

Supporting Information for

**Cage-type Hexanuclear Platinum(0) Clusters with Diphosphine and Isocyanide
Ligands Including Two Mercury(0) Atoms**Tomoaki Tanase,^{*,a} Eri Goto,^a Hiroe Takenaka,^aTakashi Horiuchi,^b Yasuhiro Yamamoto,^b Junpei Kuwabara,^c and Kotaro Osakada^c

Department of Chemistry, Faculty of Science, Nara Women's University, Kitauoya-higashi-machi, Nara 630-8285, Japan, Department of Chemistry, Faculty of Science, Toho University, 2-2-1 Miyama, Funabashi, Chiba 274-8510, Japan, and Research Laboratory of Resources Utilization, Tokyo Institute of Technology, 4259 Nagatsuda, Midori-ku, Yokohama 226-8503, Japan

- Table S1-1.** Crystallographic and Experimental Data for **8a**·CH₃(CH₂)₄CH₃
Table S1-2. Final Positional Parameters and B_{eq} for **8a**·CH₃(CH₂)₄CH₃
Table S1-3. Final Anisotropic Thermal Parameters for **8a**·CH₃(CH₂)₄CH₃
Table S1-4. Bond Lengths for Non-hydrogen Atoms of **8a**·CH₃(CH₂)₄CH₃
Table S1-5. Bond Angles for Non-hydrogen Atoms of **8a**·CH₃(CH₂)₄CH₃
Table S2-1. Crystallographic and Experimental Data for **6a**
Table S2-2. Final Positional Parameters and B_{eq} for **6a**
Table S2-3. Final Anisotropic Thermal Parameters for **6a**
Table S2-4. Bond Lengths for Non-hydrogen Atoms of **6a**
Table S2-5. Bond Angles for Non-hydrogen Atoms of **6a**
Table S3-1. Crystallographic and Experimental Data for **11**·3.5C₆H₆
Table S3-2. Final Positional Parameters and B_{eq} for **11**·3.5C₆H₆
Table S3-3. Final Anisotropic Thermal Parameters for **11**·3.5C₆H₆
Table S3-4. Bond Lengths for Non-hydrogen Atoms of **11**·3.5C₆H₆
Table S3-5. Bond Angles for Non-hydrogen Atoms of **11**·3.5C₆H₆

Table S1-1. Crystallographic and Experimental Data for **8a**-CH₃(CH₂)₄CH₃

formula	C ₁₄₇ H ₁₅₈ N ₆ P ₆ Pt ₆ Hg ₂
formula weight	3766.47
color	dark green
size, mm	0.35 x 0.35 x 0.30
cryst. system	monoclinic
space group	P2/n (No. 13)
no. refs used for cell determination	20574 (6 < 2 < 55 °)
lattice const.	a = 16.571(2) Å b = 15.024(2) Å c = 21.980(2) Å = 90 ° = 96.519(6) ° = 90 °
Z	V = 8431(1) Å ³ 2
D _{calc.} , g cm ⁻³	1.483
F(000)	3600
μ (Mo Kα), cm ⁻¹	68.54
diffractometer	An empirical absorption correction was applied (multi-scan spherical method). Rigaku/MSM Mercury CCD (50 kV 190 mA)
radiation	Mo Kα (λ = 0.71069 Å)
monochromator	graphite
temp, °C	-120
2θ range, °	6 < 2θ < 55
detector aperture, mm	70 x 70
data images	2160
oscillation range (φ = 45, ω = 90), °	-62 -118
exposure rate, °sec ⁻¹	120
detector swing angle, °	28
detector position, mm	60.7
solution	Heavy Atom Methods (DIRDIF94 Patty)
refinement	full-matrix least-squares (Shelxl-97) All non-hydrogen atoms, except the solvent, were refined with anisotropic temperature factors.
hydrogen atoms	All H atoms were calcd with C-H = 0.95 Å, and were not refined.
function minimized	w(F _o ² - F _c ²) ²
weighting scheme	w = 1/[σ ² (F _o) + (0.1178P) ² + 111.2125P] P = (F _o ² + 2F _c ²)/3
anomalous dispersion	all non-hydrogen atoms
no. unique reflections	19860
R _{int}	0.069
no. obsd. unique reflections	12879 (I > 2σ(I))
no. variables	739
data / param ratio	17.43
R ^a	0.079
wR ² ^b	0.243
GOF ^c	1.03
ρ _{max.} , eÅ ⁻³	2.61, -2.34

^a $R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$. ^b $wR2 = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right]^{1/2}$ for all data ($w = 1/[\sigma^2(F_o) + (0.0601P)^2 + 0.0205P]$). ^c $GOF = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{(N_o - N_p)} \right]^{1/2}$ ($N_o =$ no. data, $N_p =$ no. variables).

Table S1-2. Final Positional Parameters and B_{eq} for **8a**-CH₃(CH₂)₄CH₃^{a,b,c}

