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**Table 1. Crystal and Intensity Collection Data for
Pt(bpy)Cl₂ at 298 K**

Formula: C ₁₀ Cl ₂ N ₂ H ₈ Pt	Formula weight: 422.17
Crystal color: Red	Habit: Diamond-shaped needle
Crystal Size: 0.10 x 0.11 x 0.23 mm	$\rho_{\text{calc}} = 2.57 \text{ g cm}^{-3}$
Crystal System: Orthorhombic	Space group: <i>Cmcm</i> (no. 63)
$a = 17.669(5) \text{ \AA}$	
$b = 9.081(2) \text{ \AA}$	
$c = 6.804(2) \text{ \AA}$	
$V = 1091.7(5) \text{ \AA}^3$	$Z = 4$
Lattice parameters: 29 reflections	$9.5^\circ \leq \theta \leq 10.5^\circ$
$\mu = 134.5 \text{ cm}^{-1}$	Transmission coeff. = 0.70 – 1.27
Variable-temperature P1 diffractometer	$\theta - 2\theta$ scan
MoK α , $\lambda = 0.7107 \text{ \AA}$	Graphite monochromator
2θ range: 2° – 60°	$-24 \leq h \leq 21, -12 \leq k \leq 12, -9 \leq l \leq 9$
$T = 294 \text{ K}$	
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	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: < 0.01	
$\Delta\rho_{\text{max}}$: 1.2 e \AA^{-3} , $\Delta\rho_{\text{min}}$: -1.7 e \AA^{-3} in final difference map	
Secondary extinction parameter: $1.09(4) \times 10^{-6}$	

**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:

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

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

Distance(Å)			Angle(°)			
Pt	-N	2.009(6)	N	-Pt	-Cl	95.4(2)
Pt	-Cl	2.302(2)	N	-Pt	-N'	80.2(2)
N	-C(1)	1.350(10)	N	-Pt	-Cl'	175.5(2)
N	-C(5)	1.352(10)	Cl	-Pt	-Cl'	89.1(1)
C(1)	-C(2)	1.383(14)	Pt	-N	-C(1)	125.4(5)
C(1)	-H(1)	0.950	Pt	-N	-C(5)	114.9(5)
C(2)	-C(3)	1.358(15)	C(5)	-N	-C(1)	119.8(7)
C(2)	-H(2)	0.950	C(2)	-C(1)	-N	120.5(8)
C(3)	-C(4)	1.374(15)	H(1)	-C(1)	-N	119.8
C(3)	-H(3)	0.950	H(1)	-C(1)	-C(2)	119.8
C(4)	-C(5)	1.373(12)	C(3)	-C(2)	-C(1)	120.3(10)
C(4)	-H(4)	0.950	H(2)	-C(2)	-C(1)	119.9
C(5)	-C(5)'	1.442(11)	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 Å 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

