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Table 1. Crystal and Intensity Collection Data for $Pt(bpy)Cl_2$ at 298 K

Formula: $C_{10}Cl_2N_2H_8Pt$	Formula weight: 422.17
Crystal color: Red	Habit: Diamond-shaped needle
Crystal Size: 0.10 x 0.11 x 0.23 mm	$\rho_{calc} = 2.57$ g cm^{-3}
Crystal System: Orthorhombic	Space group: *Cmcm* (no. 63)
$a = 17.669(5)$ Å	
$b = 9.081(2)$ Å	
$c = 6.804(2)$ Å	
V = 1091.7(5) Å^3	$Z = 4$
Lattice parameters: 29 reflections	$9.5° \leq \theta \leq 10.5°$
$\mu = 134.5$ cm^{-1}	Transmission coeff. $= 0.70 - 1.27$
Variable-temperature $P\bar{1}$ diffractometer	$\theta - 2\theta$ scan
MoKα, $\lambda = 0.7107$Å	Graphite monochromator
2θ range: 2°–60°	$-24 \leq h \leq 21, -12 \leq k \leq 12, -9 \leq l \leq 9$
T = 294K	
Number of reflections measured: 6993	Number of independent reflections: 880
Number with $F_o^2 > 0$: 868	Number with $F_o^2 > 3\sigma(F_o^2)$: 804
Standard reflections: 3 every 97 data	Variation: within counting statistics
GOF_{merge}: 1.06 for 877 multiples	R_{merge}: 0.018 for 97 duplicates
Number used in refinement: 880	Criterion: All reflections used

Final R: 0.029 for 804 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final R: 0.033 for 868 reflections with $F_o^2 > 0$

Final weighted R: 0.067

Final GOF: 1.74 for 48 parameters and 880 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: < 0.01

$\Delta\rho_{max}$: 1.2 eÅ^{-3}, $\Delta\rho_{min}$: -1.7 eÅ^{-3} in final difference map

Secondary extinction parameter: 1.09(4) x 10^{-6}

Table 2. Final Heavy Atom Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 294 K

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
Pt	0	−313(.5)	2500	261(1)
Cl	914(1)	−2119(3)	2500	452(5)
N	732(3)	1380(7)	2500	293(14)
C(1)	1494(5)	1258(10)	2500	455(22)
C(2)	1944(5)	2503(14)	2500	623(29)
C(3)	1625(6)	3863(13)	2500	646(30)
C(4)	850(6)	3974(10)	2500	527(27)
C(5)	408(4)	2729(9)	2500	343(18)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table 3. Assigned Hydrogen Atom Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 294 K

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

Atom	x	y	z	B
H(1)	1721	310	2500	4.1
H(2)	2480	2406	2500	5.7
H(3)	1932	4722	2500	5.9
H(4)	617	4917	2500	4.8

Table 4. Heavy Atom Anisotropic Displacement Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 294 K

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	295(2)	184(2)	303(2)	0	0	0
Cl	529(12)	302(11)	524(14)	158(9)	0	0
N	335(30)	189(30)	354(35)	−58(24)	0	0
C(1)	305(38)	381(52)	678(64)	−26(34)	0	0
C(2)	360(47)	753(84)	757(79)	−215(50)	0	0
C(3)	552(58)	469(65)	918(89)	−265(50)	0	0
C(4)	586(55)	218(42)	777(75)	−115(41)	0	0
C(5)	419(42)	241(40)	369(44)	−14(31)	0	0

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

The form of the displacement factor is:

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

Table 5. Complete Distances and Angles for Platinum(Bipyridyl)-*bis*-Chloride at 294 K

		Distance(Å)
Pt	–N	2.009(6)
Pt	–Cl	2.302(2)
N	–C(1)	1.350(10)
N	–C(5)	1.352(10)
C(1)	–C(2)	1.383(14)
C(1)	–H(1)	0.950
C(2)	–C(3)	1.358(15)
C(2)	–H(2)	0.950
C(3)	–C(4)	1.374(15)
C(3)	–H(3)	0.950
C(4)	–C(5)	1.373(12)
C(4)	–H(4)	0.950
C(5)	–C(5)'	1.442(11)