atom	x	y	z	B_{eq}
Hg(1)	-0.29914(1)	-0.28596(1)	-0.2870	1.889(3)
Pt(1)	-0.35024(1)	-0.19864(1)	-0.3631	1.635(3)
Pt(2)	-0.34737(1)	-0.37620(1)	-0.3630	1.472(2)
Pt(3)	-0.46277(1)	-0.29022(1)	-0.3295	1.601(2)
P(1)	-0.28448(7)	-0.06863(7)	-0.36820(3)	2.10(2)
P(2)	-0.27095(6)	-0.49914(6)	-0.36861(3)	1.70(2)
P(3)	-0.55830(6)	-0.28634(7)	-0.28750(3)	1.95(2)
N(1)	-0.2632(2)	-0.2913(3)	-0.4288(1)	2.66(8)
N(2)	-0.5032(2)	-0.4861(3)	-0.3501(1)	2.63(8)
N(3)	-0.5054(2)	-0.0934(3)	-0.3556(1)	2.78(9)
C(1)	-0.2914(2)	-0.2855(3)	-0.3977(1)	2.04(8)
C(2)	-0.4578(2)	-0.4263(3)	-0.3415(1)	2.01(8)
C(3)	-0.4637(3)	-0.1609(3)	-0.3497(1)	2.21(9)
C(11)	-0.2537(3)	-0.2399(3)	-0.4632(2)	3.2(1)
C(12)	-0.3236(3)	-0.2036(3)	-0.4853(2)	3.4(1)
C(13)	-0.3093(4)	-0.1588(5)	-0.5202(2)	5.4(2)
C(14)	-0.2365(5)	-0.1514(5)	-0.5313(2)	6.3(2)
C(15)	-0.1682(6)	-0.1826(6)	-0.5097(3)	7.2(2)
C(16)	-0.1779(4)	-0.2305(4)	-0.4744(2)	4.2(1)
C(17)	-0.4089(3)	-0.2179(4)	-0.4729(2)	3.7(1)
C(18)	-0.1041(5)	-0.2726(5)	-0.4507(3)	6.5(2)
C(21)	-0.5026(3)	-0.5636(3)	-0.3722(1)	2.63(9)
C(22)	-0.4981(3)	-0.6477(4)	-0.3543(2)	3.5(1)
C(23)	-0.5034(4)	-0.7250(4)	-0.3771(2)	4.7(2)
C(24)	-0.5075(4)	-0.7193(4)	-0.4177(2)	4.9(2)
C(25)	-0.5142(4)	-0.6380(4)	-0.4355(2)	4.7(2)
C(26)	-0.5088(3)	-0.5584(4)	-0.4155(2)	3.9(1)
C(27)	-0.4932(4)	-0.6529(4)	-0.3084(2)	4.6(2)
C(28)	-0.5138(3)	-0.4680(4)	-0.4340(2)	3.7(1)
C(31)	-0.5874(3)	-0.0680(3)	-0.3632(2)	3.1(1)
C(32)	-0.6087(3)	0.0100(3)	-0.3444(2)	3.3(1)
C(33)	-0.6913(4)	0.0389(4)	-0.3529(2)	4.4(1)
C(34)	-0.7439(4)	-0.0049(4)	-0.3802(2)	4.3(1)
C(35)	-0.7209(3)	-0.0810(4)	-0.3984(2)	3.8(1)
C(36)	-0.6412(3)	-0.1139(3)	-0.3909(1)	2.8(1)
C(37)	-0.5477(4)	0.0580(4)	-0.3160(2)	4.6(2)
C(38)	-0.6133(4)	-0.1932(4)	-0.4118(2)	4.0(1)
C(41)	-0.1732(3)	-0.0748(3)	-0.3585(2)	3.0(1)
C(42)	-0.1468(3)	-0.1274(3)	-0.3207(1)	2.59(9)
C(43)	-0.0553(3)	-0.1291(3)	-0.3067(1)	2.57(9)
C(44)	-0.0415(3)	-0.1929(3)	-0.2712(2)	2.9(1)
C(45)	-0.5473(3)	-0.1964(3)	-0.2496(1)	2.35(9)
C(46)	-0.2680(3)	-0.5766(3)	-0.3267(1)	2.27(9)
C(47)	-0.2559(3)	-0.5269(3)	-0.2861(1)	2.45(9)
C(48)	-0.2500	-0.5868(4)	-0.2500	2.5(1)
C(111)	-0.3055(3)	-0.0122(3)	-0.4153(1)	2.53(9)
C(112)	-0.2484(3)	0.0103(4)	-0.4410(2)	3.8(1)
C(113)	-0.2725(4)	0.0462(4)	-0.4779(2)	4.6(2)
C(114)	-0.3501(4)	0.0660(4)	-0.4887(2)	5.1(2)
C(115)	-0.4108(3)	0.0461(4)	-0.4657(2)	3.8(1)
C(116)	-0.3887(3)	0.0091(3)	-0.4285(2)	3.2(1)
C(121)	-0.3098(3)	0.0169(3)	-0.3321(1)	2.57(9)
C(122)	-0.3015(3)	0.1065(4)	-0.3409(2)	3.6(1)
C(123)	-0.3221(4)	0.1711(4)	-0.3122(2)	4.4(1)
C(124)	-0.3447(4)	0.1439(4)	-0.2768(2)	4.5(1)
C(125)	-0.3510(3)	0.0534(3)	-0.2688(1)	2.9(1)
C(126)	-0.3336(3)	-0.0090(3)	-0.2961(2)	3.0(1)
C(211)	-0.1621(3)	-0.4752(3)	-0.3710(1)	2.63(10)
C(212)	-0.1266(3)	-0.3973(3)	-0.3521(1)	2.9(1)
C(213)	-0.0408(3)	-0.3794(4)	-0.3546(2)	3.5(1)

C(214)	0.0038(3)	-0.4347(4)	-0.3737(2)	3.8(1)
C(215)	-0.0324(4)	-0.5127(4)	-0.3914(2)	4.7(2)
C(216)	-0.1125(3)	-0.5322(4)	-0.3900(2)	3.6(1)
C(221)	-0.2931(3)	-0.5685(3)	-0.4131(1)	2.67(10)
C(222)	-0.3032(3)	-0.5257(4)	-0.4489(2)	3.8(1)
C(223)	-0.3216(4)	-0.5744(4)	-0.4842(2)	4.7(2)
C(224)	-0.3313(4)	-0.6609(5)	-0.4823(2)	5.8(2)
C(225)	-0.3205(5)	-0.7131(5)	-0.4455(2)	5.8(2)
C(226)	-0.3010(4)	-0.6617(4)	-0.4106(2)	4.2(1)
C(311)	-0.6628(3)	-0.2763(3)	-0.3114(1)	2.34(9)
C(312)	-0.7148(3)	-0.2039(3)	-0.3039(1)	2.83(10)
C(313)	-0.7942(3)	-0.1997(3)	-0.3249(2)	3.3(1)
C(314)	-0.8199(3)	-0.2667(4)	-0.3523(2)	4.0(1)
C(315)	-0.7682(3)	-0.3375(4)	-0.3592(2)	4.0(1)
C(316)	-0.6890(3)	-0.3408(4)	-0.3398(2)	3.6(1)
C(321)	-0.5641(3)	-0.3840(3)	-0.2556(1)	2.57(9)
C(322)	-0.6348(3)	-0.4038(4)	-0.2382(2)	3.6(1)
C(323)	-0.6414(4)	-0.4788(5)	-0.2158(2)	5.3(2)
C(324)	-0.5745(4)	-0.5388(4)	-0.2104(2)	4.7(2)
C(325)	-0.5023(4)	-0.5192(4)	-0.2253(2)	4.5(1)
C(326)	-0.4990(3)	-0.4432(3)	-0.2490(2)	3.1(1)
C(401)	0.4850(5)	0.0151(6)	0.0202(3)	6.962(2)
C(402)	0.5549(8)	0.0346(8)	0.0520(4)	11.563(4)
C(403)	0.5299(6)	0.0649(6)	0.0915(3)	8.088(3)
H(1)	-0.1900	-0.0002	-0.4328	4.8
H(2)	-0.2336	0.0565	-0.4964	6.6
H(3)	-0.3686	0.0939	-0.5145	6.5
H(4)	-0.4678	0.0584	-0.4739	4.8
H(5)	-0.4310	-0.0029	-0.4112	4.4
H(6)	-0.2822	0.1253	-0.3655	4.1
H(7)	-0.3201	0.2342	-0.3178	5.1
H(8)	-0.3576	0.1876	-0.2571	5.2
H(9)	-0.3699	0.0343	-0.2439	3.6
H(10)	-0.3351	-0.0717	-0.2906	3.6
H(11)	-0.6970	-0.1594	-0.2847	3.3
H(12)	-0.8307	-0.1513	-0.3204	4.2
H(13)	-0.8724	-0.2617	-0.3665	5.3
H(14)	-0.7882	-0.3860	-0.3766	4.9
H(15)	-0.6516	-0.3870	-0.3471	4.2
H(16)	-0.6779	-0.3616	-0.2413	4.4
H(17)	-0.6906	-0.4864	-0.2029	6.6
H(18)	-0.5798	-0.5965	-0.1981	5.7
H(19)	-0.4556	-0.5556	-0.2191	6.0
H(20)	-0.4500	-0.4294	-0.2604	3.6
H(21)	-0.1589	-0.3588	-0.3377	3.4
H(22)	-0.0155	-0.3285	-0.3420	4.3
H(23)	0.0627	-0.4234	-0.3751	4.3
H(24)	0.0008	-0.5520	-0.4054	5.8
H(25)	-0.1346	-0.5871	-0.4018	4.4
H(26)	-0.3003	-0.4613	-0.4506	4.4
H(27)	-0.3272	-0.5426	-0.5089	5.8
H(28)	-0.3478	-0.6922	-0.5070	7.5
H(29)	-0.3301	-0.7766	-0.4446	8.4
H(30)	-0.2904	-0.6904	-0.3852	4.9
H(31)	-0.5023	-0.7841	-0.3636	5.9
H(32)	-0.5029	-0.7738	-0.4326	6.2
H(33)	-0.5223	-0.6363	-0.4644	6.6
H(34)	-0.5410	-0.6261	-0.2999	6.0
H(35)	-0.4911	-0.7133	-0.3005	6.0
H(36)	-0.4469	-0.6221	-0.2966	6.0
H(37)	-0.4658	-0.4326	-0.4252	4.5
H(38)	-0.5181	-0.4709	-0.4620	4.5
H(39)	-0.5597	-0.4344	-0.4268	4.5

