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Central Research & Development Dept.
Experimental Station , 10-MAR-1998

$Pt(PEt_3)_2Me_2$ (**3b**)

TO: K. Moloy, CRD, E328/215, x52083
NOTEBOOK REF: E91930-38a

FROM: W. Marshall, CRD/CCAS, E228/326, (302)695-2128
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X-RAY CRYSTAL STRUCTURE ANALYSIS **98033**

cis-dimethyl bis(triethyl_phosphine platinum(II)

CRYSTAL DATA: C14 H36 Pt1 P2 from methanol , light amber , irregular block , ~0.18 x 0.24 x 0.25mm, monoclinic , P21/n (No. 14), a = 8.148(2)Å, b = 17.543(5)Å, c = 12.780(5)Å, beta = 93.67(3)°, T = -75°C, Vol = 1823.0Å3, Z = 4, Formula weight = 461.48, Density = 1.681g/cc, μ(Mo) = 79.34cm-1

DATA COLLECTION: Enraf-Nonius CAD4 diffractometer, MoKalpha radiation , data collected = 8276, 2-theta range = 2.3° - 55.0°, maximum hkl = 10 22 16, data octants = +++, ++-, -++, -+-, W scan method, scan width = 1.20°- 1.90°W, scan speed = 1.70-5.00°/min, typical half-height peak width = 0.16°W, 2 standards collected 41 times, 1.0% fluctuation, 2579 duplicates, 2.6% R-merge, 28.5% variation in azimuthal scan, corrected for absorption (azimuthal), range of transmission factors = 0.15- 0.23, 2963 unique reflections with I> 3.0sig(I), Unit cell refined from 25 reflections with 2-theta range=20.56-31.10

SOLUTION AND REFINEMENT: Structure solved by direct methods (MULTAN), refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, including anomalous terms for Pt, P , biweight ~ [sigma 2(I)+0.0009I 2]-1/2, refined 17 of 53 atoms, 17 atoms refined anisotropic, 154 parameters, data/parameter ratio = 19.00, final R1 = 0.029, Rw = 0.025, error of fit = 0.87, max shift/error = 0.00, largest residual density = 1.39e/Å3, near PT1 , Because the refinement for a few of the methyl hydrogens gave unrealistic C-H bond distances(1.22A), all of the hydrogens have been idealized close to their previously refined positions.

RESULTS: This study determines the structure of cis-dimethyl bis(triethyl)-phosphine platinum(II) for hydrocyantion and carbonylation catalysis research. The asymmetric unit contains one molecule as shown in figure 1 with thermal ellipsoids drawn to the 50% probability level. The structure is cis rather than the predicted trans structure.

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7.

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
Pt(1)	2363.3(2)	1941.6(1)	6915.9(2)	1.4(0)'
P(1)	3465(2)	761(1)	7263(1)	1.6(0)'
P(2)	4718(2)	2620(1)	6674(1)	1.7(0)'
C(1)	76(7)	1437(3)	7150(5)	2.4(1)'
C(2)	938(7)	2932(3)	6691(5)	2.5(1)'
C(3)	3193(7)	445(3)	8602(4)	2.1(1)'
C(4)	4027(9)	958(4)	9426(5)	3.6(2)'
C(5)	5653(7)	572(3)	7106(4)	2.1(1)'
C(6)	6325(8)	-218(3)	7385(5)	3.3(2)'
C(7)	2435(7)	-16(3)	6526(5)	2.5(1)'
C(8)	2389(8)	94(3)	5340(5)	3.0(2)'
C(9)	6063(7)	2711(3)	7879(5)	2.4(1)'
C(10)	5242(8)	3111(4)	8760(5)	3.1(2)'
C(11)	4539(8)	3626(3)	6272(5)	2.7(2)'
C(12)	4007(9)	3756(4)	5129(6)	3.9(2)'
C(13)	6146(7)	2255(3)	5739(4)	2.0(1)'
C(14)	5326(8)	1921(4)	4737(5)	3.0(2)'
H(1)	-646	1801	7426	2.4
H(1')	208	1022	7625	2.4
H(1")	-407	1255	6501	2.4
H(2)	1405	3248	6183	2.5
H(2')	926	3208	7331	2.5
H(2")	-155	2802	6456	2.5
H(3)	3593	-60	8702	2.1
H(3')	2052	416	8718	2.1
H(4)	5066	756	9664	3.6
H(4')	3367	1005	10010	3.6
H(4")	4176	1454	9147	3.6
H(5)	6307	944	7478	2.1
H(5')	5913	703	6416	2.1
H(6)	7187	-335	6944	3.3
H(6')	5490	-591	7258	3.3
H(6")	6742	-238	8096	3.3
H(7)	1337	-74	6726	2.5
H(7')	2928	-493	6706	2.5
H(8)	1828	-327	5012	3.0
H(8')	3485	91	5123	3.0
H(8")	1834	552	5145	3.0
H(9)	7039	2975	7725	2.4
H(9')	6416	2220	8110	2.4
H(10)	5961	3107	9375	3.1
H(10')	4233	2867	8887	3.1
H(10")	5036	3627	8562	3.1
H(11)	5568	3870	6431	2.7
H(11')	3838	3891	6713	2.7
H(12)	3845	4288	5026	3.9
H(12')	3017	3486	4949	3.9
H(12")	4859	3601	4701	3.9
H(13)	6878	1893	6067	2.0
H(13')	6872	2652	5557	2.0
H(14)	6139	1661	4370	3.0
H(14')	4869	2317	4307	3.0
H(14")	4509	1566	4916	3.0

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TABLE II. Anisotropic Thermal Parameters (Å² X 1000)

exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
Pt(1)	15.1(1)	18.8(1)	20.0(1)	2.2(1)	-1.1(1)	-1.8(1)
P(1)	20.2(7)	17.9(6)	22.3(7)	-0.3(5)	-0.4(5)	-0.8(5)
P(2)	20.1(7)	18.6(7)	26.3(7)	0.6(6)	0.2(6)	-1.8(6)
C(1)	17(3)	32(3)	41(3)	0(2)	3(2)	-2(3)
C(2)	26(3)	32(3)	38(3)	11(2)	4(2)	10(3)
C(3)	26(3)	28(3)	23(3)	0(2)	-2(2)	5(2)
C(4)	72(5)	42(4)	22(3)	-5(4)	-8(3)	-3(3)
C(5)	26(3)	20(3)	33(3)	4(2)	4(2)	1(2)
C(6)	41(4)	33(3)	51(4)	14(3)	6(3)	11(3)
C(7)	36(3)	24(3)	33(3)	-3(3)	-2(3)	-6(2)
C(8)	43(4)	39(3)	30(3)	-3(3)	-4(3)	-9(3)
C(9)	27(3)	26(3)	36(3)	-1(2)	-9(2)	-1(3)
C(10)	46(4)	37(3)	33(3)	3(3)	-6(3)	-8(3)
C(11)	38(4)	23(3)	42(4)	4(3)	1(3)	3(3)
C(12)	58(5)	34(4)	55(4)	12(3)	7(4)	10(3)
C(13)	25(3)	23(3)	30(3)	-1(2)	8(2)	4(2)
C(14)	43(4)	36(3)	37(3)	-1(3)	12(3)	3(3)

TABLE III. Interatomic Distances (A)

Pt(1)-P(1)	2.290 (1)	C(4)-H(4")	0.950 (0)
Pt(1)-P(2)	2.295 (2)	C(5)-H(5)	0.951 (0)
Pt(1)-C(1)	2.102 (5)	C(5)-H(5')	0.949 (0)
Pt(1)-C(2)	2.099 (5)	C(6)-H(6)	0.951 (0)
P(1)-C(3)	1.826 (5)	C(6)-H(6')	0.950 (0)
P(1)-C(5)	1.837 (5)	C(6)-H(6")	0.951 (0)
P(1)-C(7)	1.830 (6)	C(7)-H(7)	0.952 (0)
P(2)-C(9)	1.839 (6)	C(7)-H(7')	0.950 (0)
P(2)-C(11)	1.841 (6)	C(8)-H(8)	0.951 (0)
P(2)-C(13)	1.836 (5)	C(8)-H(8')	0.952 (0)
C(3)-C(4)	1.514 (8)	C(8)-H(8")	0.948 (0)
C(5)-C(6)	1.523 (7)	C(9)-H(9)	0.952 (0)
C(7)-C(8)	1.525 (8)	C(9)-H(9')	0.950 (0)
C(9)-C(10)	1.519 (8)	C(10)-H(10)	0.950 (0)
C(11)-C(12)	1.514 (9)	C(10)-H(10')	0.950 (0)
C(13)-C(14)	1.524 (8)	C(10)-H(10")	0.951 (0)
C(1)-H(1)	0.951 (0)	C(11)-H(11)	0.951 (0)
C(1)-H(1')	0.950 (0)	C(11)-H(11')	0.950 (0)
C(1)-H(1")	0.951 (0)	C(12)-H(12)	0.950 (0)
C(2)-H(2)	0.952 (0)	C(12)-H(12')	0.950 (0)
C(2)-H(2')	0.951 (0)	C(12)-H(12")	0.950 (0)
C(2)-H(2")	0.949 (0)	C(13)-H(13)	0.951 (0)
C(3)-H(3)	0.950 (0)	C(13)-H(13')	0.951 (0)
C(3)-H(3')	0.952 (0)	C(14)-H(14)	0.952 (0)
C(4)-H(4)	0.950 (0)	C(14)-H(14')	0.949 (0)
C(4)-H(4')	0.950 (0)	C(14)-H(14")	0.950 (0)

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TABLE IV. Intramolecular Angles (Deg)