			Angle(°)
N	–Pt	–Cl	95.4(2)
N	–Pt	–N'	80.2(2)
N	–Pt	–Cl'	175.5(2)
Cl	–Pt	–Cl'	89.1(1)
Pt	–N	–C(1)	125.4(5)
Pt	–N	–C(5)	114.9(5)
C(5)	–N	–C(1)	119.8(7)
C(2)	–C(1)	–N	120.5(8)
H(1)	–C(1)	–N	119.8
H(1)	–C(1)	–C(2)	119.8
C(3)	–C(2)	–C(1)	120.3(10)
H(2)	–C(2)	–C(1)	119.9
H(2)	–C(2)	–C(3)	119.9
C(4)	–C(3)	–C(2)	118.8(10)
H(3)	–C(3)	–C(2)	120.6
H(3)	–C(3)	–C(4)	120.6
C(5)	–C(4)	–C(3)	120.4(9)
H(4)	–C(4)	–C(3)	119.8
H(4)	–C(4)	–C(5)	119.8
C(4)	–C(5)	–N	120.3(8)
C(5)'	–C(5)	–N	115.1(7)
C(5)'	–C(5)	–C(4)	124.6(8)

Symmetry code: (') $-x, y, z$

Table 6. Intermolecular Distances Less Than 4.0 A for Platinum(Bipyridyl)-*bis*-Chloride at 294 K

		Distance(Å)
Pt	–Pt	3.4492(6)
Pt	–N	3.766(6)
Cl	–C(3)	3.859(11)
Cl	–C(4)	3.550(10)
Cl	–H(3)	3.387
Cl	–H(4)	2.742
Cl	–C(2)	3.800(11)
Cl	–H(2)	2.871
Cl	–H(4)	3.816
Cl	–N	3.482(6)
Cl	–C(1)	3.638(9)
Cl	–C(2)	3.875(11)
Cl	–C(3)	3.957(11)
Cl	–C(4)	3.798(10)
Cl	–C(5)	3.561(8)
C(1)	–C(3)	3.973(14)
C(1)	–H(2)	3.941
C(1)	–H(3)	3.112
C(1)	–H(1)	3.710
C(2)	–C(2)	3.928(15)
C(2)	–H(2)	3.552
C(2)	–H(1)	3.473
C(2)	–H(3)	3.212
C(3)	–H(2)	3.925
C(3)	–H(1)	3.204
C(3)	–H(2)	3.585
C(3)	–C(3)	3.980(15)
C(3)	–H(3)	3.677
C(3)	–H(4)	3.997
C(4)	–C(4)	3.879(13)
C(4)	–H(4)	3.572
H(1)	–H(2)	2.991
H(1)	–H(3)	2.439
H(1)	–H(1)	3.448
H(2)	–H(2)	3.407
H(2)	–H(3)	2.650
H(3)	–H(3)	3.439
H(4)	–H(4)	3.405