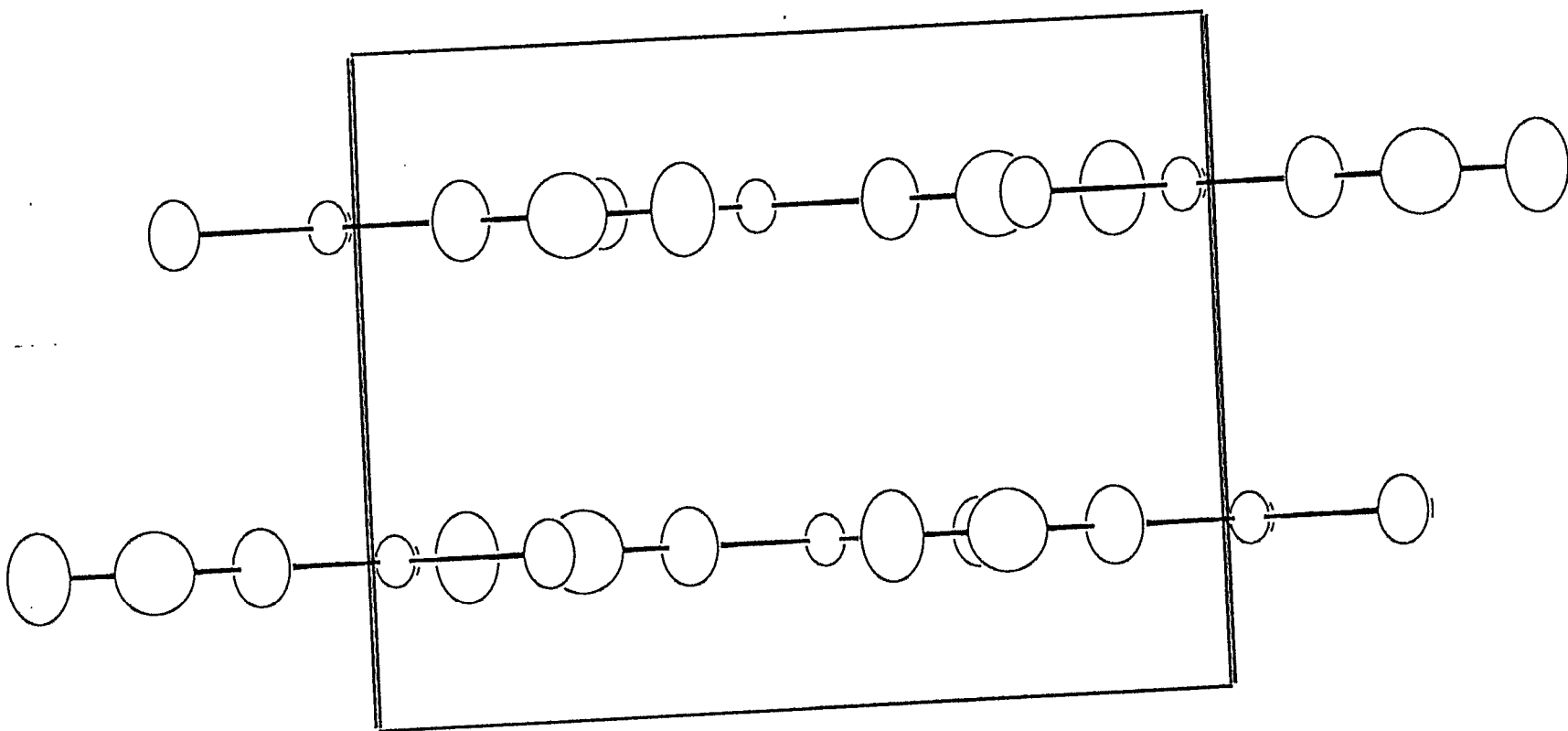


Figure 1a. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *bc* plane (projection down *a*).

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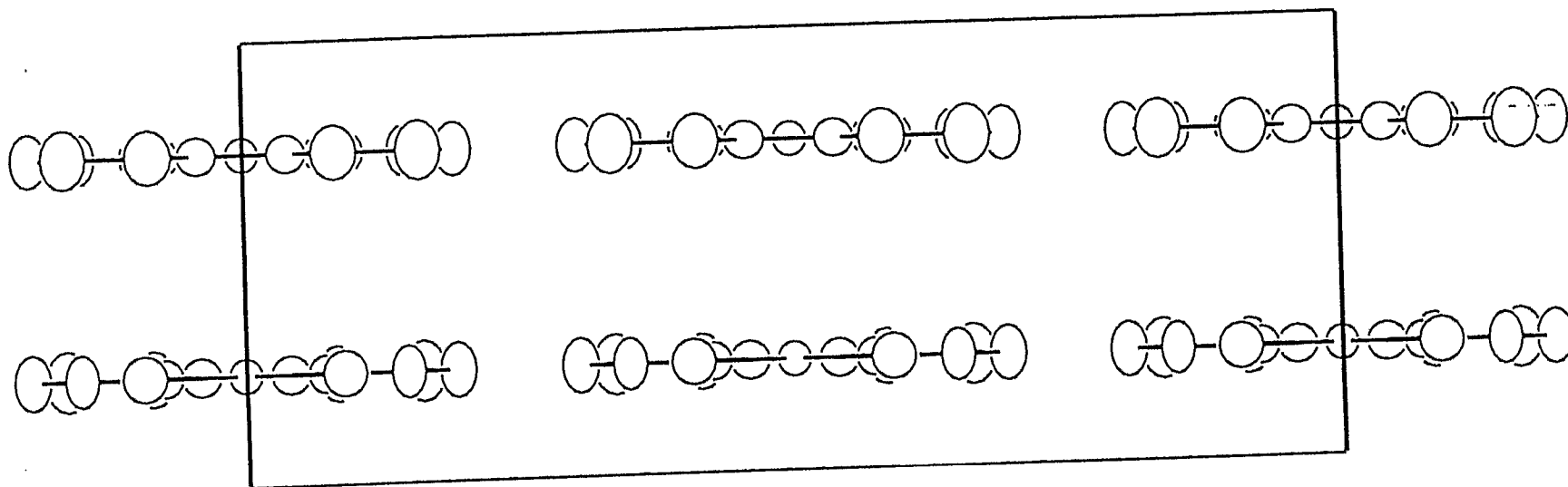