P(1)-Pt(1)-P(2)	100.03 (5)	C(5)-C(6)-H(6")	111 (0)
P(1)-Pt(1)-C(1)	86.1 (2)	C(8)-C(7)-H(7)	108 (0)
P(1)-Pt(1)-C(2)	169.1 (2)	C(8)-C(7)-H(7')	110 (0)
P(2)-Pt(1)-C(1)	173.7 (2)	C(7)-C(8)-H(8)	109 (0)
P(2)-Pt(1)-C(2)	90.7 (2)	C(7)-C(8)-H(8')	109 (0)
C(1)-Pt(1)-C(2)	83.1 (2)	C(7)-C(8)-H(8")	110 (0)
Pt(1)-P(1)-C(3)	112.7 (2)	C(10)-C(9)-H(9)	110 (0)
Pt(1)-P(1)-C(5)	120.9 (2)	C(10)-C(9)-H(9')	109 (0)
Pt(1)-P(1)-C(7)	114.4 (2)	C(9)-C(10)-H(10)	109 (0)
Pt(1)-P(2)-C(9)	113.0 (2)	C(9)-C(10)-H(10')	110 (0)
Pt(1)-P(2)-C(11)	118.9 (2)	C(9)-C(10)-H(10")	109 (0)
Pt(1)-P(2)-C(13)	118.5 (2)	C(12)-C(11)-H(11)	109 (0)
C(3)-P(1)-C(5)	103.0 (2)	C(12)-C(11)-H(11')	111 (0)
C(3)-P(1)-C(7)	100.2 (3)	C(11)-C(12)-H(12)	108 (0)
C(5)-P(1)-C(7)	103.1 (3)	C(11)-C(12)-H(12')	110 (0)
C(9)-P(2)-C(11)	100.5 (3)	C(11)-C(12)-H(12")	110 (0)
C(9)-P(2)-C(13)	101.9 (3)	C(14)-C(13)-H(13)	110 (0)
C(11)-P(2)-C(13)	101.2 (3)	C(14)-C(13)-H(13')	109 (0)
Pt(1)-C(1)-H(1)	110 (0)	C(13)-C(14)-H(14)	108 (0)
Pt(1)-C(1)-H(1')	110 (0)	C(13)-C(14)-H(14')	110 (0)
Pt(1)-C(1)-H(1")	110 (0)	C(13)-C(14)-H(14")	109 (0)
Pt(1)-C(2)-H(2)	110 (0)	H(1)-C(1)-H(1')	109 (0)
Pt(1)-C(2)-H(2')	110 (0)	H(1)-C(1)-H(1")	109 (0)
Pt(1)-C(2)-H(2")	110 (0)	H(1')-C(1)-H(1")	109 (0)
P(1)-C(3)-C(4)	113.3 (4)	H(2)-C(2)-H(2')	108 (0)
P(1)-C(5)-C(6)	118.4 (4)	H(2)-C(2)-H(2")	109 (0)
P(1)-C(7)-C(8)	113.5 (4)	H(2')-C(2)-H(2")	109 (0)
P(2)-C(9)-C(10)	113.2 (4)	H(3)-C(3)-H(3')	105 (0)
P(2)-C(11)-C(12)	115.2 (4)	H(4)-C(4)-H(4')	109 (0)
P(2)-C(13)-C(14)	114.8 (4)	H(4)-C(4)-H(4")	109 (0)
P(1)-C(3)-H(3)	110 (0)	H(4')-C(4)-H(4")	108 (0)
P(1)-C(3)-H(3')	110 (0)	H(5)-C(5)-H(5')	98 (0)
P(1)-C(5)-H(5)	110 (0)	H(6)-C(6)-H(6')	107 (0)
P(1)-C(5)-H(5')	109 (0)	H(6)-C(6)-H(6")	109 (0)
P(1)-C(7)-H(7)	110 (0)	H(6')-C(6)-H(6")	110 (0)
P(1)-C(7)-H(7')	111 (0)	H(7)-C(7)-H(7')	103 (0)
P(2)-C(9)-H(9)	109 (0)	H(8)-C(8)-H(8')	108 (0)
P(2)-C(9)-H(9')	109 (0)	H(8)-C(8)-H(8")	110 (0)
P(2)-C(11)-H(11)	109 (0)	H(8')-C(8)-H(8")	112 (0)
P(2)-C(11)-H(11')	110 (0)	H(9)-C(9)-H(9')	105 (0)
P(2)-C(13)-H(13)	111 (0)	H(10)-C(10)-H(10')	110 (0)
P(2)-C(13)-H(13')	110 (0)	H(10)-C(10)-H(10")	108 (0)
C(4)-C(3)-H(3)	109 (0)	H(10')-C(10)-H(10")	110 (0)
C(4)-C(3)-H(3')	109 (0)	H(11)-C(11)-H(11')	102 (0)
C(3)-C(4)-H(4)	111 (0)	H(12)-C(12)-H(12')	110 (0)
C(3)-C(4)-H(4')	110 (0)	H(12)-C(12)-H(12")	107 (0)
C(3)-C(4)-H(4")	110 (0)	H(12')-C(12)-H(12")	111 (0)
C(6)-C(5)-H(5)	109 (0)	H(13)-C(13)-H(13')	102 (0)
C(6)-C(5)-H(5')	110 (0)	H(14)-C(14)-H(14')	109 (0)
C(5)-C(6)-H(6)	109 (0)	H(14)-C(14)-H(14")	109 (0)
C(5)-C(6)-H(6')	110 (0)	H(14')-C(14)-H(14")	111 (0)

TABLE V. Intramolecular Non-Bonding Distances (A)

C(2)...C(12)	3.601 (9)	C(12)...C(14)	3.441 (9)
C(5)...C(13)	3.469 (7)		

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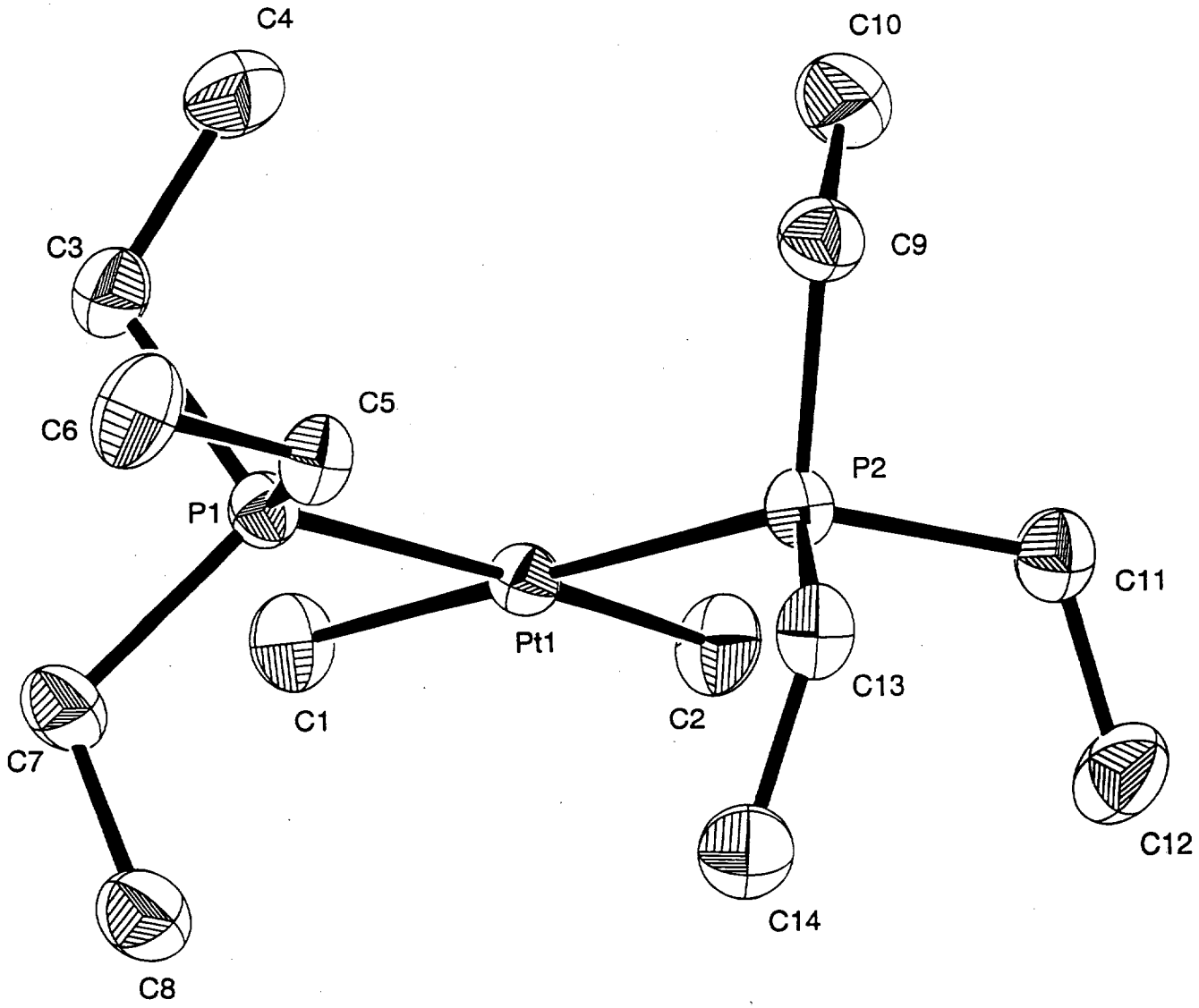

E. I. DUPONT DE NEMOURS & CO., INC.
Central Research & Development Dept.
Experimental Station , 10-MAR-1998

$Pt(PMe_2Ph)_2Me_2$ (**3c**)

TO: K. Moloy, CRD, E328/215, x52083
NOTEBOOK REF: E91930-38c

FROM: W. Marshall, CRD/CCAS, E228/326, (302)695-2128
EMAIL: Will.Marshall@usa.dupont.com marshawj@esvax

X-RAY CRYSTAL STRUCTURE ANALYSIS **98032**

cis-dimethylbis(dimethylphenyl)phosphine platinum(II)

CRYSTAL DATA: C18 H28 Pt1 P2 from methanol , faint amber , irregular block , ~0.12 x 0.18 x 0.22mm, monoclinic , C2/c (No. 15), a = 17.098(4)Å, b = 13.949(3)Å, c = 17.040(3)Å, beta = 108.73(2)°, T = -75°C, Vol = 3848.8Å3, Z = 8, Formula weight = 501.46, Density = 1.731g/cc, μ(Mo) = 75.24cm-1

DATA COLLECTION: Enraf-Nonius CAD4 diffractometer, MoKalpha radiation , data collected = 9194, 2-theta range = 2.5° - 55.0°, maximum hkl = 22 18 22, data octants = +++, ++-, -++, -+-, W scan method, scan width = 1.20°- 2.20°W, scan speed = 1.70-5.00°/min, typical half-height peak width = 0.16°W, 2 standards collected 68 times, 52.0% fluctuation, 1876 duplicates, 3.2% R-merge, 31.8% variation in azimuthal scan, corrected for absorption (azimuthal), range of transmission factors = 0.21- 0.35, 2276 unique reflections with I> 3.0sig(I), Unit cell refined from 25 reflections with 2-theta range=24.56-29.62

SOLUTION AND REFINEMENT: Structure solved by direct methods (MULTAN), refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, including anomalous terms for Pt, P , biweight ~ [sigma 2(I)+0.0009I 2]-1/2, two-theta limit for refinement = 0.0- 50.0, refined 21 of 49 atoms, 21 atoms refined anisotropic, 190 parameters, data/parameter ratio = 10.00, final R1 = 0.040, Rw = 0.030, error of fit = 0.85, max shift/error = 0.03, largest residual density = 1.07e/Å3, near C24 , Because the refinement for a few of the methyl hydrogens gave unrealistic C-H bond distances(1.14A), all of the hydrogens have been idealized close to their previously refined positions.

RESULTS: This study determines the structure of cis-dimethyl bis(dimethylphenyl)-phosphineplatinum(II) for hydrocyantion and carbonylation catalysis research. The asymmetric unit contains one molecule as shown in figure 1 with thermal ellipsoids drawn to the 50% probability level. The structure is cis rather than the predicted trans structure. The molecule contains a non-crystallographic 2-fold axis but cannot be converted to a higher symmetry.

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TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
Pt(1)	3727.0(3)	3631.1(3)	4726.2(3)	2.5(0)'
P(1)	3556(2)	4368(2)	3486(2)	3.0(1)'
P(2)	3877(2)	2128(2)	4261(2)	2.9(1)'
C(1)	3555(7)	4945(8)	5245(7)	4.8(4)'
C(2)	3895(7)	3076(8)	5899(6)	4.4(4)'
C(11)	2579(5)	4102(7)	2698(5)	2.4(3)'
C(12)	2475(7)	4082(8)	1857(7)	3.8(4)'
C(13)	1735(7)	3787(8)	1301(6)	3.8(4)'
C(14)	1101(7)	3506(9)	1561(7)	4.1(4)'
C(15)	1189(6)	3528(9)	2387(7)	4.3(4)'
C(16)	1913(6)	3822(8)	2948(6)	3.4(3)'
C(17)	4319(7)	4099(10)	2973(7)	5.8(5)'
C(18)	3609(7)	5667(8)	3461(8)	5.4(4)'
C(21)	4885(6)	1897(7)	4134(6)	2.6(3)'
C(22)	5052(8)	1078(8)	3751(7)	4.6(4)'
C(23)	5808(9)	932(10)	3628(8)	5.9(5)'
C(24)	6393(8)	1667(10)	3906(8)	5.4(5)'
C(25)	6248(7)	2460(9)	4302(7)	3.9(4)'
C(26)	5506(6)	2553(7)	4399(6)	3.1(3)'
C(27)	3144(6)	1779(8)	3278(7)	4.2(4)'
C(28)	3741(7)	1133(7)	4889(7)	4.5(4)'
H(1)	3028	5176	4917	4.9
H(1')	3986	5368	5231	4.9
H(1")	3548	4817	5790	4.9
H(2)	3928	3603	6261	4.4
H(2')	4406	2739	6072	4.4
H(2")	3439	2676	5881	4.4
H(12)	2912	4260	1655	3.8
H(13)	1669	3788	725	3.8
H(14)	595	3306	1168	4.1
H(15)	745	3326	2570	4.3
H(16)	1967	3846	3521	3.4
H(17)	4229	4474	2487	5.8
H(17')	4292	3438	2827	5.8
H(17")	4861	4219	3340	5.8
H(18)	3487	5878	2905	5.4
H(18')	4139	5875	3801	5.4
H(18")	3203	5914	3679	5.4
H(22)	4634	607	3549	4.6
H(23)	5924	375	3361	5.9
H(24)	6919	1596	3834	5.4
H(25)	6661	2942	4493	3.9
H(26)	5405	3111	4672	3.1
H(27)	3208	1116	3186	4.2
H(27')	3258	2140	2853	4.2
H(27")	2599	1917	3276	4.2
H(28)	3220	1167	4973	4.6
H(28')	4185	1150	5397	4.6
H(28")	3801	558	4613	4.6