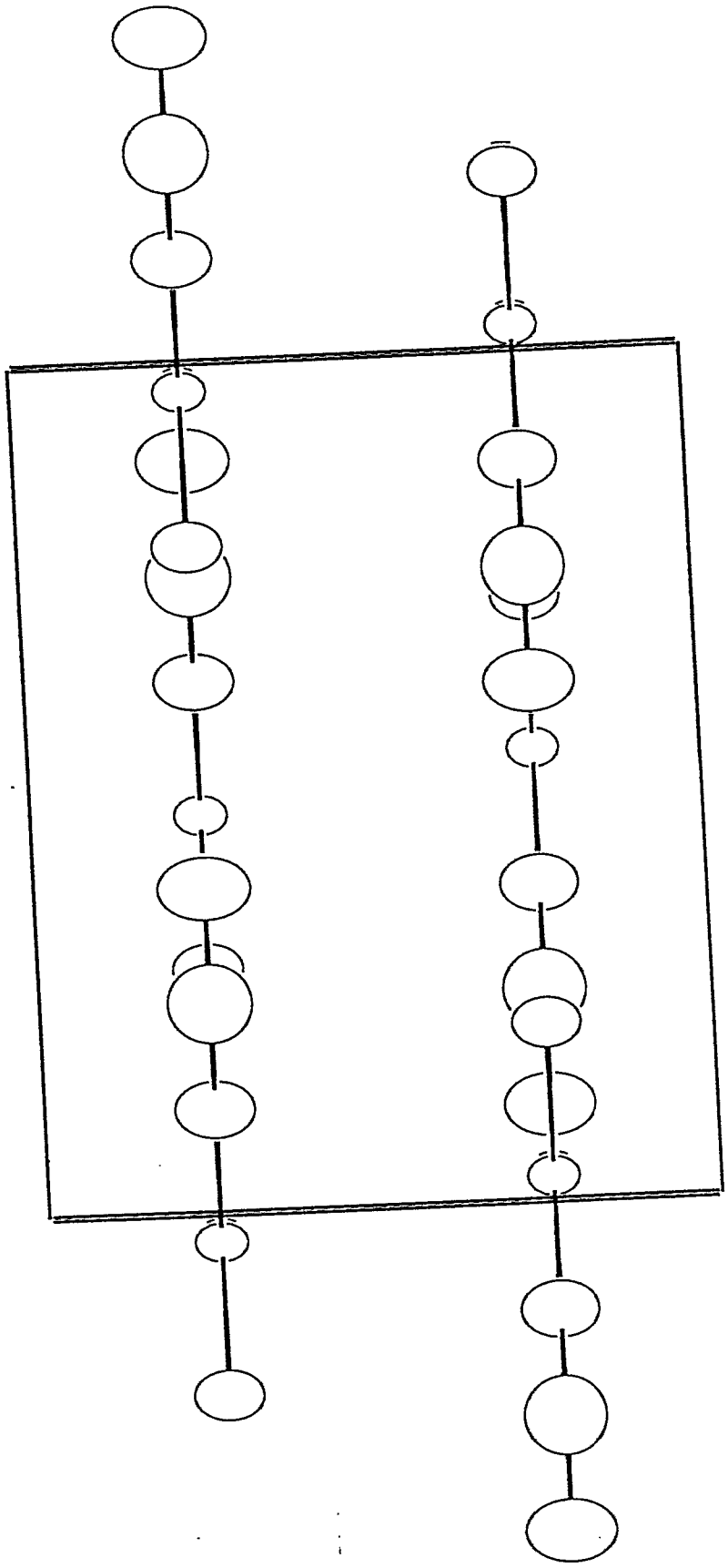

Figure 1a. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *bc* plane (projection down *a*).