H(40)	-0.7106	0.0886	-0.3388	5.3
H(41)	-0.7984	0.0214	-0.3867	5.8
H(42)	-0.7603	-0.1141	-0.4158	5.0
H(43)	-0.5277	0.0195	-0.2946	5.7
H(44)	-0.5025	0.0760	-0.3293	5.7
H(45)	-0.5710	0.1092	-0.3054	5.7
H(46)	-0.6554	-0.2187	-0.4305	5.3
H(47)	-0.5677	-0.1810	-0.4263	5.3
H(48)	-0.5955	-0.2413	-0.3934	5.3
H(49)	-0.3553	-0.1333	-0.5365	6.6
H(50)	-0.2300	-0.1229	-0.5565	7.9
H(51)	-0.1155	-0.1705	-0.5173	10.1
H(52)	-0.4345	-0.1617	-0.4697	4.4
H(53)	-0.4417	-0.2515	-0.4922	4.4
H(54)	-0.4049	-0.2489	-0.4483	4.4
H(55)	-0.1080	-0.3337	-0.4482	8.2
H(56)	-0.0540	-0.2571	-0.4610	8.2
H(57)	-0.0972	-0.2473	-0.4232	8.2
H(58)	-0.1523	-0.1041	-0.3807	3.6
H(59)	-0.1508	-0.0167	-0.3564	3.6
H(60)	-0.1753	-0.1036	-0.3002	3.1
H(61)	-0.1645	-0.1884	-0.3251	3.1
H(62)	-0.0252	-0.1481	-0.3271	3.1
H(63)	-0.0375	-0.0699	-0.2987	3.1
H(64)	-0.0737	-0.1724	-0.2509	3.6
H(65)	-0.0610	-0.2505	-0.2793	3.6
H(67)	-0.3183	-0.6094	-0.3282	2.7
H(68)	-0.2251	-0.6189	-0.3279	2.7
H(69)	-0.2059	-0.4937	-0.2855	2.9
H(70)	-0.2993	-0.4866	-0.2851	2.9
H(71)	-0.2992	-0.6200	-0.2501	2.9
H(75)	-0.5442	-0.1397	-0.2628	2.7
H(76)	-0.5948	-0.1951	-0.2360	2.7

^a Estimated standard deviations are given in parentheses. ^b All non-hydrogen atoms except for those of solvent hexane were assigned with anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos + 2U_{13}aa^*cc^*\cos + 2U_{23}bb^*cc^*\cos)$. ^c The positions of all hydrogen atoms except for solvent molecules were calculated with C-H = 0.95 Å and were not refined with the appropriate B_{iso} .

Table S1-3. Final Anisotropic Thermal Parameters for **8a**·CH₃(CH₂)₄CH₃^{a,b}

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg(1)	0.02656(6)	0.02416(7)	0.01897(6)	0.00031(6)	-0.00647(5)	-0.00004(6)
Pt(1)	0.02575(6)	0.01531(6)	0.01993(6)	0.00048(5)	-0.00236(5)	0.00234(5)
Pt(2)	0.02144(6)	0.01756(6)	0.01629(6)	0.00048(5)	-0.00077(5)	-0.00098(5)
Pt(3)	0.01966(6)	0.02022(6)	0.01998(6)	0.00029(5)	-0.00199(5)	-0.00180(6)
P(1)	0.0343(5)	0.0201(4)	0.0237(5)	-0.0050(4)	-0.0036(4)	0.0044(4)
P(2)	0.0283(5)	0.0174(4)	0.0179(4)	0.0044(4)	-0.0013(4)	-0.0033(4)
P(3)	0.0187(4)	0.0308(5)	0.0238(5)	0.0015(4)	-0.0003(4)	-0.0022(4)
N(1)	0.036(2)	0.033(2)	0.033(2)	0.000(2)	0.006(2)	-0.002(2)
N(2)	0.034(2)	0.032(2)	0.035(2)	-0.004(2)	0.004(2)	0.000(2)
N(3)	0.036(2)	0.033(2)	0.036(2)	0.005(2)	0.001(2)	0.004(2)
C(1)	0.028(2)	0.025(2)	0.024(2)	0.004(2)	0.004(2)	0.003(2)
C(2)	0.019(2)	0.025(2)	0.031(2)	0.001(1)	-0.002(2)	-0.009(2)
C(3)	0.033(2)	0.025(2)	0.024(2)	-0.004(2)	-0.007(2)	-0.007(2)
C(11)	0.047(3)	0.036(2)	0.040(2)	-0.002(2)	0.007(2)	-0.002(2)
C(12)	0.048(3)	0.040(3)	0.041(3)	0.001(2)	-0.001(2)	-0.005(2)
C(13)	0.078(4)	0.064(4)	0.063(4)	-0.004(3)	0.009(3)	0.005(3)
C(14)	0.089(5)	0.075(5)	0.076(5)	-0.003(4)	0.014(4)	0.009(4)
C(15)	0.105(6)	0.089(5)	0.085(5)	-0.008(5)	0.027(5)	0.010(5)