Figure 1b. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *ac* plane (projection down *b*).

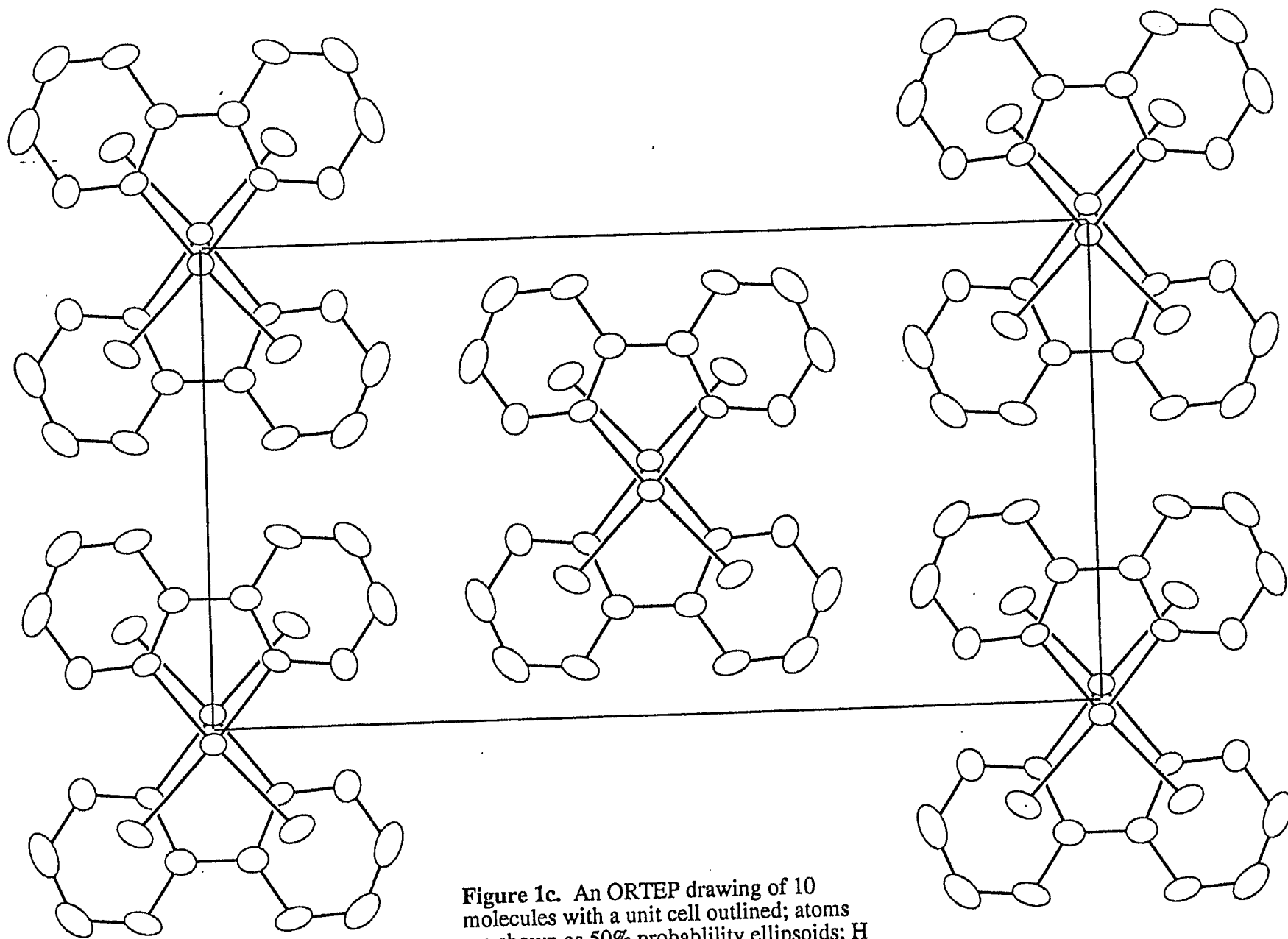


Figure 1c. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *ab* plane (projection down *c*).

**Table 7. Crystal and Intensity Collection Data for
Pt(bpy)Cl₂ at 20 K**

Formula: C ₁₀ Cl ₂ N ₂ H ₈ Pt	Formula weight: 422.17
Crystal color: Red	Habit: Diamond-shaped needle
Crystal Size: 0.10 x 0.11 x 0.23 mm	$\rho_{\text{calc}} = 2.65 \text{ g cm}^{-3}$
Crystal System: Orthorhombic	Space group: <i>Cmcm</i> (no. 63)
$a = 17.598(10) \text{ \AA}$	
$b = 9.059(4) \text{ \AA}$	
$c = 6.643(3) \text{ \AA}$	
$V = 1059.0(9) \text{ \AA}^3$	$Z = 4$
Lattice parameters: 28 reflections	$9.5^\circ \leq \theta \leq 10.5^\circ$
$\mu = 138.6 \text{ cm}^{-1}$	Transmission coeff. = 0.70 – 1.27
Variable-temperature P1 diffractometer	$\theta - 2\theta$ scan
MoK α , $\lambda = 0.7107 \text{ \AA}$	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	
$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: < 0.01	
$\Delta\rho_{\text{max}}$: 4.3 e \AA^{-3} , $\Delta\rho_{\text{min}}$: -4.3 e \AA^{-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 Å 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			