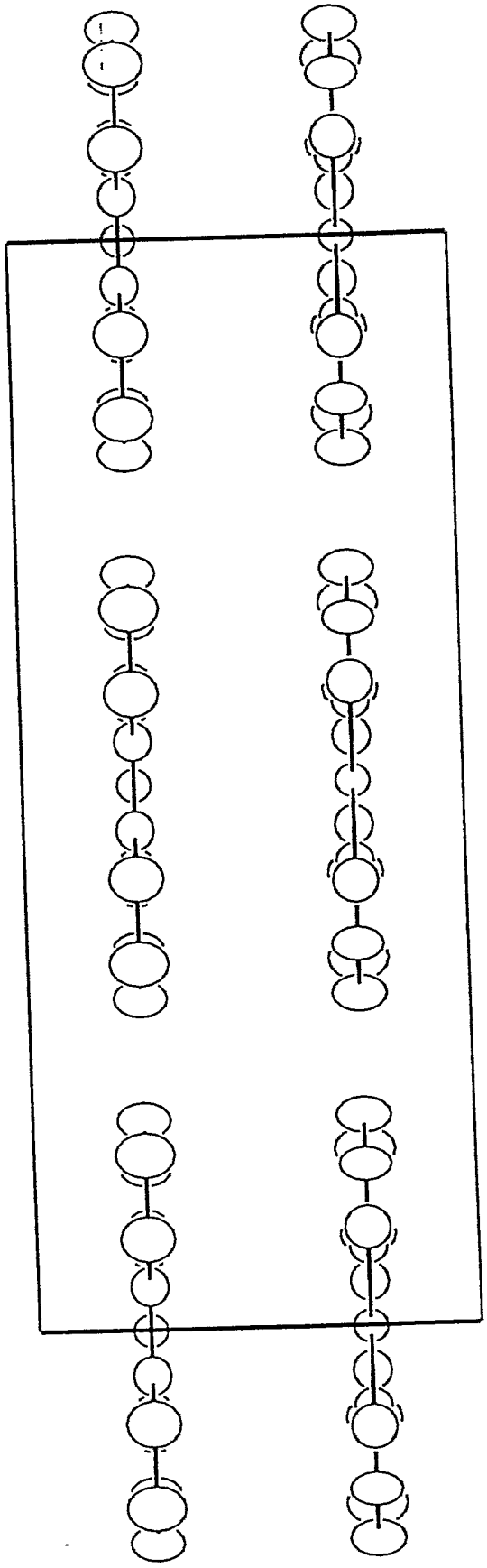

Figure 1b. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *ac* plane (projection down *b*).