C(16)	0.056(3)	0.053(3)	0.054(3)	-0.003(3)	0.016(3)	0.005(3)
C(17)	0.051(3)	0.048(3)	0.039(3)	0.000(2)	-0.001(2)	-0.001(2)
C(18)	0.078(4)	0.090(5)	0.086(5)	0.002(4)	0.031(4)	0.009(4)
C(21)	0.033(2)	0.033(2)	0.034(2)	-0.003(2)	0.001(2)	-0.002(2)
C(22)	0.050(3)	0.041(3)	0.044(3)	-0.006(2)	0.005(2)	-0.001(2)
C(23)	0.062(3)	0.052(3)	0.063(4)	-0.006(3)	0.001(3)	-0.003(3)
C(24)	0.068(4)	0.049(3)	0.067(4)	-0.003(3)	0.003(3)	-0.007(3)
C(25)	0.060(3)	0.058(3)	0.060(4)	-0.007(3)	-0.001(3)	-0.006(3)
C(26)	0.050(3)	0.049(3)	0.048(3)	-0.002(3)	0.001(2)	-0.004(3)
C(27)	0.066(3)	0.054(3)	0.055(3)	-0.003(3)	0.005(3)	0.001(3)
C(28)	0.049(3)	0.048(3)	0.041(3)	0.001(2)	-0.003(2)	-0.004(2)
C(31)	0.038(2)	0.038(2)	0.040(2)	0.003(2)	0.003(2)	0.005(2)
C(32)	0.042(2)	0.040(2)	0.043(3)	0.007(2)	0.005(2)	0.004(2)
C(33)	0.051(3)	0.055(3)	0.059(3)	0.009(3)	0.005(3)	0.002(3)
C(34)	0.053(3)	0.054(3)	0.058(3)	0.005(3)	0.007(3)	0.007(3)
C(35)	0.046(3)	0.054(3)	0.045(3)	0.001(2)	0.007(2)	0.005(2)
C(36)	0.037(2)	0.037(2)	0.031(2)	0.002(2)	0.001(2)	0.006(2)
C(37)	0.069(4)	0.052(3)	0.056(3)	0.002(3)	0.009(3)	-0.003(3)
C(38)	0.052(3)	0.056(3)	0.045(3)	-0.004(3)	-0.001(3)	0.002(3)
C(41)	0.038(2)	0.036(2)	0.038(2)	-0.004(2)	-0.001(2)	0.003(2)
C(42)	0.034(2)	0.033(2)	0.032(2)	-0.004(2)	0.002(2)	0.004(2)
C(43)	0.032(2)	0.034(2)	0.031(2)	-0.003(2)	0.002(2)	0.002(2)
C(44)	0.035(2)	0.038(2)	0.036(2)	0.001(2)	0.000(2)	0.004(2)
C(45)	0.030(2)	0.030(2)	0.030(2)	0.001(2)	0.005(2)	-0.005(2)
C(46)	0.032(2)	0.025(2)	0.029(2)	0.003(2)	0.001(2)	0.001(2)
C(47)	0.034(2)	0.028(2)	0.030(2)	0.001(2)	0.000(2)	0.003(2)
C(48)	0.033(3)	0.028(3)	0.033(3)	0.0000	0.002(3)	0.0000
C(111)	0.035(2)	0.028(2)	0.032(2)	0.001(2)	-0.003(2)	0.003(2)
C(112)	0.054(3)	0.045(3)	0.046(3)	0.000(2)	0.004(2)	0.001(2)
C(113)	0.067(3)	0.058(3)	0.050(3)	0.001(3)	0.008(3)	0.002(3)
C(114)	0.076(4)	0.059(4)	0.057(4)	-0.002(3)	0.000(3)	0.003(3)
C(115)	0.051(3)	0.045(3)	0.047(3)	0.003(2)	-0.007(2)	0.000(2)
C(116)	0.046(3)	0.034(2)	0.041(3)	0.001(2)	-0.002(2)	0.000(2)
C(121)	0.033(2)	0.028(2)	0.035(2)	-0.003(2)	-0.004(2)	0.003(2)
C(122)	0.051(3)	0.041(3)	0.046(3)	-0.004(2)	0.001(2)	0.002(2)
C(123)	0.069(4)	0.047(3)	0.052(3)	-0.001(3)	0.002(3)	0.001(3)
C(124)	0.062(3)	0.055(3)	0.053(3)	0.005(3)	0.008(3)	-0.005(3)
C(125)	0.041(2)	0.032(2)	0.035(2)	0.001(2)	-0.001(2)	0.003(2)
C(126)	0.040(2)	0.033(2)	0.037(2)	-0.002(2)	-0.002(2)	-0.001(2)
C(211)	0.034(2)	0.032(2)	0.033(2)	0.000(2)	0.001(2)	0.001(2)
C(212)	0.038(2)	0.038(2)	0.035(2)	0.001(2)	0.005(2)	-0.002(2)
C(213)	0.045(3)	0.043(3)	0.045(3)	-0.005(2)	-0.001(2)	-0.004(2)
C(214)	0.042(3)	0.055(3)	0.046(3)	-0.002(2)	0.008(2)	-0.002(3)
C(215)	0.058(3)	0.062(4)	0.062(4)	0.007(3)	0.013(3)	-0.004(3)
C(216)	0.045(3)	0.046(3)	0.046(3)	0.004(2)	0.005(2)	-0.004(2)
C(221)	0.036(2)	0.032(2)	0.033(2)	0.000(2)	0.002(2)	-0.005(2)
C(222)	0.048(3)	0.051(3)	0.046(3)	0.004(2)	0.005(2)	-0.005(2)
C(223)	0.060(3)	0.063(4)	0.054(3)	-0.002(3)	0.002(3)	-0.006(3)
C(224)	0.072(4)	0.084(5)	0.063(4)	0.005(4)	0.004(3)	-0.018(4)
C(225)	0.078(4)	0.076(4)	0.068(4)	-0.001(4)	0.009(4)	-0.019(4)
C(226)	0.058(3)	0.050(3)	0.053(3)	0.000(3)	0.005(3)	-0.008(3)
C(311)	0.026(2)	0.034(2)	0.030(2)	-0.001(2)	0.003(2)	0.000(2)
C(312)	0.035(2)	0.036(2)	0.036(2)	0.000(2)	0.004(2)	0.000(2)
C(313)	0.037(2)	0.044(3)	0.044(3)	0.001(2)	0.003(2)	0.007(2)
C(314)	0.046(3)	0.058(3)	0.048(3)	0.000(3)	0.002(2)	0.008(3)
C(315)	0.050(3)	0.052(3)	0.049(3)	-0.002(3)	0.000(3)	-0.001(3)
C(316)	0.044(3)	0.047(3)	0.044(3)	-0.003(2)	0.001(2)	-0.002(2)
C(321)	0.033(2)	0.034(2)	0.031(2)	0.002(2)	0.004(2)	0.001(2)
C(322)	0.044(3)	0.050(3)	0.044(3)	0.003(2)	0.005(2)	0.004(2)
C(323)	0.064(4)	0.073(4)	0.067(4)	-0.005(3)	0.010(3)	0.012(3)
C(324)	0.067(4)	0.054(3)	0.056(3)	-0.005(3)	0.003(3)	0.006(3)
C(325)	0.063(3)	0.058(3)	0.048(3)	0.002(3)	0.005(3)	0.005(3)
C(326)	0.038(2)	0.041(2)	0.039(2)	0.003(2)	0.004(2)	0.001(2)