TABLE II. Anisotropic Thermal Parameters (Å² X 1000)

exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
Pt(1)	28.0(2)	39.0(2)	29.3(2)	-4.2(3)	11.0(1)	-3.7(3)
P(1)	31(2)	45(2)	40(2)	-1(1)	14(1)	9(1)
P(2)	41(2)	39(2)	30(2)	-7(1)	9(1)	-2(1)
C(1)	69(8)	60(8)	64(9)	7(7)	35(7)	-9(7)
C(2)	80(9)	54(8)	36(7)	2(7)	23(6)	-7(6)
C(11)	32(5)	35(6)	28(6)	11(5)	14(5)	9(5)
C(12)	70(9)	37(7)	43(8)	2(6)	28(7)	3(6)
C(13)	71(8)	44(8)	22(6)	8(7)	5(6)	6(6)
C(14)	45(7)	49(8)	45(7)	17(7)	-12(6)	8(7)
C(15)	41(6)	68(8)	58(8)	12(7)	18(6)	16(8)
C(16)	29(5)	71(9)	33(6)	6(6)	18(5)	6(6)
C(17)	56(8)	116(11)	65(8)	28(8)	41(7)	46(8)
C(18)	48(7)	51(8)	91(10)	-29(7)	2(7)	15(7)
C(21)	33(6)	35(6)	29(6)	7(5)	7(5)	2(5)
C(22)	70(9)	40(8)	48(8)	1(6)	-2(7)	-8(6)
C(23)	72(10)	85(11)	78(10)	41(9)	37(8)	-8(9)
C(24)	64(9)	89(13)	69(10)	13(9)	46(8)	31(8)
C(25)	35(6)	59(8)	54(8)	13(6)	12(6)	10(7)
C(26)	34(6)	36(6)	40(6)	11(5)	1(5)	8(5)
C(27)	44(7)	52(7)	51(7)	4(6)	-4(6)	-16(6)
C(28)	76(8)	37(7)	58(8)	-23(7)	19(7)	1(6)

TABLE III. Interatomic Distances (A)

Pt(1)-P(1)	2.284 (3)	C(2)-H(2)	0.950 (0)
Pt(1)-P(2)	2.285 (3)	C(2)-H(2')	0.951 (0)
Pt(1)-C(1)	2.096 (11)	C(2)-H(2")	0.951 (0)
Pt(1)-C(2)	2.075 (11)	C(12)-H(12)	0.951 (0)
P(1)-C(11)	1.813 (9)	C(13)-H(13)	0.950 (0)
P(1)-C(17)	1.829 (11)	C(14)-H(14)	0.951 (0)
P(1)-C(18)	1.815 (11)	C(15)-H(15)	0.951 (0)
P(2)-C(21)	1.833 (10)	C(16)-H(16)	0.951 (0)
P(2)-C(27)	1.807 (10)	C(17)-H(17)	0.949 (0)
P(2)-C(28)	1.811 (10)	C(17)-H(17')	0.952 (0)
C(11)-C(12)	1.386 (13)	C(17)-H(17")	0.951 (0)
C(11)-C(16)	1.395 (12)	C(18)-H(18)	0.950 (0)
C(12)-C(13)	1.378 (14)	C(18)-H(18')	0.950 (0)
C(13)-C(14)	1.354 (15)	C(18)-H(18")	0.951 (0)
C(14)-C(15)	1.368 (14)	C(22)-H(22)	0.951 (0)
C(15)-C(16)	1.361 (13)	C(23)-H(23)	0.953 (0)
C(21)-C(22)	1.389 (13)	C(24)-H(24)	0.951 (0)
C(21)-C(26)	1.363 (13)	C(25)-H(25)	0.953 (0)
C(22)-C(23)	1.391 (16)	C(26)-H(26)	0.952 (0)
C(23)-C(24)	1.404 (17)	C(27)-H(27)	0.950 (0)
C(24)-C(25)	1.360 (16)	C(27)-H(27')	0.952 (0)
C(25)-C(26)	1.338 (14)	C(27)-H(27")	0.950 (0)
C(1)-H(1)	0.951 (0)	C(28)-H(28)	0.949 (0)
C(1)-H(1')	0.949 (0)	C(28)-H(28')	0.951 (0)
C(1)-H(1")	0.951 (0)	C(28)-H(28")	0.952 (0)

TABLE IV. Intramolecular Angles (Deg)

P(1)-Pt(1)-P(2)	95.0 (1)	C(11)-C(16)-C(15)	121 (1)
P(1)-Pt(1)-C(1)	90.2 (3)	C(22)-C(21)-C(26)	117 (1)
P(1)-Pt(1)-C(2)	175.1 (3)	C(21)-C(22)-C(23)	122 (1)
P(2)-Pt(1)-C(1)	174.4 (3)	C(22)-C(23)-C(24)	116 (1)
P(2)-Pt(1)-C(2)	89.7 (3)	C(23)-C(24)-C(25)	123 (1)
C(1)-Pt(1)-C(2)	85.1 (4)	C(24)-C(25)-C(26)	118 (1)
Pt(1)-P(1)-C(11)	114.0 (3)	C(21)-C(26)-C(25)	124 (1)
Pt(1)-P(1)-C(17)	116.8 (4)	C(11)-C(12)-H(12)	121 (0)
Pt(1)-P(1)-C(18)	118.6 (4)	C(13)-C(12)-H(12)	119 (0)
Pt(1)-P(2)-C(21)	114.6 (3)	C(12)-C(13)-H(13)	119 (0)
Pt(1)-P(2)-C(27)	116.5 (4)	C(14)-C(13)-H(13)	120 (0)
Pt(1)-P(2)-C(28)	116.6 (4)	C(13)-C(14)-H(14)	120 (0)
C(11)-P(1)-C(17)	103.5 (5)	C(15)-C(14)-H(14)	120 (0)
C(11)-P(1)-C(18)	103.2 (5)	C(14)-C(15)-H(15)	120 (0)
C(17)-P(1)-C(18)	98.4 (6)	C(16)-C(15)-H(15)	120 (0)
C(21)-P(2)-C(27)	104.0 (5)	C(11)-C(16)-H(16)	119 (0)
C(21)-P(2)-C(28)	103.8 (5)	C(15)-C(16)-H(16)	120 (0)
C(27)-P(2)-C(28)	99.2 (5)	C(21)-C(22)-H(22)	120 (0)
Pt(1)-C(1)-H(1)	106 (0)	C(23)-C(22)-H(22)	118 (0)
Pt(1)-C(1)-H(1')	109 (0)	C(22)-C(23)-H(23)	122 (0)
Pt(1)-C(1)-H(1")	107 (0)	C(24)-C(23)-H(23)	121 (0)
Pt(1)-C(2)-H(2)	107 (0)	C(23)-C(24)-H(24)	119 (0)
Pt(1)-C(2)-H(2')	108 (0)	C(25)-C(24)-H(24)	119 (0)
Pt(1)-C(2)-H(2")	109 (0)	C(24)-C(25)-H(25)	121 (0)
P(1)-C(11)-C(12)	123.5 (8)	C(26)-C(25)-H(25)	121 (0)
P(1)-C(11)-C(16)	118.7 (7)	C(21)-C(26)-H(26)	118 (0)
P(2)-C(21)-C(22)	122.8 (9)	C(25)-C(26)-H(26)	118 (0)
P(2)-C(21)-C(26)	120.3 (8)	H(1)-C(1)-H(1')	112 (0)
P(1)-C(17)-H(17)	111 (0)	H(1)-C(1)-H(1")	109 (0)
P(1)-C(17)-H(17')	110 (0)	H(1')-C(1)-H(1")	113 (0)
P(1)-C(17)-H(17")	110 (0)	H(2)-C(2)-H(2')	109 (0)
P(1)-C(18)-H(18)	110 (0)	H(2)-C(2)-H(2")	111 (0)
P(1)-C(18)-H(18')	110 (0)	H(2')-C(2)-H(2")	112 (0)
P(1)-C(18)-H(18")	108 (0)	H(17)-C(17)-H(17')	109 (0)
P(2)-C(27)-H(27)	109 (0)	H(17)-C(17)-H(17")	109 (0)
P(2)-C(27)-H(27')	108 (0)	H(17')-C(17)-H(17")	107 (0)
P(2)-C(27)-H(27")	110 (0)	H(18)-C(18)-H(18')	112 (0)
P(2)-C(28)-H(28)	111 (0)	H(18)-C(18)-H(18")	109 (0)
P(2)-C(28)-H(28')	108 (0)	H(18')-C(18)-H(18")	109 (0)
P(2)-C(28)-H(28")	107 (0)	H(27)-C(27)-H(27')	109 (0)
C(12)-C(11)-C(16)	117.6 (9)	H(27)-C(27)-H(27")	111 (0)
C(11)-C(12)-C(13)	120 (1)	H(27')-C(27)-H(27")	109 (0)
C(12)-C(13)-C(14)	121 (1)	H(28)-C(28)-H(28')	112 (0)
C(13)-C(14)-C(15)	120 (1)	H(28)-C(28)-H(28")	112 (0)
C(14)-C(15)-C(16)	120 (1)	H(28')-C(28)-H(28")	107 (0)

TABLE V. Intramolecular Non-Bonding Distances (A)

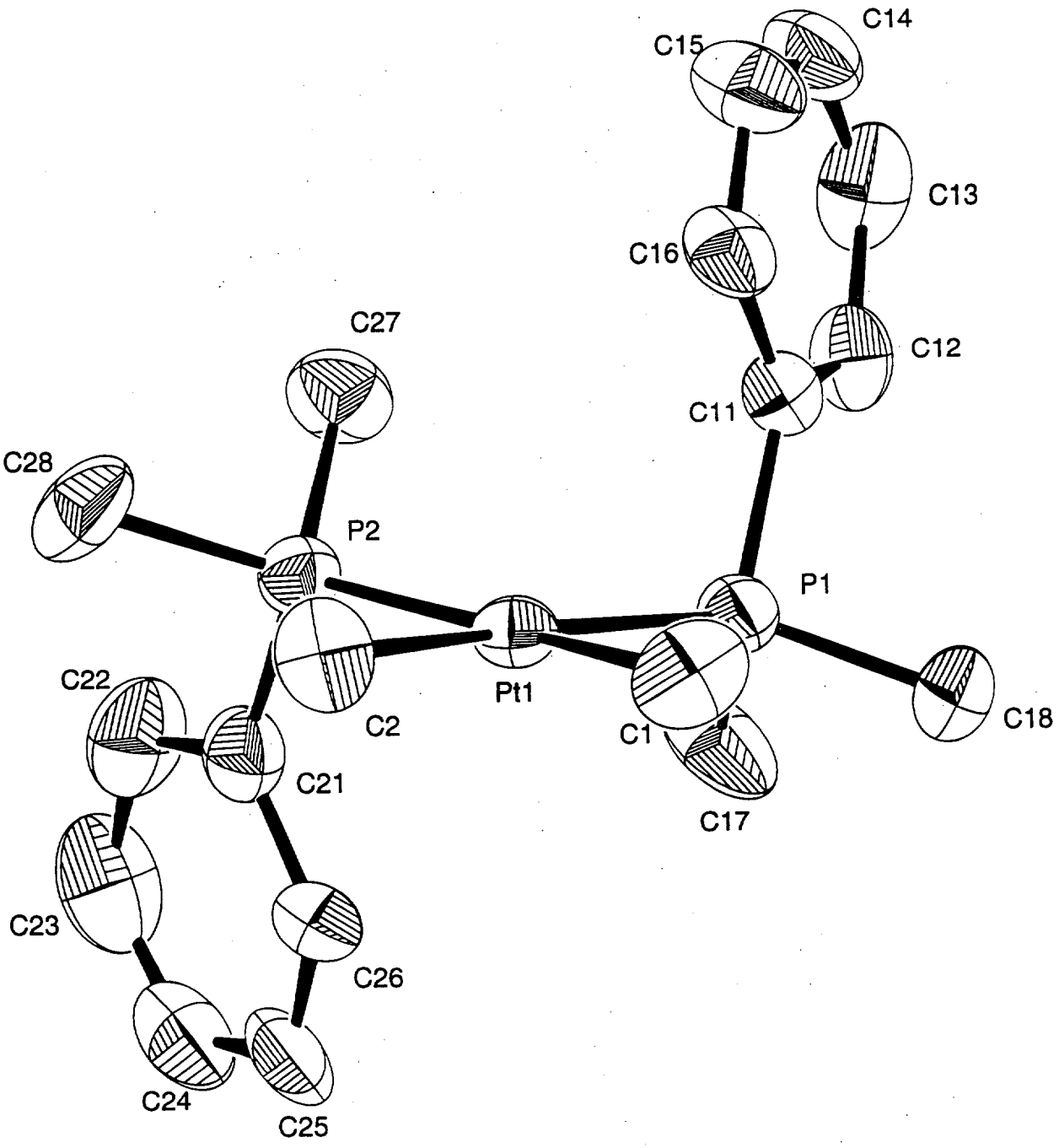
C(11)...C(27)	3.434 (14)
C(16)...C(27)	3.479 (15)
C(17)...C(21)	3.614 (15)
C(17)...C(26)	3.392 (14)