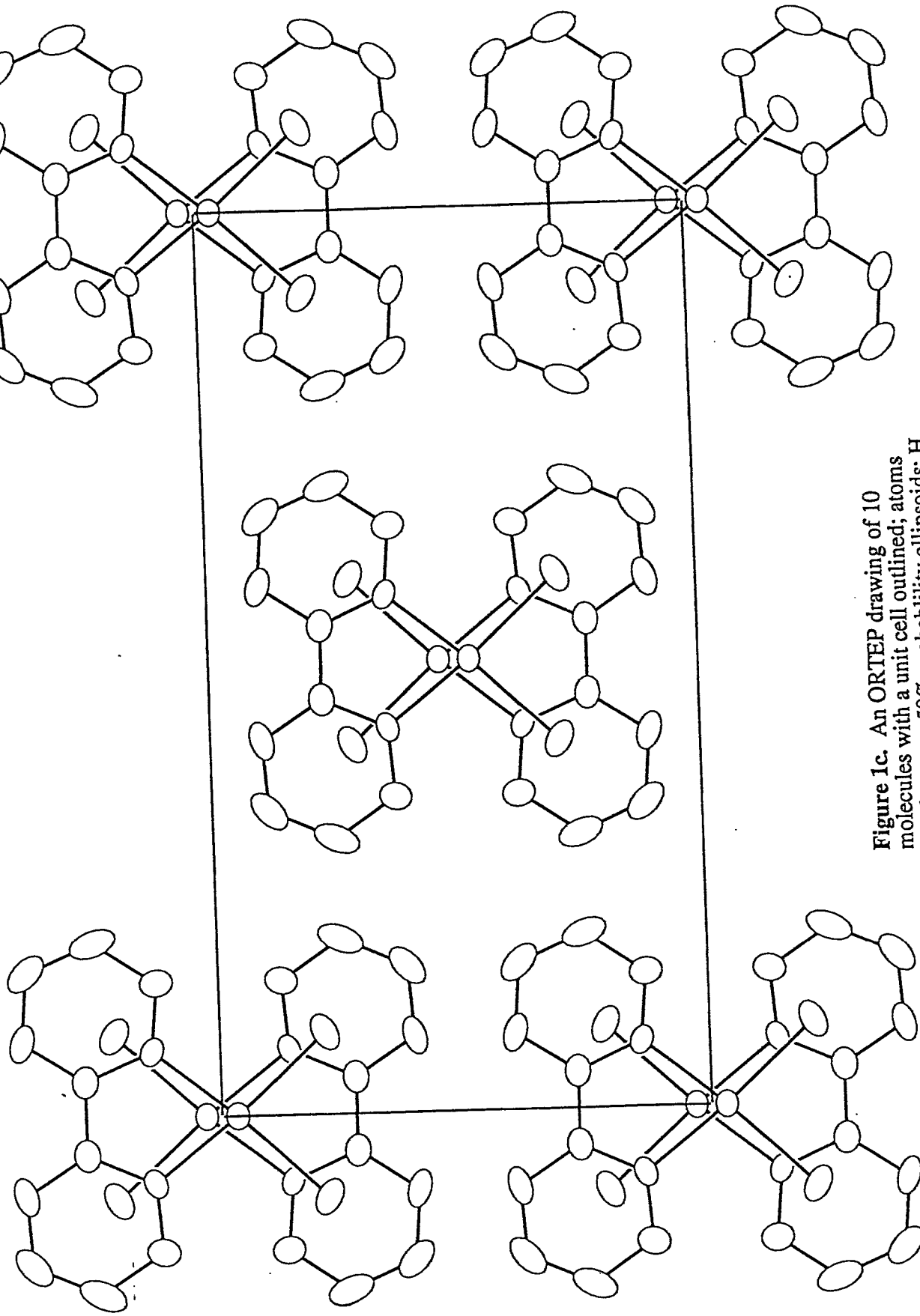

Figure 1c. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *ab* plane (projection down *c*).

Table 7. Crystal and Intensity Collection Data for $Pt(bpy)Cl_2$ at 20 K

Formula: $C_{10}Cl_2N_2H_8Pt$	Formula weight: 422.17
Crystal color: Red	Habit: Diamond-shaped needle
Crystal Size: 0.10 x 0.11 x 0.23 mm	$\rho_{calc} = 2.65$ g cm^{-3}
Crystal System: Orthorhombic	Space group: *Cmcm* (no. 63)
$a = 17.598(10)$ Å	
$b = 9.059(4)$ Å	
$c = 6.643(3)$ Å	
V = 1059.0(9) Å^3	$Z = 4$
Lattice parameters: 28 reflections	$9.5° \leq \theta \leq 10.5°$
$\mu = 138.6$ cm^{-1}	Transmission coeff. $= 0.70 - 1.27$
Variable-temperature $P\bar{1}$ diffractometer	$\theta - 2\theta$ scan
MoKα, $\lambda = 0.7107$Å	Graphite monochromator
2θ range: 2–81.0°	$-32 \leq h \leq 29, -16 \leq k \leq 16, -12 \leq l \leq 12$
T = 20 K	
Number of reflections measured: 7503	Number of independent reflections: 1844
Number with $F_o^2 > 0$: 1797	Number with $F_o^2 > 3\sigma(F_o^2)$: 1714
Standard reflections: 3 every 97 data	Variation: within counting statistics
GOF_{merge}: 1.30 for 1840 multiples	R_{merge}: 0.026 for 174 duplicates
Number used in refinement: 1844	Criterion: All reflections used

Final R: 0.032 for 1714 reflections with $F_o^2 > 3\sigma(F_o^2)$

Final R: 0.034 for 1797 reflections with $F_o^2 > 0$

Final weighted R: 0.077

Final GOF: 2.19 for 48 parameters and 1844 reflections

$(\Delta/\sigma)_{max}$ in final least squares cycle: < 0.01

$\Delta\rho_{max}$: 4.3 eÅ^{-3}, $\Delta\rho_{min}$: -4.3 eÅ^{-3} in final difference map

Secondary extinction parameter: 1.28(4) x 10^{-6}

Table 8. Final Heavy Atom Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 20 K

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
Pt	0	−314(.3)	2500	32(1)
Cl	921(1)	−2127(1)	2500	70(2)
N	739(2)	1384(4)	2500	47(7)
C(1)	1501(3)	1273(6)	2500	93(7)
C(2)	1966(3)	2503(6)	2500	91(8)
C(3)	1638(3)	3889(6)	2500	94(8)
C(4)	850(3)	4016(6)	2500	84(7)
C(5)	415(3)	2746(5)	2500	66(9)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table 9. Assigned Hydrogen Atom Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 20 K

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

Atom	x	y	z	B
H(1)	1726	320	2500	0.8
H(2)	2503	2397	2500	0.8
H(3)	1947	4748	2500	0.9
H(4)	615	4960	2500	0.8

Table 10. Heavy Atom Anisotropic Displacement Parameters for Platinum(Bipyridyl)-*bis*-Chloride at 20 K