^a Estimated standard deviations are given in parentheses. ^b Parameters have the form $\exp(-2 \sqrt{U_{11}h^2a^2 + \dots + 2U_{12}hka^*b^*\cos \dots})$.

Table S1-4. Bond Lengths for Non-hydrogen Atoms of **8a**·CH₃(CH₂)₄CH₃^a

atom	atom	distance	atom	atom	distance
Hg(1)	Hg(1)*	2.8424(2)	N(1)	C(11)	1.431(6)
Hg(1)	Pt(1)	2.9448(1)	N(2)	C(2)	1.188(5)
Hg(1)	Pt(2)	2.9541(1)	N(2)	C(21)	1.386(6)
Hg(1)	Pt(3)	2.9263(4)	N(3)	C(3)	1.231(6)
Pt(1)	Pt(2)	2.6680(2)	N(3)	C(31)	1.408(6)
Pt(1)	Pt(3)	2.6775(3)	C(11)	C(12)	1.416(7)
Pt(1)	P(1)	2.253(1)	C(11)	C(16)	1.361(8)
Pt(1)	C(1)	2.074(4)	C(12)	C(13)	1.408(9)
Pt(1)	C(3)	2.064(4)	C(12)	C(17)	1.536(8)
Pt(2)	Pt(3)	2.6702(3)	C(13)	C(14)	1.31(1)
Pt(2)	P(2)	2.260(1)	C(14)	C(15)	1.36(1)
Pt(2)	C(1)	2.088(4)	C(15)	C(16)	1.43(1)
Pt(2)	C(2)	2.181(4)	C(16)	C(18)	1.52(1)
Pt(3)	P(3)	2.252(1)	C(21)	C(22)	1.400(7)
Pt(3)	C(2)	2.088(4)	C(21)	C(26)	1.470(8)
Pt(3)	C(3)	2.061(4)	C(22)	C(23)	1.397(8)
P(1)	C(41)	1.838(5)	C(22)	C(27)	1.557(9)
P(1)	C(111)	1.815(5)	C(23)	C(24)	1.38(1)
P(1)	C(121)	1.860(5)	C(24)	C(25)	1.364(9)
P(2)	C(46)	1.839(5)	C(25)	C(26)	1.376(9)
P(2)	C(211)	1.851(5)	C(26)	C(28)	1.497(8)
P(2)	C(221)	1.842(5)	C(31)	C(32)	1.400(7)
P(3)	C(45)	1.864(4)	C(31)	C(36)	1.405(7)
P(3)	C(311)	1.835(4)	C(32)	C(33)	1.434(8)
P(3)	C(321)	1.835(5)	C(32)	C(37)	1.500(8)
N(1)	C(1)	1.209(6)	C(33)	C(34)	1.370(8)
C(34)	C(35)	1.375(8)	C(215)	C(216)	1.366(8)
C(35)	C(36)	1.405(7)	C(221)	C(222)	1.373(7)
C(36)	C(38)	1.489(8)	C(221)	C(226)	1.410(7)
C(41)	C(42)	1.534(7)	C(222)	C(223)	1.411(9)
C(42)	C(43)	1.537(6)	C(223)	C(224)	1.31(1)
C(43)	C(44)	1.538(7)	C(224)	C(225)	1.47(1)
C(44)	C(45)*	1.560(6)	C(225)	C(226)	1.42(1)
C(46)	C(47)	1.563(6)	C(311)	C(312)	1.428(6)
C(47)	C(48)	1.519(6)	C(311)	C(316)	1.404(7)
C(111)	C(112)	1.401(8)	C(312)	C(313)	1.426(7)
C(111)	C(116)	1.436(7)	C(313)	C(314)	1.405(8)
C(112)	C(113)	1.387(8)	C(314)	C(315)	1.402(8)
C(113)	C(114)	1.331(9)	C(315)	C(316)	1.401(7)
C(114)	C(115)	1.376(9)	C(321)	C(322)	1.403(7)
C(115)	C(116)	1.396(8)	C(321)	C(326)	1.396(7)
C(121)	C(122)	1.390(7)	C(322)	C(323)	1.374(9)
C(121)	C(126)	1.388(7)	C(323)	C(324)	1.424(9)
C(122)	C(123)	1.446(8)	C(324)	C(325)	1.38(1)
C(123)	C(124)	1.365(9)	C(325)	C(326)	1.404(8)
C(124)	C(125)	1.393(8)	C(401)	C(401)*	1.58(2)
C(125)	C(126)	1.373(7)	C(401)	C(402)	1.52(1)
C(211)	C(212)	1.430(7)	C(402)	C(403)	1.52(2)
C(211)	C(216)	1.396(7)			
C(212)	C(213)	1.459(7)			
C(213)	C(214)	1.328(8)			
C(214)	C(215)	1.421(9)			

^a Estimated standard deviations are given in parentheses.

