—N	1·353 (12)	1·367 (13)	1·339 (6)	1·348 (7)
C(3)—C(7)	1·404 (17)			
C(7)—C(7′)	1·371 (36)			
N—O(1)	1·170 (12)		N—O(1)	1·238 (6)
N—O(2)	1·257 (17)		N—O(2)	1·236 (7)
N—O(3)	1·208 (14)		N—O(3)	1·228 (7)
	Ring 1	Ring 2	Ring 1	Ring 2
Pt—N—C(2)	115·1 (6)	116·6 (7)	115·9 (3)	115·0 (3)
Pt—N—C(6)	127·1 (7)	125·6 (7)	125·4 (3)	125·7 (4)
N—C(2)—C(3)	123·8 (8)	123·5 (11)	122·6 (4)	121·2 (5)
N—C(2)—C(2′)	114·8 (5)	113·7 (6)	114·0 (2)	114·6 (3)
C(3)—C(2)—C(2′)	121·4 (6)	122·7 (7)	123·3 (3)	124·2 (3)
C(2)—C(3)—C(4)	118·1 (9)	118·8 (11)	118·3 (5)	119·2 (5)
C(3)—C(4)—C(5)	118·1 (9)	118·9 (10)	119·7 (5)	119·4 (5)
C(4)—C(5)—C(6)	121·7 (9)	119·4 (12)	119·1 (5)	119·5 (6)
C(5)—C(6)—N	121·1 (10)	122·3 (11)	121·9 (5)	122·6 (6)
C(6)—N—C(2)	117·1 (9)	116·9 (8)	118·0 (4)	118·0 (5)
C(2)—C(3)—C(7)	116·6 (10)			
C(4)—C(3)—C(7)	125·2 (10)			
C(3)—C(7)—C(7′)	121·5 (8)			
O(1)—N—O(2)	112·5 (1·5)		O(1)—N—O(2)	118·7 (6)
O(1)—N—O(3)	131·6 (1·6)		O(1)—N—O(3)	121·8 (6)
O(2)—N—O(3)	115·7 (1·3)		O(2)—N—O(3)	119·5 (6)

	N(1)—Pt—N(1′)	N(2)—Pt—N(2′)	N(1)—Pt—N(2)	N(1)—Pt—N(2′)
$[Pt(bpy)(phen)]^{2+}$	80·2 (4)	79·0 (5)	102·3 (3)	165·3 (3)
$[Pt(bpy)_2]^{2+}$	80·1 (2)	80·0 (2)	102·0 (2)	164·6 (2)

Symmetry code: (′) $-x, y, \frac{1}{2}-z$; N(1) is the N of ring 1 *etc.*

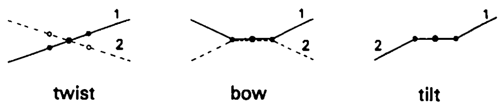
complexes are not, as might have been expected, isomorphous with the corresponding Pd and the Ag bis(bipyridine) monohydrates.

The water molecules are in the plane of the bipyridine groups and close to the hydrogen atoms on C(3) and C(3′); C(3)—O is 3·226 (8) Å for (2). Constable & Seddon (1982) have shown that it is just these hydrogens which are the most acidic. $[Ir(bpy)_3]^{2+}$ forms a monohydrate which has a similarly placed water molecule (Wickramasinghe, Bird & Serpone, 1981). The authors suggested the cyclometallation of one bipyridine group and the formation of an N—H···O hydrogen bond. This was confirmed by further studies on both the acid (Hazell & Hazell, 1984) and base (Nord, Hazell, Hazell & Farver, 1983) forms of the iridium complex. However, in the platinum complexes there is no evidence for Pt—C bonding, the Pt—N bonds have the expected lengths and the thermal parameters for the atoms assumed to be N and C show no abnormalities. Thus the close positioning of a water molecule in the plane of, and close to, the atoms which are nominally C(3) and C(3′) is not in itself sufficient evidence for cyclometallation.

The nitrate ions are hydrogen-bonded to the water molecule. $O(2)—H_2O = 2{\cdot}868$ (8) Å in (2), and $N—O(2)—H_2O$ [110·5 (4)°] and $O(2)—H_2O—O(2)$ [107·5 (3)°] are close to tetrahedral. In $[Pt(bpy)(phen)]^{2+}$, there would be no hydrogen-bonding and the nitrate ions could vibrate more freely. In (1), which has an average of 0·30 water molecules per cation, the nitrate oxygens have larger temperature parameters than those in (2). The hydrogen bonding could be responsible for (2) crystallizing so much more readily than (1) and it may be that the inclusion of $[Pt(bpy)_2](NO_3)_2.H_2O$ in the only good crystal of (1) is the reason for the difference in crystal quality.