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	42(1)	14(1)	39(1)	0	0	0
Cl	86(4)	47(4)	76(4)	13(3)	0	0
N	68(13)	22(13)	51(14)	−9(10)	0	0
C(1)	85(16)	76(17)	118(19)	1(13)	0	0
C(2)	57(15)	101(19)	114(19)	−21(13)	0	0
C(3)	92(17)	63(17)	126(19)	−13(13)	0	0
C(4)	89(16)	56(16)	107(18)	−8(14)	0	0
C(5)	56(14)	27(15)	114(18)	−1(12)	0	0

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

The form of the displacement factor is:

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

Table 11. Complete Distances and Angles for Platinum(Bipyridyl)-*bis*-Chloride at 20 K

Distance(Å)			Angle(°)			
Pt	–Cl	2.308(1)	N	–Pt	–Cl	95.2(1)
Pt	–N	2.015(4)	N	–Pt	–N'	80.5(2)
N	–C(1)	1.343(6)	N	–Pt	–Cl'	175.6(1)
N	–C(5)	1.360(6)	Cl	–Pt	–Cl'	89.2(1)
C(1)	–C(2)	1.383(7)	Pt	–N	–C(1)	125.9(3)
C(1)	–H(1)	0.950	Pt	–N	–C(5)	114.9(3)
C(2)	–C(3)	1.382(7)	C(1)	–N	–C(5)	119.2(4)
C(2)	–H(2)	0.950	C(2)	–C(1)	–N	122.0(5)
C(3)	–C(4)	1.391(7)	H(1)	–C(1)	–N	119.0
C(3)	–H(3)	0.950	H(1)	–C(1)	–C(2)	119.0
C(4)	–C(5)	1.382(7)	C(3)	–C(2)	–C(1)	119.0(5)
C(4)	–H(4)	0.950	H(2)	–C(2)	–C(1)	120.5
C(5)	–C(5)'	1.459(6)	H(2)	–C(2)	–C(3)	120.5
			C(4)	–C(3)	–C(2)	119.4(5)
			H(3)	–C(3)	–C(2)	120.3
			H(3)	–C(3)	–C(4)	120.3
			C(5)	–C(4)	–C(3)	118.9(4)
			H(4)	–C(4)	–C(3)	120.5
			H(4)	–C(4)	–C(5)	120.5
			C(4)	–C(5)	–N	121.5(4)
			C(5)'	–C(5)	–N	114.9(4)
			C(5)'	–C(5)	–C(4)	123.7(4)

Symmetry code: (') $-x, y, z$

Table 12. Intermolecular Distances Less Than 4.0 A for Platinum(Bipyridyl)-*bis*-Chloride at 20 K

		Distance(Å)			Distance(Å)
Pt	–Pt	3.3697(3)	H(3)	–H(3)	3.353
Pt	–N	3.697(4)	H(4)	–H(4)	3.965
Cl	–C(3)	3.823(5)	H(4)	–H(4)	3.322
Cl	–C(4)	3.497(5)			
Cl	–H(3)	3.358			
Cl	–H(4)	2.693			
Cl	–C(2)	3.734(5)			
Cl	–H(2)	2.807			
Cl	–H(4)	3.778			
Cl	–N	3.404(4)			
Cl	–C(1)	3.560(5)			
Cl	–C(2)	3.812(5)			
Cl	–C(3)	3.895(5)			
Cl	–C(4)	3.738(5)			
Cl	–C(5)	3.484(5)			
Cl	–H(1)	3.965			
C(1)	–H(2)	3.945			
C(1)	–C(3)	3.924(7)			
C(1)	–H(2)	3.924			
C(1)	–H(3)	3.061			
C(1)	–H(1)	3.643			
C(2)	–C(2)	3.817(7)			
C(2)	–H(2)	3.452			
C(2)	–H(3)	3.145			
C(2)	–H(1)	3.437			
C(3)	–H(2)	3.831			
C(3)	–H(1)	3.158			
C(3)	–H(2)	3.520			
C(3)	–C(3)	3.884(7)			
C(3)	–H(3)	3.585			
C(3)	–H(4)	3.919			
C(4)	–C(4)	3.770(7)			
C(4)	–H(4)	3.474			
C(5)	–H(4)	3.934			
H(1)	–H(2)	2.975			
H(1)	–H(3)	2.391			
H(1)	–H(1)	3.372			
H(2)	–H(2)	3.327			
H(2)	–H(3)	3.968			
H(2)	–H(3)	2.588			
H(2)	–H(4)	3.981			