Table S1-5. Bond Angles for Non-hydrogen Atoms of **8a**·CH₃(CH₂)₄CH₃^a

atom	atom	atom	angle	atom	atom	atom	angle
Hg(1)*	Hg(1)	Pt(1)	149.341(6)	Pt(1)	Pt(2)	Pt(3)	60.208(6)
Hg(1)*	Hg(1)	Pt(2)	148.130(6)	Pt(1)	Pt(2)	P(2)	145.82(3)
Hg(1)*	Hg(1)	Pt(3)	147.629(8)	Pt(1)	Pt(2)	C(1)	49.9(1)
Pt(1)	Hg(1)	Pt(2)	53.781(4)	Pt(1)	Pt(2)	C(2)	109.2(1)
Pt(1)	Hg(1)	Pt(3)	54.263(4)	Pt(3)	Pt(2)	P(2)	150.10(3)
Pt(2)	Hg(1)	Pt(3)	54.009(4)	Pt(3)	Pt(2)	C(1)	108.2(1)
Hg(1)	Pt(1)	Pt(2)	63.288(4)	Pt(3)	Pt(2)	C(2)	49.7(1)
Hg(1)	Pt(1)	Pt(3)	62.517(7)	P(2)	Pt(2)	C(1)	101.4(1)
Hg(1)	Pt(1)	P(1)	111.15(3)	P(2)	Pt(2)	C(2)	104.2(1)
Hg(1)	Pt(1)	C(1)	96.5(1)	C(1)	Pt(2)	C(2)	149.1(1)
Hg(1)	Pt(1)	C(3)	96.1(1)	Hg(1)	Pt(3)	Pt(1)	63.221(7)
Pt(2)	Pt(1)	Pt(3)	59.937(6)	Hg(1)	Pt(3)	Pt(2)	63.526(8)
Pt(2)	Pt(1)	P(1)	149.11(3)	Hg(1)	Pt(3)	P(3)	111.31(3)
Pt(2)	Pt(1)	C(1)	50.4(1)	Hg(1)	Pt(3)	C(2)	93.7(1)
Pt(2)	Pt(1)	C(3)	106.9(1)	Hg(1)	Pt(3)	C(3)	96.7(1)
Pt(3)	Pt(1)	P(1)	147.67(3)	Pt(1)	Pt(3)	Pt(2)	59.856(7)
Pt(3)	Pt(1)	C(1)	108.4(1)	Pt(1)	Pt(3)	P(3)	146.37(3)
Pt(3)	Pt(1)	C(3)	49.5(1)	Pt(1)	Pt(3)	C(2)	112.0(1)
P(1)	Pt(1)	C(1)	103.8(1)	Pt(1)	Pt(3)	C(3)	49.6(1)
P(1)	Pt(1)	C(3)	103.9(1)	Pt(2)	Pt(3)	P(3)	150.92(3)
C(1)	Pt(1)	C(3)	142.9(2)	Pt(2)	Pt(3)	C(2)	52.9(1)
Hg(1)	Pt(2)	Pt(1)	62.932(4)	Pt(2)	Pt(3)	C(3)	106.9(1)
Hg(1)	Pt(2)	Pt(3)	62.464(7)	P(3)	Pt(3)	C(2)	101.3(1)
Hg(1)	Pt(2)	P(2)	110.52(3)	P(3)	Pt(3)	C(3)	102.1(1)
Hg(1)	Pt(2)	C(1)	95.9(1)	C(2)	Pt(3)	C(3)	148.8(2)
Hg(1)	Pt(2)	C(2)	91.0(1)	Pt(1)	P(1)	C(41)	115.2(2)
Pt(1)	P(1)	C(111)	115.3(1)	Pt(1)	C(3)	Pt(3)	80.9(1)
Pt(1)	P(1)	C(121)	113.6(2)	Pt(1)	C(3)	N(3)	134.3(3)
C(41)	P(1)	C(111)	105.7(2)	Pt(3)	C(3)	N(3)	144.5(4)
C(41)	P(1)	C(121)	102.3(2)	N(1)	C(11)	C(12)	119.0(5)
C(111)	P(1)	C(121)	103.2(2)	N(1)	C(11)	C(16)	118.5(4)
Pt(2)	P(2)	C(46)	114.7(1)	C(12)	C(11)	C(16)	122.4(5)
Pt(2)	P(2)	C(211)	113.8(1)	C(11)	C(12)	C(13)	115.2(5)
Pt(2)	P(2)	C(221)	118.0(1)	C(11)	C(12)	C(17)	121.5(5)
C(46)	P(2)	C(211)	102.5(2)	C(13)	C(12)	C(17)	123.2(5)
C(46)	P(2)	C(221)	105.5(2)	C(12)	C(13)	C(14)	122.3(6)
C(211)	P(2)	C(221)	100.3(2)	C(13)	C(14)	C(15)	123.3(8)
Pt(3)	P(3)	C(45)	116.0(1)	C(14)	C(15)	C(16)	117.6(8)
Pt(3)	P(3)	C(311)	114.6(2)	C(11)	C(16)	C(15)	119.0(6)
Pt(3)	P(3)	C(321)	116.3(2)	C(11)	C(16)	C(18)	121.2(6)
C(45)	P(3)	C(311)	105.1(2)	C(15)	C(16)	C(18)	119.8(6)
C(45)	P(3)	C(321)	100.2(2)	N(2)	C(21)	C(22)	121.7(4)
C(311)	P(3)	C(321)	102.6(2)	N(2)	C(21)	C(26)	119.6(4)
C(1)	N(1)	C(11)	140.4(4)	C(22)	C(21)	C(26)	118.7(4)
C(2)	N(2)	C(21)	136.5(4)	C(21)	C(22)	C(23)	120.7(5)
C(3)	N(3)	C(31)	140.0(4)	C(21)	C(22)	C(27)	118.5(5)
Pt(1)	C(1)	Pt(2)	79.7(2)	C(23)	C(22)	C(27)	120.7(5)
Pt(1)	C(1)	N(1)	142.9(3)	C(22)	C(23)	C(24)	120.0(6)
Pt(2)	C(1)	N(1)	133.5(3)	C(23)	C(24)	C(25)	119.8(6)
Pt(2)	C(2)	Pt(3)	77.4(1)	C(24)	C(25)	C(26)	124.0(6)
Pt(2)	C(2)	N(2)	135.3(3)	C(21)	C(26)	C(25)	116.5(5)
Pt(3)	C(2)	N(2)	138.7(3)	C(21)	C(26)	C(28)	117.9(5)
C(25)	C(26)	C(28)	125.5(5)	C(113)	C(114)	C(115)	122.7(6)
N(3)	C(31)	C(32)	115.5(4)	C(114)	C(115)	C(116)	118.2(5)
N(3)	C(31)	C(36)	121.1(4)	C(111)	C(116)	C(115)	121.0(5)
C(32)	C(31)	C(36)	123.1(4)	P(1)	C(121)	C(122)	119.4(4)
C(31)	C(32)	C(33)	116.4(5)	P(1)	C(121)	C(126)	120.0(3)
C(31)	C(32)	C(37)	120.8(5)	C(122)	C(121)	C(126)	120.5(5)