TABLE VI. Intermolecular Distances (A)

C(17)...C(17)a 3.227 (20)

Symmetry Operation Codes

a 1-X,Y,1/2-Z


C14
C15
C13
C16
C12
C27
C11
C28
P2
P1
Pt1
C22
C2
C1
C18
C21
C17
C23
C26
C24
C25

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Central Research & Development Dept.
Experimental Station , 10-MAR-1998

$Pt(Ppyrl_3)_2Me_2$ (**3n**)

TO: K. Moloy, CRD, E328/215, x52083
NOTEBOOK REF: E91930-38b

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X-RAY CRYSTAL STRUCTURE ANALYSIS **98031**

cis-dimethyl bis(tri-n-pyrrolyl)-phosphineplatinum(II)

CRYSTAL DATA: C26 H30 Pt1 P2 N6 from dichloromethane/pentane , light amber , irregular block , ~0.21 x 0.22 x 0.23mm, monoclinic , P21/c (No. 14), a = 9.252(1)Å, b = 15.607(4)Å, c = 18.638(3)Å, beta = 95.04(1)°, T = -75°C, Vol = 2680.9Å3, Z = 4, Formula weight = 683.61, Density = 1.694g/cc, μ(Mo) = 54.31cm-1

DATA COLLECTION: Enraf-Nonius CAD4 diffractometer, MoKalpha radiation , data collected = 6563, 2-theta range = 2.2° - 55.0°, maximum hkl = 12 20 24, data octants = +++, -++, W scan method, scan width = 1.20°- 2.40°W, scan speed = 1.70- 5.00°/min, typical half-height peak width = 0.19°W, 2 standards collected 32 times, 8.0% fluctuation, 127 duplicates, 1.5% R-merge, 13.5% variation in azimuthal scan, corrected for absorption (azimuthal), range of transmission factors = 0.24- 0.26, 3940 unique reflections with I> 3.0sig(I), Unit cell refined from 25 reflections with 2-theta range=22.04-27.12

SOLUTION AND REFINEMENT: Structure solved by direct methods (MULTAN), refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, including anomalous terms for Pt, P , biweight ~ [sigma 2(I)+0.0009I 2]-1/2, refined 35 of 65 atoms, 35 atoms refined anisotropic, 316 parameters, data/parameter ratio = 12.00, final R1 = 0.036, Rw = 0.033, error of fit = 1.07, max shift/error = 0.00, largest residual density = 1.79e/Å3, near PT1 , Because the refinement for a few of the methyl hydrogens gave unrealistic C-H bond distances(0.70A), all of the hydrogens have been idealized close to their previously refined positions.

RESULTS: This study determines the structure of cis-dimethyl bis(tri-n-pyrrolyl)-phosphineplatinum(II) for hydrocyantion and carbonylation catalysis research. The asymmetric unit contains one molecule as shown in figure 1 with thermal ellipsoids drawn to the 50% probability level. The structure is cis rather than the predicted trans structure.

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TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
Pt(1)	1679.6(3)	1507.7(2)	5091.2(1)	1.7(0)'
P(1)	2005(2)	1464(1)	3910(1)	1.8(0)'
P(2)	924(2)	2877(1)	5129(1)	1.8(0)'
N(11)	2730(6)	580(4)	3537(3)	2.0(1)'
N(21)	3159(6)	2223(3)	3661(3)	2.1(1)'
N(31)	474(5)	1543(4)	3347(3)	2.2(1)'
N(41)	1854(5)	3473(4)	5782(2)	2.1(1)'
N(51)	-837(6)	2974(3)	5275(3)	2.0(1)'
N(61)	952(6)	3590(4)	4435(3)	2.1(1)'
C(1)	2298(9)	225(5)	5189(4)	3.4(2)'
C(2)	1480(8)	1407(6)	6214(3)	3.3(2)'
C(12)	4174(8)	392(5)	3566(4)	3.5(2)'
C(13)	4325(9)	-449(6)	3353(5)	4.3(2)'
C(14)	2905(9)	-779(4)	3204(4)	3.2(2)'
C(15)	1968(8)	-156(5)	3329(4)	2.7(2)'
C(22)	4323(7)	2459(5)	4134(4)	2.6(2)'
C(23)	5300(8)	2899(5)	3768(4)	3.4(2)'
C(24)	4735(9)	2922(6)	3046(4)	3.8(2)'
C(25)	3438(8)	2515(5)	2991(4)	3.0(2)'
C(32)	-917(7)	1537(5)	3585(4)	2.8(2)'
C(33)	-1872(7)	1542(6)	3000(4)	3.5(2)'
C(34)	-1094(8)	1515(6)	2383(4)	3.6(2)'
C(35)	304(7)	1514(6)	2596(3)	3.1(2)'
C(42)	3243(7)	3262(5)	6064(4)	2.9(2)'
C(43)	3776(8)	3936(6)	6467(4)	3.6(2)'
C(44)	2725(8)	4597(5)	6430(4)	3.1(2)'
C(45)	1553(8)	4304(5)	6010(4)	2.8(2)'
C(52)	-1703(8)	3695(4)	5247(4)	2.5(2)'
C(53)	-3035(7)	3495(6)	5450(4)	3.1(2)'
C(54)	-3007(7)	2616(5)	5613(4)	2.7(2)'
C(55)	-1678(7)	2297(5)	5511(3)	2.4(2)'
C(62)	28(8)	3562(5)	3794(4)	3.0(2)'
C(63)	643(10)	4053(5)	3300(4)	3.6(2)'
C(64)	1963(10)	4369(5)	3613(4)	3.8(2)'
C(65)	2141(8)	4084(4)	4294(4)	2.7(2)'
H(1)	2511	90	5679	4.3
H(1')	3147	142	4937	4.3
H(1")	1540	-124	4981	4.3
H(2)	1066	1926	6379	4.1
H(2')	2420	1336	6461	4.1
H(2")	884	941	6307	4.1
H(12)	4953	770	3709	4.4
H(13)	5206	-759	3325	5.3
H(14)	2688	-1344	3040	4.3
H(15)	943	-212	3288	3.8
H(22)	4421	2334	4634	3.7
H(23)	6186	3139	3959	4.6
H(24)	5181	3197	2664	4.9
H(25)	2816	2446	2566	4.1
H(32)	-1128	1527	4077	3.9
H(33)	-2907	1560	2991	4.5
H(34)	-1524	1516	1899	4.6

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters (

H(35)	1083	1498	2297	4.2
H(42)	3731	2739	5990	3.8
H(43)	4701	3971	6733	4.6
H(44)	2844	5144	6654	4.1
H(45)	673	4614	5886	3.8
H(52)	-1418	4239	5097	3.5
H(53)	-3833	3867	5487	4.1
H(54)	-3790	2302	5773	3.8
H(55)	-1350	1718	5587	3.3
H(62)	-862	3252	3724	4.1
H(63)	259	4167	2820	4.5
H(64)	2612	4713	3380	4.9
H(65)	2948	4195	4635	3.7

TABLE II. Anisotropic Thermal Parameters (Å² X 1000)

exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
Pt(1)	23.1(1)	25.2(1)	16.5(1)	3.4(2)	2.9(1)	2.3(2)
P(1)	25.0(8)	25.8(8)	17.2(7)	2.8(9)	3.7(6)	-1.6(8)
P(2)	24(1)	26(1)	19(1)	3(1)	5(1)	1(1)
N(11)	24(3)	26(3)	27(3)	5(2)	4(2)	-5(2)
N(21)	30(3)	28(3)	23(3)	6(3)	6(2)	3(2)
N(31)	24(3)	36(3)	22(2)	4(3)	5(2)	-3(3)
N(41)	28(3)	34(3)	19(2)	-3(3)	4(2)	-4(3)
N(51)	26(3)	26(3)	25(3)	1(2)	3(2)	-3(2)
N(61)	31(3)	28(3)	21(2)	5(3)	6(2)	4(3)
C(1)	57(5)	35(4)	36(4)	6(4)	-1(4)	6(3)
C(2)	45(4)	69(6)	12(3)	4(4)	9(3)	14(4)
C(12)	26(4)	47(5)	59(5)	2(4)	3(4)	-19(4)
C(13)	55(5)	48(5)	59(5)	26(5)	2(4)	-12(5)
C(14)	59(5)	27(4)	35(4)	8(4)	8(4)	-4(3)
C(15)	42(4)	33(4)	28(4)	-4(3)	7(3)	-6(3)
C(22)	27(4)	45(4)	27(4)	-4(3)	5(3)	-5(3)
C(23)	31(4)	59(5)	43(4)	-14(4)	13(3)	-5(4)
C(24)	50(5)	64(6)	34(4)	-7(4)	16(4)	12(4)
C(25)	42(4)	52(5)	21(3)	-8(4)	1(3)	13(3)
C(32)	32(4)	40(4)	35(4)	-2(4)	1(3)	-5(4)
C(33)	23(3)	59(5)	50(4)	-4(4)	-3(3)	-3(5)
C(34)	43(4)	55(5)	35(4)	5(5)	-11(3)	5(4)
C(35)	41(4)	53(5)	24(3)	0(4)	6(3)	0(4)
C(42)	28(4)	57(6)	25(3)	0(3)	2(3)	-2(3)
C(43)	32(4)	74(6)	30(4)	-19(4)	-1(3)	-3(4)
C(44)	45(4)	49(5)	25(4)	-17(4)	13(3)	-11(3)
C(45)	50(5)	36(4)	23(4)	5(4)	9(3)	-4(3)
C(52)	38(4)	24(4)	34(4)	4(3)	5(3)	2(3)
C(53)	31(4)	51(5)	37(4)	12(4)	2(3)	-2(4)
C(54)	24(4)	47(5)	33(4)	-3(3)	0(3)	1(3)
C(55)	32(4)	39(4)	19(3)	-5(3)	-1(3)	3(3)
C(62)	45(4)	38(4)	30(3)	12(4)	-5(3)	2(4)
C(63)	77(6)	40(5)	20(4)	23(4)	8(4)	7(3)
C(64)	73(6)	42(5)	35(4)	15(5)	24(4)	13(4)

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C(65)	41(4)	26(4)	35(4)	1(3)	9(3)	-1(3)

TABLE III. Interatomic Distances (A)