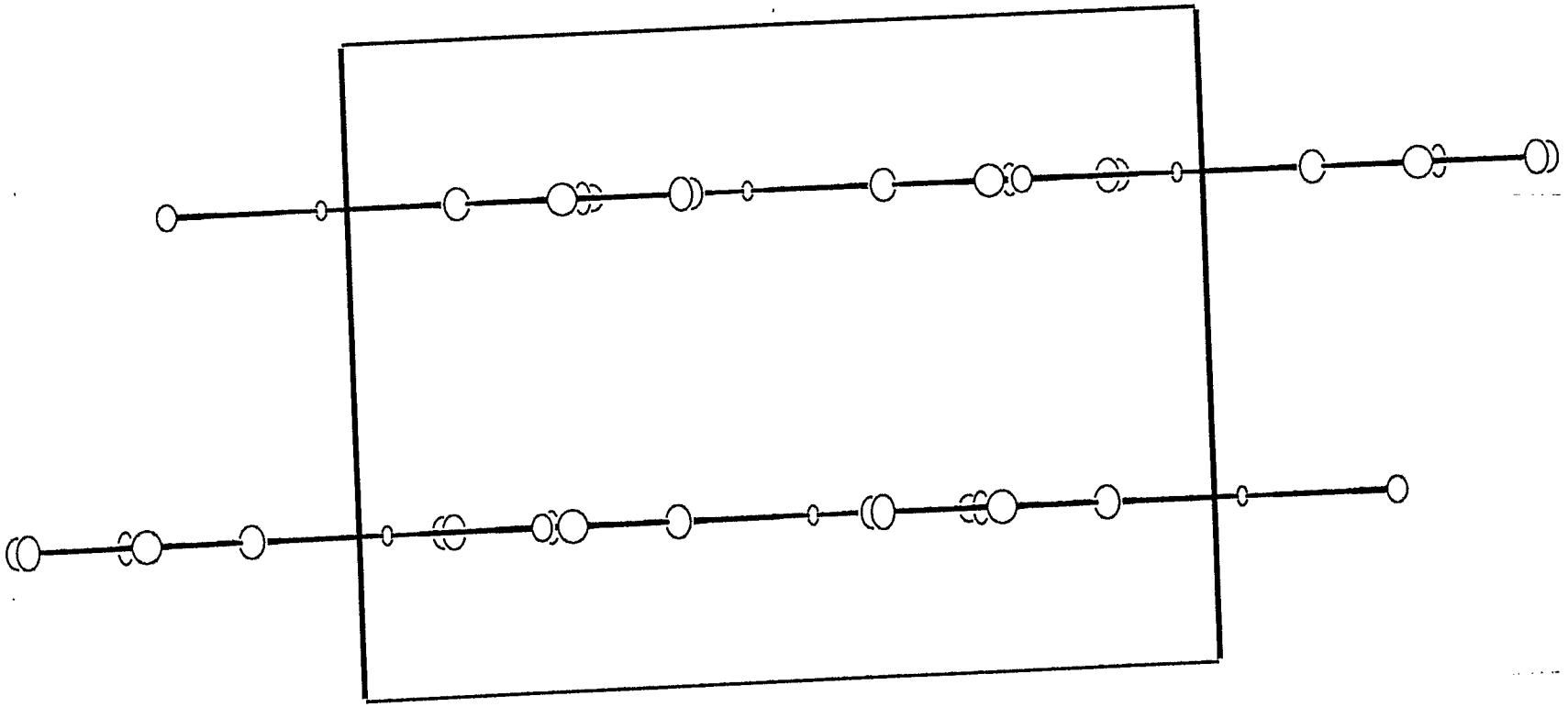

Figure 2a. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *bc* plane (projection down *a*).