For the tetrahedrally distorted complexes $[M(bpy)_x(phen)_{2-x}]^{2+}$, M = Pt, Pd, both the distortion at the metal and the torsion angle between the ligands are greatest for the bis(bipyridine) complexes. The values for the mixed-ligand complex are intermediate between those for the bis(bipyridine) and for the bis(phenanthroline) complexes. When 2,2′-bipyridine is in the *cis* conformation the hydrogen atoms on C(3) and C(3′) are too close. The strain is reduced by the pyridines being twisted about C(2)—C(2′) and by an in-plane bending which pushes the hydrogens on C(5) towards the opposite ligand so that the overcrowding and hence the distortion is slightly larger for the

Table 3. *Configurations of trans-dipyridine complexes, and their M*—N *distances*



	Twist	Bow	Tilt	Planar	M—N(Å)
$[Pt(bpy)_{1.3}(phen)_{0.7}](NO_3)_2.0{\cdot}3H_2O$	*a*				2·013 (6)
$[Pt(bpy)_2](NO_3)_2.H_2O$	*a*				2·026 (3)
$[Pt(phen)_2]Cl_2.3H_2O$	*b*				2·033 (6)
$[Pt(bpy)_2]TCNQ_2$		*c*			2·02 (1)
$[Pt(bpy)_2]TCNQ_3$		*d*			2·02 (2)
$[Pt(phpy)_2]$		*e*			2·127 (4)*
$[Pd(bpy)_2](NO_3)_2.H_2O$	*f,g*				2·034 (4)
$[Pd(phen)_2](ClO_4)_2$	*h*				2·051 (3)
$[Ru(bpy)_2(OH_2)(OH)](ClO_4)_2$	*i*				2·095 (2)
$[Ru(bpy)_2(Pph_3)_2](PF_6)_2$		*j*			2·080 (6)
$[Ru(Me_2bpy)_2(py)_2](PF_6)_2$		*j*			2·095 (1)
$[Ru(phen)_2(py)_2](PF_6)_2$			*k*		2·098 (4)
$[Cu(bpy)_2](ClO_4)_2$	*l*				1·99 (1)
$[Cu(bpy)_2]S_3O_6$	*m*				1·983
$[Ag(bpy)_2](NO_3)_2.H_2O$	*n*				2·160 (5)
$[Hg(phen)_2](NO_3)_2$	*o*				2·339 (5)
$[Sr(phen)_2(OH)_4](ClO_4)_2.2phen$				*p*	2·793 (7)
$[Ba(phen)_2(OH)_4](ClO_4)_2.2phen$				*p*	2·956 (7)

References: (*a*) this work; (*b*) Hazell & Mukhopadhyay (1980); (*c*) Dong, Endres, Keller, Moroni & Nöthe (1977), TCNQ = tetracyanoquinodimethane; (*d*) Endres, Keller, Moroni, Nöthe & Dong (1978); (*e*) Chassot, Müller & von Zelewsky (1984), phpy = 2-phenylpyridine; (*f*) Chieh (1972); (*g*) Hinamoto, Ooi & Kuraya (1972); (*h*) Rund & Hazell (1980); (*i*) Durham, Wilson, Hodgson & Meyer (1980); (*j*) Cordes, Durham, Swepston, Pennington, Condren, Jensen & Walsh (1982), Pph_3 = triphenylphosphine, Me_2bpy = 4,4′-dimethyl- 2,2′-bipyridine; (*k*) Bonneson, Walsh, Pennington, Cordes & Durham (1983); (*l*) Nakai (1971); (*m*) Ferrari, Fava & Pelizzi (1977); (*n*) Atwood, Simms & Satko (1973); (*o*) Grdenić, Kamenar & Hergold-Brundić (1978); (*p*) Smith, O'Reilly, Kennard & White (1977).

* Pt—C = 1·988 (3) Å.

bipyridine than for the phenanthroline complexes. The in-plane bending can be seen from the discrepancy between C(3)—C(2)—C(2′) and N—C(2)—C(2′) of 8–10°. The twisting of the ligands is in keeping with mechanisms for hydrolysis in which the ligands are twisted even more and the nucleophile attached to the central metal atom (Nord, 1975); *cf.* $[Pt(phen)_2CN^-]$ (Wernberg & Hazell, 1980) where the angle between the ligands is 76° and CN^- is bonded to Pt. Table 3 summarizes the geometries so far found for complexes with *trans* polypyridyl ligands. Although the tetrahedral, or twist, deformation is the commonest there are a surprising number with bow or tilt deformations in which the planar configuration at the metal atom is retained. So far no phenanthroline complexes have been reported with the bow deformation.

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The Structure of Bis(2,4,6-trimethoxyphenyl)mercury*

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Abstract. $[Hg(C_9H_{11}O_3)_2]$, $M_r = 534.96$, monoclinic, $P2_1/c$, $a = 14.624\ (4)$, $b = 17.731\ (5)$, $c = 7.221\ (3)$ Å, $\beta = 93.98\ (3)°$, $V = 1868\ (1)$ Å^3, $Z = 4$, $D_m = 1.93\ (2)$, $D_x = 1.90$ g cm^{-3}, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 82.4$ cm^{-1}, $F(000) = 1032$, $T = 293$ K. Final $R = 0.045$ for 2292 observed reflections. Molecules of the title compound have near linear stereochemistry at Hg, C—Hg—C 176.7 (4)°, both Hg—C bonds 2.07 (1) Å, with an angle of 63.5 (4)° between the aromatic rings.

* Organomercury Compounds. XXIX.

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