Pt(1)-P(1)	2.249 (1)	C(53)-C(54)	1.406 (10)
Pt(1)-P(2)	2.252 (2)	C(54)-C(55)	1.355 (9)
Pt(1)-C(1)	2.086 (7)	C(62)-C(63)	1.361 (10)
Pt(1)-C(2)	2.123 (6)	C(63)-C(64)	1.396 (11)
P(1)-N(11)	1.710 (5)	C(64)-C(65)	1.341 (10)
P(1)-N(21)	1.686 (6)	C(1)-H(1)	0.941 (0)
P(1)-N(31)	1.691 (5)	C(1)-H(1')	0.958 (0)
P(2)-N(41)	1.703 (5)	C(1)-H(1")	0.944 (0)
P(2)-N(51)	1.681 (5)	C(2)-H(2)	0.958 (0)
P(2)-N(61)	1.708 (5)	C(2)-H(2')	0.953 (0)
N(11)-C(12)	1.364 (8)	C(2)-H(2")	0.938 (0)
N(11)-C(15)	1.385 (8)	C(12)-H(12)	0.951 (0)
N(21)-C(22)	1.379 (8)	C(13)-H(13)	0.954 (0)
N(21)-C(25)	1.375 (8)	C(14)-H(14)	0.949 (0)
N(31)-C(32)	1.397 (8)	C(15)-H(15)	0.948 (0)
N(31)-C(35)	1.396 (7)	C(22)-H(22)	0.949 (0)
N(41)-C(42)	1.385 (8)	C(23)-H(23)	0.942 (0)
N(41)-C(45)	1.399 (8)	C(24)-H(24)	0.956 (0)
N(51)-C(52)	1.380 (8)	C(25)-H(25)	0.944 (0)
N(51)-C(55)	1.406 (8)	C(32)-H(32)	0.954 (0)
N(61)-C(62)	1.408 (8)	C(33)-H(33)	0.956 (0)
N(61)-C(65)	1.389 (8)	C(34)-H(34)	0.954 (0)
C(12)-C(13)	1.382 (11)	C(35)-H(35)	0.949 (0)
C(13)-C(14)	1.415 (11)	C(42)-H(42)	0.949 (0)
C(14)-C(15)	1.337 (9)	C(43)-H(43)	0.953 (0)
C(22)-C(23)	1.364 (9)	C(44)-H(44)	0.951 (0)
C(23)-C(24)	1.401 (10)	C(45)-H(45)	0.958 (0)
C(24)-C(25)	1.354 (10)	C(52)-H(52)	0.939 (0)
C(32)-C(33)	1.342 (9)	C(53)-H(53)	0.946 (0)
C(33)-C(34)	1.411 (10)	C(54)-H(54)	0.944 (0)
C(34)-C(35)	1.319 (9)	C(55)-H(55)	0.960 (0)
C(42)-C(43)	1.359 (10)	C(62)-H(62)	0.954 (0)
C(43)-C(44)	1.416 (11)	C(63)-H(63)	0.951 (0)
C(44)-C(45)	1.361 (9)	C(64)-H(64)	0.940 (0)
C(52)-C(53)	1.357 (9)	C(65)-H(65)	0.953 (0)

TABLE IV. Intramolecular Angles (Deg)

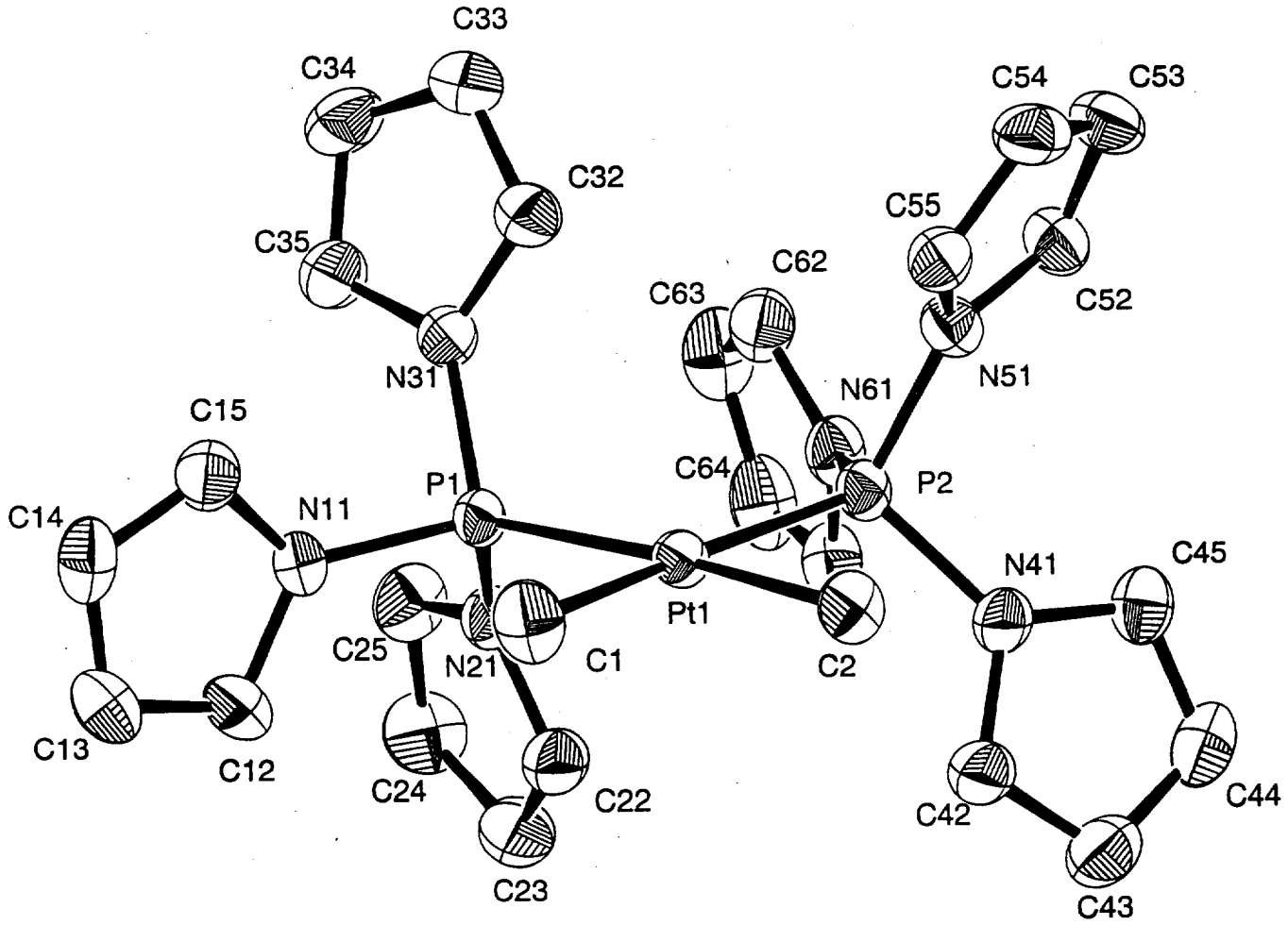
P(1)-Pt(1)-P(2)	97.36 (7)	N(51)-P(2)-N(61)	98.2 (3)
P(1)-Pt(1)-C(1)	89.8 (2)	P(1)-N(11)-C(12)	125.1 (5)
P(1)-Pt(1)-C(2)	173.5 (2)	P(1)-N(11)-C(15)	125.1 (5)
P(2)-Pt(1)-C(1)	172.7 (2)	P(1)-N(21)-C(22)	119.3 (5)
P(2)-Pt(1)-C(2)	89.1 (2)	P(1)-N(21)-C(25)	131.0 (5)
C(1)-Pt(1)-C(2)	83.7 (3)	P(1)-N(31)-C(32)	123.2 (4)
Pt(1)-P(1)-N(11)	120.9 (2)	P(1)-N(31)-C(35)	129.3 (4)
Pt(1)-P(1)-N(21)	113.0 (2)	P(2)-N(41)-C(42)	122.3 (5)
Pt(1)-P(1)-N(31)	115.3 (2)	P(2)-N(41)-C(45)	128.4 (5)
Pt(1)-P(2)-N(41)	113.7 (2)	P(2)-N(51)-C(52)	129.4 (5)
Pt(1)-P(2)-N(51)	113.5 (2)	P(2)-N(51)-C(55)	123.6 (5)
Pt(1)-P(2)-N(61)	124.7 (2)	P(2)-N(61)-C(62)	125.1 (5)
N(11)-P(1)-N(21)	100.0 (3)	P(2)-N(61)-C(65)	124.8 (5)
N(11)-P(1)-N(31)	98.3 (3)	C(12)-N(11)-C(15)	107.9 (6)

N(21)-P(1)-N(31)	107.2 (3)	C(22)-N(21)-C(25)	107.0 (6)
N(41)-P(2)-N(51)	105.7 (3)	C(32)-N(31)-C(35)	107.0 (5)
N(41)-P(2)-N(61)	98.3 (3)	C(42)-N(41)-C(45)	107.9 (6)
C(52)-N(51)-C(55)	106.8 (5)	C(63)-C(64)-C(65)	107.9 (7)
C(62)-N(61)-C(65)	106.7 (5)	C(13)-C(12)-H(12)	125 (0)
Pt(1)-C(1)-H(1)	109 (0)	C(12)-C(13)-H(13)	127 (0)
Pt(1)-C(1)-H(1')	108 (0)	C(14)-C(13)-H(13)	126 (0)
Pt(1)-C(1)-H(1")	109 (0)	C(13)-C(14)-H(14)	125 (0)
Pt(1)-C(2)-H(2)	109 (0)	C(15)-C(14)-H(14)	128 (0)
Pt(1)-C(2)-H(2')	109 (0)	C(14)-C(15)-H(15)	125 (0)
Pt(1)-C(2)-H(2")	110 (0)	C(23)-C(22)-H(22)	126 (0)
N(11)-C(12)-C(13)	108.4 (7)	C(22)-C(23)-H(23)	127 (0)
N(11)-C(15)-C(14)	109.2 (6)	C(24)-C(23)-H(23)	126 (0)
N(21)-C(22)-C(23)	109.3 (6)	C(23)-C(24)-H(24)	125 (0)
N(21)-C(25)-C(24)	108.8 (6)	C(25)-C(24)-H(24)	126 (0)
N(31)-C(32)-C(33)	107.6 (6)	C(24)-C(25)-H(25)	126 (0)
N(31)-C(35)-C(34)	108.9 (6)	C(33)-C(32)-H(32)	127 (0)
N(41)-C(42)-C(43)	107.8 (7)	C(32)-C(33)-H(33)	127 (0)
N(41)-C(45)-C(44)	108.5 (6)	C(34)-C(33)-H(33)	125 (0)
N(51)-C(52)-C(53)	109.9 (6)	C(33)-C(34)-H(34)	125 (0)
N(51)-C(55)-C(54)	107.6 (6)	C(35)-C(34)-H(34)	127 (0)
N(61)-C(62)-C(63)	107.3 (7)	C(34)-C(35)-H(35)	127 (0)
N(61)-C(65)-C(64)	109.3 (7)	C(43)-C(42)-H(42)	126 (0)
N(11)-C(12)-H(12)	126 (0)	C(42)-C(43)-H(43)	127 (0)
N(11)-C(15)-H(15)	125 (0)	C(44)-C(43)-H(43)	124 (0)
N(21)-C(22)-H(22)	125 (0)	C(43)-C(44)-H(44)	125 (0)
N(21)-C(25)-H(25)	125 (0)	C(45)-C(44)-H(44)	128 (0)
N(31)-C(32)-H(32)	125 (0)	C(44)-C(45)-H(45)	126 (0)
N(31)-C(35)-H(35)	124 (0)	C(53)-C(52)-H(52)	125 (0)
N(41)-C(42)-H(42)	126 (0)	C(52)-C(53)-H(53)	128 (0)
N(41)-C(45)-H(45)	126 (0)	C(54)-C(53)-H(53)	126 (0)
N(51)-C(52)-H(52)	125 (0)	C(53)-C(54)-H(54)	125 (0)
N(51)-C(55)-H(55)	125 (0)	C(55)-C(54)-H(54)	126 (0)
N(61)-C(62)-H(62)	126 (0)	C(54)-C(55)-H(55)	127 (0)
N(61)-C(65)-H(65)	124 (0)	C(63)-C(62)-H(62)	127 (0)
C(12)-C(13)-C(14)	106.7 (7)	C(62)-C(63)-H(63)	127 (0)
C(13)-C(14)-C(15)	107.8 (7)	C(64)-C(63)-H(63)	125 (0)
C(22)-C(23)-C(24)	106.6 (6)	C(63)-C(64)-H(64)	126 (0)
C(23)-C(24)-C(25)	108.3 (6)	C(65)-C(64)-H(64)	127 (0)
C(32)-C(33)-C(34)	108.4 (6)	C(64)-C(65)-H(65)	127 (0)
C(33)-C(34)-C(35)	108.1 (6)	H(1)-C(1)-H(1')	110 (0)
C(42)-C(43)-C(44)	108.8 (6)	H(1)-C(1)-H(1")	111 (0)
C(43)-C(44)-C(45)	107.0 (7)	H(1')-C(1)-H(1")	109 (0)
C(52)-C(53)-C(54)	106.6 (6)	H(2)-C(2)-H(2')	109 (0)
C(53)-C(54)-C(55)	109.1 (6)	H(2)-C(2)-H(2")	110 (0)
C(62)-C(63)-C(64)	108.6 (6)	H(2')-C(2)-H(2")	110 (0)