Figure 2b. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *ac* plane (projection down *b*).

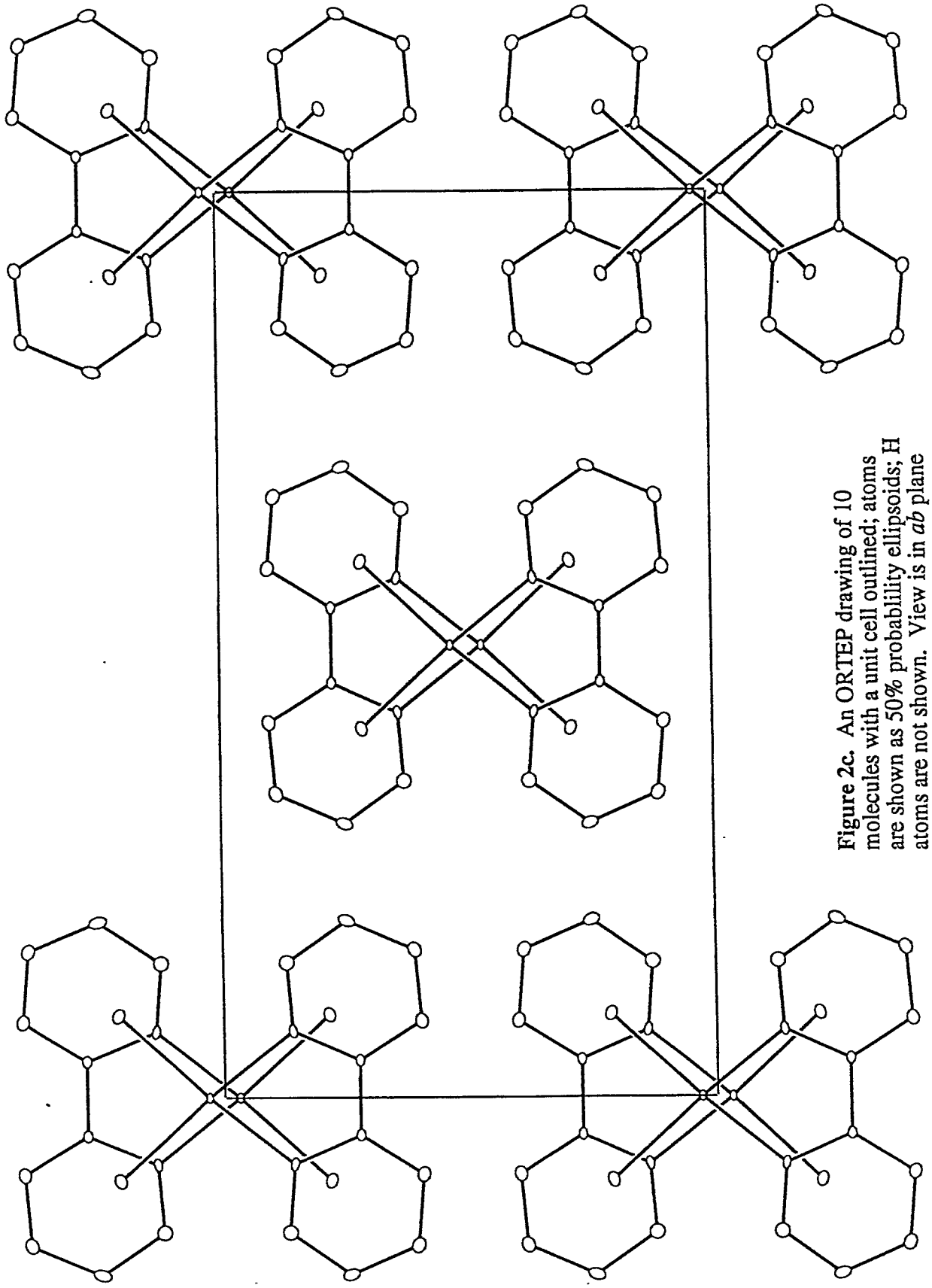

Figure 2c. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probablility ellipsoids; H atoms are not shown. View is in *ab* plane (projection down *c*).