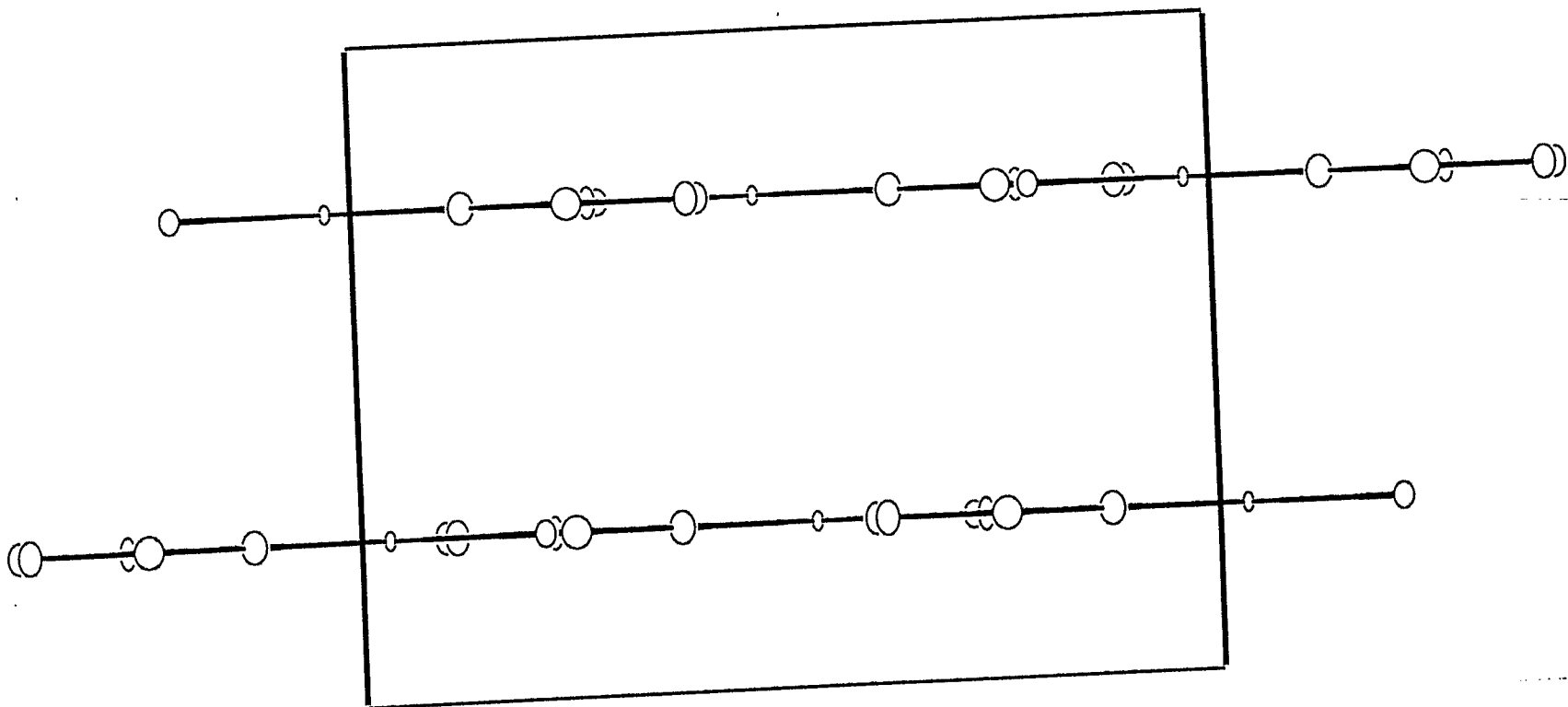


Figure 2a. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *bc* plane (projection down *a*).

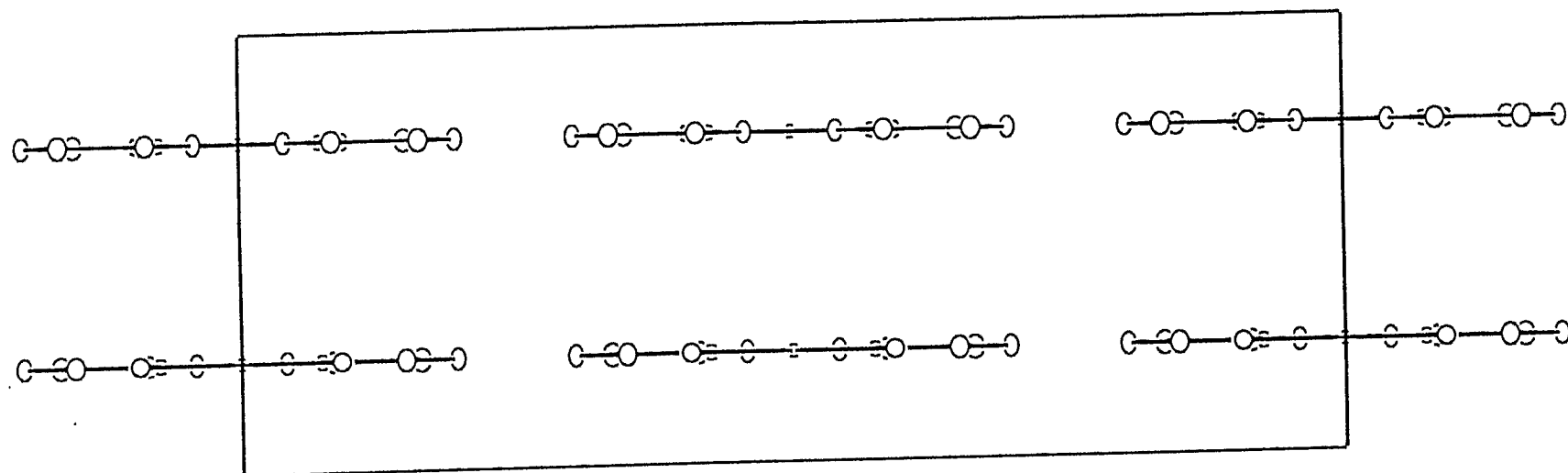


Figure 2b. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *ac* plane (projection down *b*).