TABLE V. Intramolecular Non-Bonding Distances (A)

P(1)...C(62)	3.747 (8)	C(12)...C(22)	3.393 (11)
P(2)...C(22)	3.846 (7)	C(12)...C(25)	3.530 (11)
P(2)...C(32)	3.834 (7)	C(15)...C(35)	3.264 (11)
N(21)...N(61)	3.365 (7)	C(22)...C(65)	3.272 (10)
N(31)...N(61)	3.789 (8)	C(23)...C(65)	3.664 (10)
N(21)...C(62)	3.598 (9)	C(24)...C(64)	3.642 (11)
N(21)...C(63)	3.709 (9)	C(25)...C(35)	3.319 (10)
N(21)...C(64)	3.527 (10)	C(25)...C(63)	3.611 (11)
N(21)...C(65)	3.304 (9)	C(25)...C(64)	3.443 (11)

N(31)...C(62)	3.294 (10)	C(25)...C(65)	3.720 (10)
N(61)...C(22)	3.670 (8)	C(32)...C(62)	3.293 (11)
C(1)...C(12)	3.628 (11)	C(42)...C(65)	3.604 (10)
C(1)...C(15)	3.504 (10)	C(45)...C(52)	3.353 (10)
C(2)...C(42)	3.346 (11)	C(45)...C(65)	3.309 (9)
C(2)...C(55)	3:393 (10)	C(52)...C(62)	3.272 (10)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C34
C32
C35
N31
C15
C14
N11
P1
C25
N21
C1
Pt1
C2
C13
C12
C24
C22
C23
C54
C53
C55
C52
C62
C63
N61
N51
C64
P2
N41
C45
C42
C44
C43

C65

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Central Research & Development Dept.
Experimental Station , 27-MAY-1998

$Pt(PCy_3)_2Me_2$ (**3p**)

TO: K. Moloy, CRD, E328/215a, x52083
NOTEBOOK REF: E91930-67

FROM: W. Marshall, CRD/CCAS, E228/326, (302)695-2128
EMAIL: Will.Marshall@usa.dupont.com marshawj@esvax

X-RAY CRYSTAL STRUCTURE ANALYSIS 98101

cis-dimethylbis(tricyclohexylphosphine)platinum(II)

CRYSTAL DATA: C39 H74 Pt1 Cl2 P2 from dichloromethane , colorless , irregular block , ~0.12 x 0.20 x 0.21mm, orthorhombic , Pbca (No. 61), a = 17.702(1)Å, b = 18.102(1)Å, c = 25.137(1)Å, T = -100°C, Vol = 8054.9Å3, Z = 8, Formula weight = 870.97, Density = 1.436g/cc, μ(Mo) = 37.56cm-1

DATA COLLECTION: Rigaku RU300, R-AXIS image plate area detector, MoKalpha radiation ,filament size = 12.0 x 2.0mm, anode power = 55kV x 240mA, crystal to plate distance = 85.0mm, 105μ pixel raster, number of frames = 90, oscillation range = 4.0%deg;, exposure time = 8.0 min/frame, box sum integration, data collected = 83404, 2-theta range = 3.6° - 55.0°, maximum hkl = 22 23 28, no absorption correction, 8153 duplicates, 2.5% R-merge, 5589 unique reflections with I> 3.0sig(I),

SOLUTION AND REFINEMENT: Structure solved by direct methods using teXsan(SIR-92), refined using Z program suite(Calabrese), refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, including anomalous terms for Pt, Cl, P , biweight ~ [sigma 2(I)+0.0009I 2]-1/2, refined 50 of 102 atoms, 50 atoms refined anisotropic, 451 parameters, data/parameter ratio = 12.37, final R1 = 0.039, Rw = 0.041, error of fit = 1.81, max shift/error = 0.04, largest residual density = 1.44e/Å3, near PT1 , Because the refinement for a few of the methyl hydrogens gave thermal parameters larger than desired(22.2), all of the hydrogens have been idealized close to their previously refined positions.

RESULTS: This study determines the structure of cis-dimethylbis(tricyclohexylphosphine) platinum(II) for hydrocyanation, carbonylation catalysis reearch. The asymmetric unit contains one molecule and one dichloromethane solvent molecule as shown in figure 1 with thermal ellipsoids drawn to the 50% probability level. Two of the cyclohexyl groups are badly disordered and no hydrogens are affixed to them.

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
Pt(1)	3337.4(1)	978.1(1)	4535.1(1)	2.1(0)'
Cl(71)	962(2)	-205(2)	2178(1)	9.4(1)'
Cl(72)	1554(3)	1039(3)	1559(2)	12.8(2)'
P(1)	2343(1)	1294(1)	5108(1)	2.2(0)'
P(2)	3056(1)	1416(1)	3686(1)	2.1(0)'
C(1)	3809(4)	416(4)	5202(3)	3.3(2)'
C(2)	4368(3)	585(4)	4206(3)	3.0(2)'
C(11)	1732(5)	489(4)	5270(3)	4.5(2)'
C(12')	2114(11)	-112(9)	5624(7)	5.8(5)'
C(12")	1401(8)	379(8)	5786(5)	3.5(3)'
C(13')	1471(12)	-672(9)	5828(6)	5.2(5)'
C(13")	772(16)	-193(14)	5804(9)	9.4(9)'
C(14)	1009(8)	-944(6)	5443(6)	9.9(5)'
C(15')	782(10)	-453(10)	4978(7)	5.1(5)'
C(15")	1309(8)	-795(6)	4963(5)	2.8(3)'
C(16')	1351(7)	137(7)	4816(4)	2.6(3)'
C(16")	1980(10)	-201(8)	4995(8)	5.1(5)'
C(21)	2734(3)	1595(3)	5763(2)	2.5(1)'
C(22)	2206(4)	1925(4)	6186(2)	3.3(2)'
C(23)	2621(4)	1985(4)	6717(3)	4.0(2)'
C(24)	3334(5)	2448(4)	6670(3)	4.5(2)'
C(25)	3850(4)	2162(4)	6234(3)	4.1(2)'
C(26)	3421(4)	2104(4)	5704(3)	3.5(2)'
C(31)	1624(3)	2005(3)	4902(2)	2.7(1)'
C(32)	875(3)	2066(4)	5205(3)	3.6(2)'
C(33)	363(4)	2623(5)	4933(3)	4.1(2)'
C(34)	731(4)	3365(5)	4874(3)	4.4(2)'
C(35)	1476(4)	3321(4)	4578(3)	4.1(2)'
C(36)	1997(4)	2751(3)	4853(2)	3.0(2)'
C(41)	3266(4)	702(4)	3162(3)	3.8(2)'
C(42)	3065(4)	-86(3)	3338(3)	3.4(2)'
C(43')	2999(11)	-652(9)	2851(7)	4.7(5)'
C(43")	3497(12)	-648(8)	3032(8)	5.0(5)'
C(44)	3587(6)	-536(5)	2454(4)	7.1(3)'
C(45)	3760(5)	256(5)	2288(3)	5.2(2)'
C(46')	3246(10)	888(8)	2615(5)	4.3(4)'
C(46")	3848(8)	746(8)	2750(5)	3.3(3)'
C(51)	3596(3)	2247(3)	3454(2)	2.3(1)'
C(52)	4457(3)	2169(3)	3486(3)	3.1(2)'
C(53)	4846(4)	2863(4)	3256(3)	3.5(2)'
C(54)	4594(4)	3556(4)	3532(3)	3.8(2)'
C(55)	3730(4)	3633(4)	3528(3)	3.5(2)'
C(56)	3360(3)	2943(3)	3755(2)	2.8(1)'
C(61)	2061(3)	1693(3)	3521(2)	2.2(1)'
C(62)	1927(3)	2108(4)	2998(2)	3.0(2)'
C(63)	1103(4)	2353(4)	2954(3)	4.2(2)'
C(64)	565(4)	1704(4)	2999(3)	4.1(2)'
C(65)	700(4)	1280(4)	3504(3)	3.9(2)'
C(66)	1526(3)	1045(3)	3554(3)	3.2(2)'

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters (

H(1")	4037	757	5437	4.4
H(2)	4513	896	3917	4.1
H(2')	4297	96	4077	4.1
H(2")	4749	590	4469	4.1
H(21)	2922	1148	5910	3.5
H(22)	1775	1616	6227	4.3
H(22')	2045	2402	6077	4.3
H(23)	2744	1504	6840	5.0
H(23')	2293	2199	6974	5.0
H(24)	3600	2438	6999	5.5
H(24')	3206	2946	6599	5.5
H(25)	4037	1691	6329	5.1
H(25')	4266	2489	6194	5.1
H(26)	3257	2585	5599	4.5
H(26')	3750	1919	5439	4.5
H(31)	1496	1857	4551	3.7
H(32)	970	2221	5560	4.6
H(32')	633	1597	5213	4.6
H(33)	-92	2674	5135	5.1
H(33')	218	2441	4594	5.1
H(34)	809	3576	5214	5.4
H(34')	398	3688	4690	5.4
H(35)	1713	3793	4581	5.1
H(35')	1389	3174	4221	5.1
H(36)	2453	2705	4656	4.0
H(36')	2131	2927	5197	4.0
H(51)	3459	2305	3090	3.3
H(52)	4613	1745	3291	4.1
H(52')	4604	2106	3848	4.1
H(53)	4739	2900	2887	4.5
H(53')	5380	2813	3289	4.5
H(54)	4816	3972	3362	4.8
H(54')	4772	3551	3889	4.8
H(55)	3562	3707	3174	4.5
H(55')	3589	4051	3734	4.5
H(56)	3493	2894	4120	3.8
H(56')	2826	2996	3741	3.8
H(61)	1929	2023	3800	3.3
H(62)	2047	1794	2706	4.0
H(62')	2248	2529	2982	4.0
H(63)	1026	2596	2623	5.2
H(63')	997	2702	3227	5.2
H(64)	632	1386	2703	5.1
H(64')	60	1879	2993	5.1
H(65)	387	851	3508	4.9
H(65')	564	1575	3802	4.9
H(66)	1600	795	3881	4.2
H(66')	1644	702	3281	4.2
H(72)	518	367	1451	8.7
H(72')	1187	-72	1306	8.7

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C(72)	1021(6)	264(7)	1582(4)	7.8(4)'
H(1)	4168	62	5087	4.4
H(1')	3411	160	5390	4.4