C(33)	C(32)	C(37)	122.9(5)	C(121)	C(122)	C(123)	117.8(5)
C(32)	C(33)	C(34)	120.8(6)	C(122)	C(123)	C(124)	120.5(5)
C(33)	C(34)	C(35)	121.2(5)	C(123)	C(124)	C(125)	119.8(6)
C(34)	C(35)	C(36)	120.9(5)	C(124)	C(125)	C(126)	120.6(5)
C(31)	C(36)	C(35)	117.4(4)	C(121)	C(126)	C(125)	120.6(4)
C(31)	C(36)	C(38)	120.5(4)	P(2)	C(211)	C(212)	119.5(4)
C(35)	C(36)	C(38)	122.1(4)	P(2)	C(211)	C(216)	121.9(4)
P(1)	C(41)	C(42)	111.2(3)	C(212)	C(211)	C(216)	118.5(4)
C(41)	C(42)	C(43)*	116.6(4)	C(211)	C(212)	C(213)	118.5(4)
C(42)	C(43)	C(44)	108.0(4)	C(212)	C(213)	C(214)	120.9(5)
C(43)	C(44)	C(45)*	115.3(4)	C(213)	C(214)	C(215)	119.5(5)
P(3)	C(45)	C(44)*	110.7(3)	C(214)	C(215)	C(216)	121.8(6)
P(2)	C(46)	C(47)	112.0(3)	C(211)	C(216)	C(215)	120.7(5)
C(46)	C(47)	C(48)	115.1(4)	P(2)	C(221)	C(222)	117.3(4)
C(47)	C(48)	C(47)*	107.4(5)	P(2)	C(221)	C(226)	121.6(4)
P(1)	C(111)	C(112)	126.1(4)	C(222)	C(221)	C(226)	121.0(5)
P(1)	C(111)	C(116)	117.5(4)	C(221)	C(222)	C(223)	120.5(5)
C(112)	C(111)	C(116)	116.4(4)	C(222)	C(223)	C(224)	119.3(6)
C(111)	C(112)	C(113)	121.1(5)	C(223)	C(224)	C(225)	124.3(7)
C(112)	C(113)	C(114)	120.5(6)	C(224)	C(225)	C(226)	114.7(6)
C(221)	C(226)	C(225)	120.2(6)				
P(3)	C(311)	C(312)	122.8(3)				
P(3)	C(311)	C(316)	116.9(3)				
C(312)	C(311)	C(316)	120.2(4)				
C(311)	C(312)	C(313)	119.0(4)				
C(312)	C(313)	C(314)	119.6(5)				
C(313)	C(314)	C(315)	120.7(5)				
C(314)	C(315)	C(316)	120.2(5)				
C(311)	C(316)	C(315)	120.1(5)				
P(3)	C(321)	C(322)	121.4(4)				
P(3)	C(321)	C(326)	120.9(4)				
C(322)	C(321)	C(326)	117.6(4)				
C(321)	C(322)	C(323)	122.1(5)				
C(322)	C(323)	C(324)	118.7(6)				
C(323)	C(324)	C(325)	120.8(6)				
C(324)	C(325)	C(326)	118.4(5)				
C(321)	C(326)	C(325)	122.1(5)				
C(401)	C(401)	C(402)	113(1)				
C(401)	C(402)	C(403)	115(1)				

^a Estimated deviations are given in parentheses.

Table S2-1. Crystallographic and Experimental Data for **6a**

formula	C ₁₄₄ H ₁₅₀ N ₆ P ₆ Pt ₆ Hg ₂
formula weight	3722.37
color	dark green
size, mm	0.20 x 0.20 x 0.20
cryst. system	monoclinic
space group	C2/c (No. 15)
no. refs used for cell determination	10093 ($6 < 2\theta < 55^\circ$)
lattice const.	$a = 38.202(4) \text{ \AA}$ $b = 14.8735(11) \text{ \AA}$ $c = 30.618(3) \text{ \AA}$ $\beta = 90^\circ$ $\alpha = 115.632(1)^\circ$ $\gamma = 90^\circ$ $V = 15685(3) \text{ \AA}^3$
Z	4
D_{calc} , g cm ⁻³	1.576
$F(000)$	7096
μ (Mo $K\alpha$), cm ⁻¹	73.67
diffractometer	An empirical absorption correction was applied (multi-scan spherical method). Rigaku/MSM Mercury CCD
radiation	(50 kV 190 mA) Mo $K\alpha$ ($\lambda = 0.71069 \text{ \AA}$)
monochromator	graphite
temp, °C	-120
2θ range, °	$6 < 2\theta < 50$
detector aperture, mm	70 x 70
data images	1440
oscillation range ($\omega = 45, \phi = 90$), °	-70 -110
exposure rate, °sec ⁻¹	128
detector swing angle, °	20
detector position, mm	59.7
solution	Direct methods (SIR92)
refinement	full-matrix least-squares (teXsan) The Hg, Pt, and P atoms were refined with anisotropic temperature factors, and other non-H atoms were refined isotropically.
hydrogen atoms	All hydrogen atoms were calcd with C-H = 0.95 Å, and were not refined.
function minimized	$w(F_o - F_c)^2$
weighting scheme	$1/\sigma^2(F_o)$
anomalous dispersion	all non-hydrogen atoms
no. unique reflections	6775
R_{int}	0.056
no. obsd. unique reflections	3688 ($I > 3\sigma(I)$)
p -factor	0.03
no. variables	418
data / param ratio	8.82
R^a	0.084
R_w^b	0.089
GOF ^c	1.18
ρ_{max} , eÅ ⁻³	1.86, -1.45

^a $R = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2}$ ($w = 1/\sigma^2(F_o)$).

^c GOF = $[\sum w(|F_o| - |F_c|)^2 / (N_o - N_p)]^{1/2}$ (N_o = no. data, N_p = no. variables).