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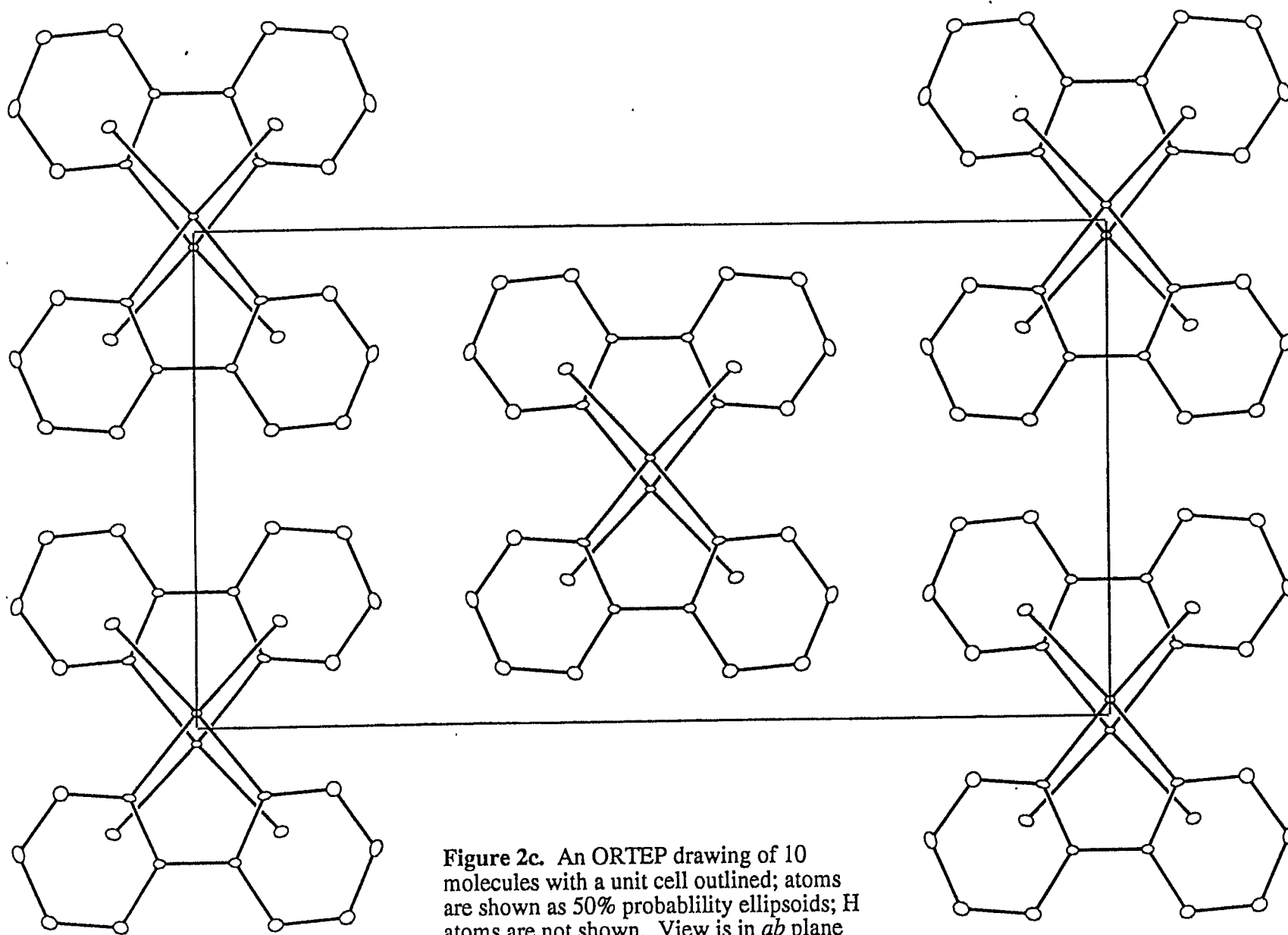


Figure 2c. An ORTEP drawing of 10 molecules with a unit cell outlined; atoms are shown as 50% probability ellipsoids; H atoms are not shown. View is in *ab* plane (projection down *c*).

Pt-Pt Distance vs. Temperature