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters (

H(1")	4037	757	5437	4.4
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H(2')	4297	96	4077	4.1
H(2")	4749	590	4469	4.1
H(21)	2922	1148	5910	3.5
H(22)	1775	1616	6227	4.3
H(22')	2045	2402	6077	4.3
H(23)	2744	1504	6840	5.0
H(23')	2293	2199	6974	5.0
H(24)	3600	2438	6999	5.5
H(24')	3206	2946	6599	5.5
H(25)	4037	1691	6329	5.1
H(25')	4266	2489	6194	5.1
H(26)	3257	2585	5599	4.5
H(26')	3750	1919	5439	4.5
H(31)	1496	1857	4551	3.7
H(32)	970	2221	5560	4.6
H(32')	633	1597	5213	4.6
H(33)	-92	2674	5135	5.1
H(33')	218	2441	4594	5.1
H(34)	809	3576	5214	5.4
H(34')	398	3688	4690	5.4
H(35)	1713	3793	4581	5.1
H(35')	1389	3174	4221	5.1
H(36)	2453	2705	4656	4.0
H(36')	2131	2927	5197	4.0
H(51)	3459	2305	3090	3.3
H(52)	4613	1745	3291	4.1
H(52')	4604	2106	3848	4.1
H(53)	4739	2900	2887	4.5
H(53')	5380	2813	3289	4.5
H(54)	4816	3972	3362	4.8
H(54')	4772	3551	3889	4.8
H(55)	3562	3707	3174	4.5
H(55')	3589	4051	3734	4.5
H(56)	3493	2894	4120	3.8
H(56')	2826	2996	3741	3.8
H(61)	1929	2023	3800	3.3
H(62)	2047	1794	2706	4.0
H(62')	2248	2529	2982	4.0
H(63)	1026	2596	2623	5.2
H(63')	997	2702	3227	5.2
H(64)	632	1386	2703	5.1
H(64')	60	1879	2993	5.1
H(65)	387	851	3508	4.9
H(65')	564	1575	3802	4.9
H(66)	1600	795	3881	4.2
H(66')	1644	702	3281	4.2
H(72)	518	367	1451	8.7
H(72')	1187	-72	1306	8.7

TABLE II. Anisotropic Thermal Parameters (Å2 X 1000)
exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
Pt(1)	23.6(1)	27.6(1)	28.2(1)	0.3(1)	-0.9(1)	2.2(1)
Cl(71)	151(3)	111(2)	93(2)	21(2)	-13(2)	-9(2)
Cl(72)	203(5)	190(4)	94(3)	-87(4)	-13(2)	-8(2)
P(1)	25(1)	33(1)	27(1)	-4(1)	1(1)	-1(1)
P(2)	28(1)	26(1)	25(1)	1(1)	1(1)	2(1)
C(1)	42(4)	50(4)	33(3)	13(3)	-10(3)	15(3)
C(2)	18(3)	46(4)	48(4)	13(2)	7(2)	-5(3)
C(11)	67(5)	52(4)	53(4)	-33(4)	18(4)	-10(3)
C(12')	89(13)	49(9)	80(13)	-16(9)	-38(10)	17(8)
C(12")	56(8)	54(8)	23(7)	-39(7)	11(5)	-17(5)
C(13')	110(15)	42(8)	46(9)	-34(9)	-39(9)	14(7)
C(13")	162(24)	105(18)	90(15)	-98(18)	67(16)	-53(14)
C(14)	143(11)	73(7)	160(13)	-56(8)	-36(10)	56(8)
C(15')	54(10)	65(11)	75(12)	-35(9)	-20(8)	20(9)
C(15")	39(7)	16(6)	49(8)	-1(5)	8(6)	-9(5)
C(16')	40(6)	45(7)	14(6)	-33(6)	-7(4)	3(5)
C(16")	74(11)	29(8)	92(13)	-9(7)	20(10)	-26(8)
C(21)	32(3)	33(3)	32(3)	-5(2)	-4(2)	2(2)
C(22)	51(4)	46(4)	28(3)	-5(3)	1(3)	-7(3)
C(23)	55(4)	63(5)	35(4)	-8(4)	0(3)	-11(3)
C(24)	73(5)	59(4)	39(4)	-23(4)	-13(4)	-5(3)
C(25)	51(4)	65(5)	41(4)	-23(4)	-5(3)	-2(3)
C(26)	41(4)	58(4)	35(3)	-21(3)	-2(3)	-3(3)
C(31)	26(3)	47(3)	28(3)	1(3)	2(2)	2(2)
C(32)	31(3)	62(4)	42(4)	0(3)	6(3)	-4(3)
C(33)	27(3)	80(6)	49(4)	21(3)	2(3)	-12(4)
C(34)	50(4)	65(5)	53(5)	23(4)	2(3)	-8(4)
C(35)	51(4)	55(4)	49(4)	19(3)	1(3)	-5(3)
C(36)	38(3)	38(4)	37(4)	9(3)	4(3)	0(3)
C(41)	74(5)	29(3)	43(4)	3(3)	29(4)	-2(3)
C(42)	46(4)	28(3)	55(4)	-4(3)	2(3)	-6(3)
C(43')	68(11)	42(9)	68(12)	-10(9)	5(9)	-27(8)
C(43")	90(15)	26(7)	74(13)	2(8)	19(10)	-21(8)
C(44)	121(9)	65(6)	85(7)	-31(6)	26(6)	-38(5)
C(45)	96(6)	64(5)	37(4)	-3(5)	14(4)	-16(4)
C(46')	84(12)	49(8)	30(8)	18(8)	-2(7)	-11(6)
C(46")	41(7)	46(8)	36(7)	-6(6)	12(6)	-6(6)
C(51)	31(3)	30(3)	27(3)	-3(2)	-1(2)	2(2)
C(52)	34(3)	34(3)	48(4)	-4(3)	6(3)	-5(3)
C(53)	39(4)	46(4)	49(4)	-7(3)	8(3)	-3(3)
C(54)	42(4)	47(4)	56(4)	-13(3)	5(3)	-2(3)
C(55)	53(4)	32(3)	46(4)	-2(3)	1(3)	4(3)
C(56)	35(3)	33(3)	40(3)	-1(3)	4(3)	-3(2)
C(61)	29(3)	29(3)	27(3)	3(2)	-3(2)	1(2)
C(62)	39(3)	39(4)	37(4)	0(3)	-6(3)	5(3)
C(63)	50(4)	60(5)	48(4)	9(3)	-16(3)	4(4)
C(64)	35(4)	64(5)	57(4)	6(3)	-13(3)	-10(4)
C(65)	29(3)	58(4)	61(5)	-9(3)	-7(3)	-4(4)
C(66)	33(3)	36(3)	52(4)	-5(3)	-2(3)	1(3)
C(72)	88(7)	145(11)	63(6)	2(7)	-24(5)	-26(6)

TABLE III. Interatomic Distances (A)

Pt(1)-P(1)	2.344 (1)	C(51)-C(56)	1.527 (8)
Pt(1)-P(2)	2.330 (1)	C(52)-C(53)	1.545 (9)
Pt(1)-C(1)	2.132 (6)	C(53)-C(54)	1.502 (9)
Pt(1)-C(2)	2.126 (5)	C(54)-C(55)	1.535 (10)
Cl(71)-C(72)	1.726 (12)	C(55)-C(56)	1.523 (9)
Cl(72)-C(72)	1.691 (13)	C(61)-C(62)	1.533 (8)
P(1)-C(11)	1.859 (7)	C(61)-C(66)	1.509 (8)
P(1)-C(21)	1.868 (6)	C(62)-C(63)	1.528 (9)
P(1)-C(31)	1.884 (6)	C(63)-C(64)	1.517 (10)
P(2)-C(41)	1.882 (6)	C(64)-C(65)	1.503 (10)
P(2)-C(51)	1.875 (6)	C(65)-C(66)	1.526 (9)
P(2)-C(61)	1.878 (5)	C(1)-H(1)	0.949 (0)
C(11)-C(12')	1.559 (18)	C(1)-H(1')	0.966 (0)
C(11)-C(12")	1.438 (14)	C(1)-H(1")	0.943 (0)
C(11)-C(16')	1.472 (12)	C(2)-H(2)	0.955 (0)
C(11)-C(16")	1.492 (15)	C(2)-H(2')	0.952 (0)
C(12')-C(12")	1.596 (25)	C(2)-H(2")	0.944 (0)
C(12')-C(13')	1.608 (24)	C(21)-H(21)	0.949 (0)
C(12')-C(16")	1.605 (25)	C(22)-H(22)	0.952 (0)
C(12")-C(13")	1.522 (20)	C(22)-H(22')	0.951 (0)
C(13')-C(13")	1.512 (33)	C(23)-H(23)	0.950 (0)
C(13')-C(14)	1.358 (18)	C(23)-H(23')	0.951 (0)
C(13")-C(14)	1.688 (26)	C(24)-H(24)	0.951 (0)
C(14)-C(15')	1.523 (19)	C(24)-H(24')	0.947 (0)
C(14)-C(15")	1.346 (18)	C(25)-H(25)	0.945 (0)
C(15')-C(15")	1.120 (21)	C(25)-H(25')	0.950 (0)
C(15')-C(16')	1.523 (17)	C(26)-H(26)	0.955 (0)
C(15")-C(16')	1.728 (17)	C(26)-H(26')	0.947 (0)
C(15")-C(16")	1.605 (19)	C(31)-H(31)	0.951 (0)
C(16')-C(16")	1.348 (22)	C(32)-H(32)	0.951 (0)
C(21)-C(22)	1.538 (8)	C(32)-H(32')	0.950 (0)
C(21)-C(26)	1.532 (8)	C(33)-H(33)	0.957 (0)
C(22)-C(23)	1.525 (9)	C(33)-H(33')	0.948 (0)
C(23)-C(24)	1.521 (10)	C(34)-H(34)	0.946 (0)
C(24)-C(25)	1.518 (11)	C(34)-H(34')	0.951 (0)
C(25)-C(26)	1.539 (9)	C(35)-H(35)	0.952 (0)
C(31)-C(32)	1.532 (8)	C(35)-H(35')	0.950 (0)
C(31)-C(36)	1.508 (9)	C(36)-H(36)	0.950 (0)
C(32)-C(33)	1.518 (10)	C(36)-H(36')	0.951 (0)
C(33)-C(34)	1.500 (11)	C(51)-H(51)	0.952 (0)
C(34)-C(35)	1.517 (10)	C(52)-H(52)	0.952 (0)
C(35)-C(36)	1.546 (9)	C(52)-H(52')	0.953 (0)
C(41)-C(42)	1.535 (9)	C(53)-H(53)	0.949 (0)
C(41)-C(46')	1.417 (16)	C(53)-H(53')	0.952 (0)
C(41)-C(46")	1.464 (13)	C(54)-H(54)	0.950 (0)
C(42)-C(43')	1.600 (17)	C(54)-H(54')	0.951 (0)
C(42)-C(43")	1.486 (16)	C(55)-H(55)	0.948 (0)
C(43')-C(43")	0.993 (22)	C(55)-H(55')	0.949 (0)
C(43')-C(44)	1.457 (20)	C(56)-H(56)	0.952 (0)
C(43")-C(44)	1.475 (22)	C(56)-H(56')	0.951 (0)

C(44)-C(45)	1.524 (13)	C(61)-H(61)	0.951 (0)
C(45)-C(46')	1.678 (15)	C(62)-H(62)	0.952 (0)
C(45)-C(46")	1.469 (14)	C(62)-H(62')	0.952 (0)
C(46')-C(46")	1.147 (19)	C(63)-H(63)	0.950 (0)
C(51)-C(52)	1.532 (8)	C(63)-H(63')	0.952 (0)
C(64)-H(64)	0.947 (0)	C(66)-H(66)	0.948 (0)
C(64)-H(64')	0.949 (0)	C(66)-H(66')	0.950 (0)
C(65)-H(65)	0.955 (0)	C(72)-H(72)	0.968 (0)
C(65)-H(65')	0.951 (0)	C(72)-H(72')	0.969 (0)

TABLE IV. Intramolecular Angles (Deg)

P(1)-Pt(1)-P(2)	108.60 (5)	C(12')-C(11)-C(16')	110 (1)
P(1)-Pt(1)-C(1)	85.8 (2)	C(12')-C(11)-C(16")	63 (1)
P(1)-Pt(1)-C(2)	164.7 (2)	C(12")-C(11)-C(16')	117.0 (7)
P(2)-Pt(1)-C(1)	165.1 (2)	C(12")-C(11)-C(16")	115 (1)
P(2)-Pt(1)-C(2)	86.6 (2)	C(16')-C(11)-C(16")	54 (1)
C(1)-Pt(1)-C(2)	79.1 (2)	C(11)-C(12')-C(12")	54.2 (8)
Pt(1)-P(1)-C(11)	112.4 (3)	C(11)-C(12')-C(13')	108 (1)
Pt(1)-P(1)-C(21)	109.5 (2)	C(11)-C(12')-C(16")	56.3 (8)
Pt(1)-P(1)-C(31)	120.4 (2)	C(12")-C(12')-C(13')	73 (1)
Pt(1)-P(2)-C(41)	111.4 (2)	C(12")-C(12')-C(16")	101 (1)
Pt(1)-P(2)-C(51)	116.7 (2)	C(13')-C(12')-C(16")	98 (1)
Pt(1)-P(2)-C(61)	119.6 (2)	C(11)-C(12")-C(12')	61.6 (8)
C(11)-P(1)-C(21)	104.5 (3)	C(11)-C(12")-C(13")	115 (1)
C(11)-P(1)-C(31)	101.7 (3)	C(12')-C(12")-C(13")	102 (1)
C(21)-P(1)-C(31)	107.0 (3)	C(12')-C(13')-C(13")	102 (1)
C(41)-P(2)-C(51)	103.5 (3)	C(12')-C(13')-C(14)	115 (1)
C(41)-P(2)-C(61)	102.3 (3)	C(13")-C(13')-C(14)	72 (1)
C(51)-P(2)-C(61)	101.3 (2)	C(12")-C(13")-C(13')	78 (2)
Pt(1)-C(1)-H(1)	110 (0)	C(12")-C(13")-C(14)	111 (2)
Pt(1)-C(1)-H(1')	109 (0)	C(13')-C(13")-C(14)	50 (1)
Pt(1)-C(1)-H(1")	110 (0)	C(13')-C(14)-C(13")	58 (1)
Pt(1)-C(2)-H(2)	109 (0)	C(13')-C(14)-C(15')	120 (1)
Pt(1)-C(2)-H(2')	109 (0)	C(13')-C(14)-C(15")	109 (1)
Pt(1)-C(2)-H(2")	110 (0)	C(13")-C(14)-C(15')	83 (1)
Cl(71)-C(72)-Cl(72)	118.0 (6)	C(13")-C(14)-C(15")	115 (1)
Cl(71)-C(72)-H(72)	110 (0)	C(15')-C(14)-C(15")	45 (1)
Cl(71)-C(72)-H(72')	109 (0)	C(14)-C(15')-C(15")	59 (1)
Cl(72)-C(72)-H(72)	110 (0)	C(14)-C(15')-C(16')	116 (1)
Cl(72)-C(72)-H(72')	109 (0)	C(15")-C(15')-C(16')	80 (1)
P(1)-C(11)-C(12')	114.8 (8)	C(14)-C(15")-C(15')	76 (1)
P(1)-C(11)-C(12")	122.9 (6)	C(14)-C(15")-C(16')	114 (1)
P(1)-C(11)-C(16')	115.8 (6)	C(14)-C(15")-C(16")	112 (1)
P(1)-C(11)-C(16")	112.5 (8)	C(15')-C(15")-C(16')	60 (1)
P(1)-C(21)-C(22)	119.9 (4)	C(15')-C(15")-C(16")	104 (1)
P(1)-C(21)-C(26)	112.6 (4)	C(16')-C(15")-C(16")	47.5 (8)
P(1)-C(31)-C(32)	119.8 (4)	C(11)-C(16')-C(15')	114 (1)
P(1)-C(31)-C(36)	109.8 (4)	C(11)-C(16')-C(15")	106.0 (9)
P(2)-C(41)-C(42)	113.1 (4)	C(11)-C(16')-C(16")	63.7 (8)
P(2)-C(41)-C(46')	120.7 (7)	C(15')-C(16')-C(15")	39.7 (8)
P(2)-C(41)-C(46")	126.6 (7)	C(15')-C(16')-C(16")	98 (1)
P(2)-C(51)-C(52)	114.6 (4)	C(15")-C(16')-C(16")	61 (1)
P(2)-C(51)-C(56)	111.5 (4)	C(11)-C(16")-C(12')	60 (1)
P(2)-C(61)-C(62)	117.7 (4)	C(11)-C(16")-C(15")	112 (1)
P(2)-C(61)-C(66)	111.7 (4)	C(11)-C(16")-C(16')	62.2 (8)
P(1)-C(21)-H(21)	103 (0)	C(12')-C(16")-C(15")	103 (1)
P(1)-C(31)-H(31)	103 (0)	C(12')-C(16")-C(16')	114 (1)
P(2)-C(51)-H(51)	105 (0)	C(15")-C(16")-C(16')	71 (1)
P(2)-C(61)-H(61)	104 (0)	C(22)-C(21)-C(26)	108.4 (5)
C(12')-C(11)-C(12")	64 (1)	C(21)-C(22)-C(23)	109.9 (5)
C(22)-C(23)-C(24)	111.9 (6)	C(23)-C(24)-H(24)	109 (0)
C(23)-C(24)-C(25)	111.5 (6)	C(23)-C(24)-H(24')	110 (0)
C(24)-C(25)-C(26)	110.6 (6)	C(25)-C(24)-H(24)	109 (0)

C(66)-C(61)-H(61)	107 (0)	H(2)-C(2)-H(2")	110 (0)
C(61)-C(62)-H(62)	110 (0)	H(2')-C(2)-H(2")	110 (0)
C(61)-C(62)-H(62')	110 (0)	H(22)-C(22)-H(22')	109 (0)
C(63)-C(62)-H(62)	109 (0)	H(23)-C(23)-H(23')	107 (0)
C(63)-C(62)-H(62')	109 (0)	H(24)-C(24)-H(24')	107 (0)
C(62)-C(63)-H(63)	110 (0)	H(25)-C(25)-H(25')	109 (0)
C(62)-C(63)-H(63')	109 (0)	H(26)-C(26)-H(26')	108 (0)
C(64)-C(63)-H(63)	110 (0)	H(32)-C(32)-H(32')	109 (0)
C(64)-C(63)-H(63')	110 (0)	H(33)-C(33)-H(33')	106 (0)
C(63)-C(64)-H(64)	109 (0)	H(34)-C(34)-H(34')	106 (0)
C(63)-C(64)-H(64')	109 (0)	H(35)-C(35)-H(35')	109 (0)
C(65)-C(64)-H(64)	110 (0)	H(36)-C(36)-H(36')	107 (0)
C(65)-C(64)-H(64')	109 (0)	H(52)-C(52)-H(52')	108 (0)
C(64)-C(65)-H(65)	109 (0)	H(53)-C(53)-H(53')	107 (0)
C(64)-C(65)-H(65')	110 (0)	H(54)-C(54)-H(54')	107 (0)
C(66)-C(65)-H(65)	109 (0)	H(55)-C(55)-H(55')	108 (0)
C(66)-C(65)-H(65')	110 (0)	H(56)-C(56)-H(56')	107 (0)
C(61)-C(66)-H(66)	109 (0)	H(62)-C(62)-H(62')	108 (0)
C(61)-C(66)-H(66')	109 (0)	H(63)-C(63)-H(63')	107 (0)
C(65)-C(66)-H(66)	110 (0)	H(64)-C(64)-H(64')	108 (0)
C(65)-C(66)-H(66')	109 (0)	H(65)-C(65)-H(65')	108 (0)
H(1)-C(1)-H(1')	108 (0)	H(66)-C(66)-H(66')	106 (0)
H(1)-C(1)-H(1")	110 (0)	H(72)-C(72)-H(72')	99 (0)
H(1')-C(1)-H(1")	109 (0)		

TABLE V. Intramolecular Non-Bonding Distances (A)

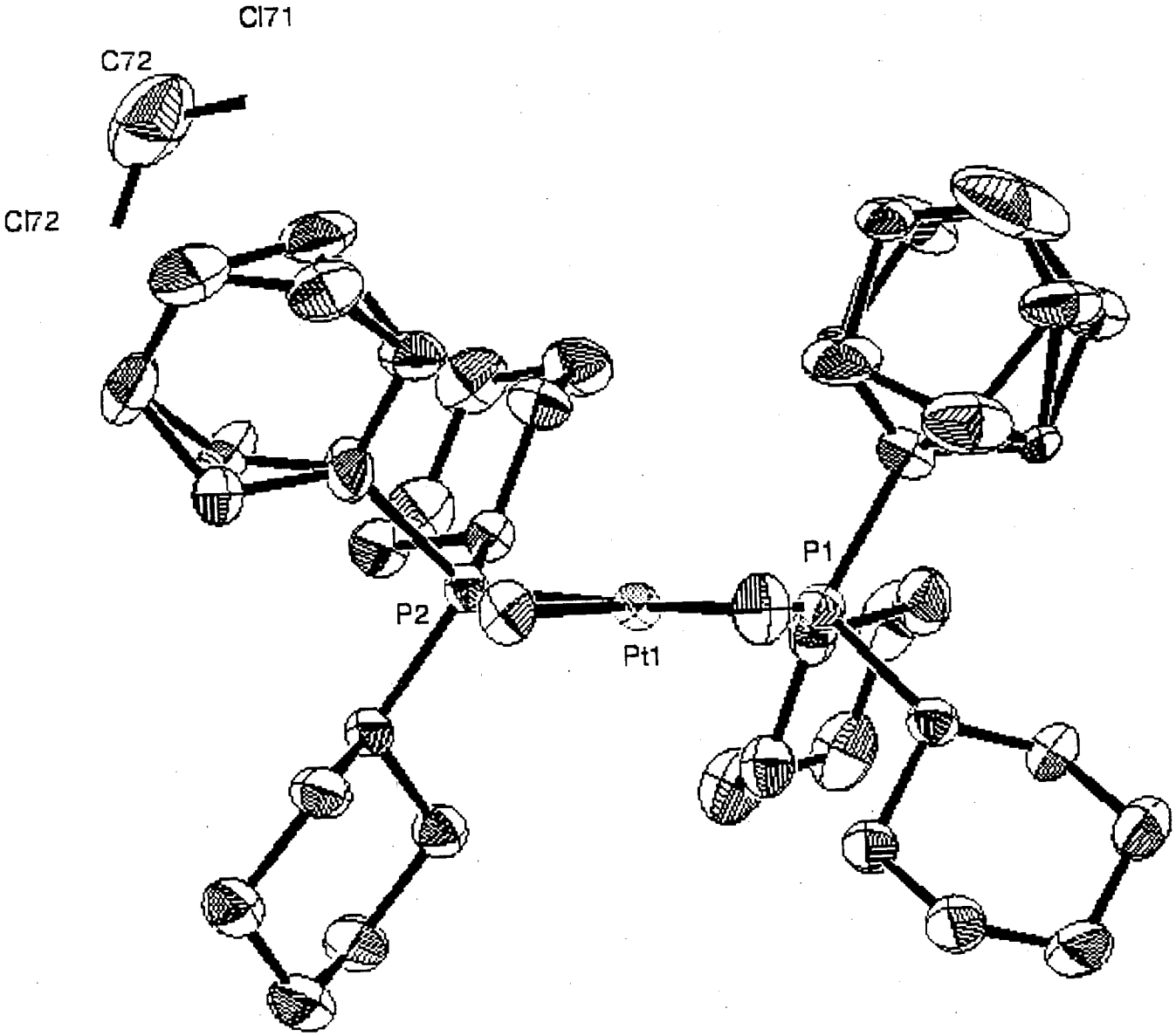
C(1)...C(12')	3.322 (21)
C(1)...C(16")	3.464 (19)
C(1)...C(26)	3.375 (10)
C(2)...C(42)	3.400 (9)
C(2)...C(52)	3.395 (9)
C(12")...C(22)	3.297 (13)
C(12")...C(32)	3.510 (18)
C(16')...C(32)	3.723 (16)
C(16')...C(66)	3.586 (13)
C(22)...C(32)	3.421 (9)
C(22)...C(36)	3.689 (9)
C(26)...C(36)	3.507 (10)
C(31)...C(61)	3.602 (8)
C(36)...C(56)	3.681 (8)
C(42)...C(66)	3.453 (9)
C(46')...C(62)	3.354 (16)
C(46")...C(52)	3.351 (14)
C(56)...C(62)	3.513 (9)

TABLE VI. Intermolecular Distances (A)

C(15')...C(15')a	3.220 (40)

Symmetry Operation Codes

a -X,-Y,1-Z


Cl71
C72
Cl72
P1
P2
Pt1