Table S2-2. Final Positional Parameters and B_{eq} for **6a**^{a,b,c}

atom	x	y	z	B_{eq}
Hg(1)	0.03771(6)	-0.0359(2)	0.28854(7)	4.34(6)
Pt(1)	0.11137(6)	0.0467(1)	0.35520(7)	3.06(5)
Pt(2)	0.07269(6)	-0.0512(2)	0.39175(7)	3.61(6)
Pt(3)	0.11149(7)	-0.1309(1)	0.34978(8)	3.63(6)
P(1)	0.1207(4)	0.1858(10)	0.3337(6)	5.2(5)
P(2)	0.0356(4)	-0.0568(8)	0.4308(4)	3.2(4)
P(3)	0.1247(5)	-0.2534(10)	0.3194(6)	4.5(5)
N(1)	0.0953(12)	0.131(3)	0.436(2)	4.8(11)
N(2)	0.0923(11)	-0.251(3)	0.420(1)	3.9(10)
N(3)	0.1672(12)	-0.045(3)	0.3274(13)	4.9(10)
C(1)	0.083(1)	0.099(3)	0.398(2)	3.5(13)
C(2)	0.090(2)	-0.181(4)	0.398(2)	5.6(15)
C(3)	0.1419(11)	-0.041(3)	0.3370(13)	1.5(8)
C(11)	0.111(2)	0.185(4)	0.474(2)	6.1(15)
C(12)	0.092(2)	0.271(4)	0.482(2)	4.8(13)
C(13)	0.108(1)	0.323(3)	0.517(2)	3.9(12)
C(14)	0.143(2)	0.300(4)	0.557(2)	6.3(15)
C(15)	0.159(2)	0.219(4)	0.555(2)	8.1(17)
C(16)	0.144(2)	0.152(3)	0.514(2)	4.1(12)
C(17)	0.050(1)	0.298(3)	0.434(2)	6.3(15)
C(18)	0.1634(12)	0.071(3)	0.512(2)	4.1(12)
C(21)	0.114(2)	-0.330(5)	0.442(3)	8.6(20)
C(22)	0.092(2)	-0.416(4)	0.433(2)	6.5(16)
C(23)	0.119(2)	-0.481(4)	0.454(2)	8.0(18)
C(24)	0.161(2)	-0.469(5)	0.472(2)	10.0(20)
C(25)	0.174(2)	-0.377(5)	0.489(3)	9.8(20)
C(26)	0.150(2)	-0.314(5)	0.467(3)	9.0(21)
C(27)	0.0520(12)	-0.404(3)	0.407(2)	3.2(11)
C(28)	0.171(2)	-0.223(4)	0.473(2)	7.2(16)
C(31)	0.202(1)	0.020(3)	0.335(2)	3.6(12)
C(32)	0.212(2)	0.046(4)	0.299(2)	5.4(13)
C(33)	0.238(2)	0.099(4)	0.304(2)	7.3(17)
C(34)	0.268(1)	0.140(3)	0.347(2)	3.7(11)
C(35)	0.2587(13)	0.114(3)	0.389(2)	3.2(11)
C(36)	0.233(2)	0.052(4)	0.382(2)	5.2(13)
C(37)	0.181(2)	0.016(4)	0.246(2)	9.7(19)
C(38)	0.224(2)	0.020(4)	0.430(2)	7.6(16)
C(41)	0.125(1)	0.178(3)	0.274(2)	3.8(12)
C(42)	0.0040(12)	0.040(3)	0.418(2)	4.2(11)
C(43)	-0.029(1)	0.055(4)	0.364(2)	5.9(14)
C(44)	-0.049(2)	0.135(4)	0.359(2)	7.7(17)
C(45)	-0.089(1)	0.156(3)	0.317(2)	5.6(14)
C(46)	-0.0859(13)	0.150(3)	0.269(2)	3.4(11)
C(47)	0.086(3)	-0.336(6)	0.299(3)	15.3(34)
C(48)	0.058(3)	-0.348(6)	0.267(3)	15.1(33)
C(49)	0.018(2)	-0.328(5)	0.260(3)	14.4(31)
C(111)	0.1639(11)	0.234(2)	0.372(1)	1.3(9)
C(112)	0.1697(13)	0.244(3)	0.420(2)	2.9(10)
C(113)	0.204(2)	0.296(4)	0.458(2)	6.2(15)
C(114)	0.227(2)	0.324(4)	0.444(2)	6.0(15)
C(115)	0.225(2)	0.318(3)	0.399(2)	5.0(14)
C(116)	0.193(2)	0.268(4)	0.360(2)	6.4(15)
C(121)	0.088(2)	0.270(4)	0.323(2)	5.0(13)
C(122)	0.090(2)	0.357(3)	0.328(2)	4.7(13)
C(123)	0.060(2)	0.424(5)	0.324(2)	9.6(20)
C(124)	0.0213(12)	0.374(3)	0.3093(13)	1.7(9)
C(125)	0.015(2)	0.289(4)	0.310(2)	7.8(17)
C(126)	0.046(1)	0.232(3)	0.315(2)	3.8(12)
C(211)	0.0646(11)	-0.042(3)	0.4967(13)	2.3(9)
C(212)	0.0887(12)	-0.128(3)	0.520(2)	3.0(11)

C(213)	0.116(2)	-0.110(4)	0.567(2)	5.3(14)
C(214)	0.117(2)	-0.031(4)	0.591(2)	6.6(15)
C(215)	0.0959(13)	0.037(4)	0.569(2)	4.0(11)
C(216)	0.0679(11)	0.038(3)	0.5239(13)	2.2(9)
C(221)	0.0044(13)	-0.153(3)	0.422(2)	2.7(11)
C(222)	-0.004(2)	-0.183(3)	0.454(2)	4.6(13)
C(223)	-0.031(2)	-0.246(4)	0.452(2)	6.9(16)
C(224)	-0.044(2)	-0.292(4)	0.412(2)	7.2(17)
C(225)	-0.036(2)	-0.270(4)	0.377(2)	7.0(16)
C(226)	-0.006(2)	-0.190(3)	0.380(2)	5.6(14)
C(311)	0.1330(11)	-0.242(3)	0.267(1)	1.4(9)
C(312)	0.113(2)	-0.179(3)	0.231(2)	5.0(13)
C(313)	0.117(2)	-0.153(4)	0.191(2)	7.7(17)
C(314)	0.136(1)	-0.213(4)	0.174(2)	5.7(14)
C(315)	0.156(2)	-0.293(4)	0.207(2)	5.8(14)
C(316)	0.151(2)	-0.296(4)	0.250(2)	5.6(14)
C(327) ^d	0.169(2)	-0.299(5)	0.352(2)	14.2(12)
C(328) ^d	0.206(2)	-0.260(3)	0.375(2)	14.2(12)
C(329) ^d	0.237(1)	-0.310(5)	0.408(2)	14.2(12)
C(330) ^d	0.231(2)	-0.399(5)	0.418(2)	14.2(12)
C(331) ^d	0.194(2)	-0.438(3)	0.395(2)	14.2(12)
C(332) ^d	0.163(1)	-0.388(5)	0.362(2)	14.2(12)
H(1)	0.1516	0.2168	0.4298	3.5
H(2)	0.2064	0.3054	0.4902	7.3
H(3)	0.2486	0.3539	0.4680	7.1
H(4)	0.2439	0.3462	0.3918	6.0
H(5)	0.1924	0.2599	0.3291	7.6
H(6)	0.1146	0.3821	0.3342	5.6
H(7)	0.0635	0.4865	0.3295	11.5
H(8)	-0.0012	0.4112	0.2979	2.0
H(9)	-0.0094	0.2668	0.3075	9.3
H(10)	0.0414	0.1693	0.3131	4.5
H(11)	0.0852	-0.1851	0.5043	3.6
H(12)	0.1351	-0.1545	0.5833	6.4
H(13)	0.1348	-0.0257	0.6239	7.9
H(14)	0.1005	0.0916	0.5863	4.8
H(15)	0.0512	0.0879	0.5109	2.6
H(16)	0.0110	-0.1589	0.4853	5.5
H(17)	-0.0396	-0.2543	0.4765	8.2
H(18)	-0.0609	-0.3421	0.4079	8.6
H(19)	-0.0473	-0.3037	0.3473	8.4
H(20)	0.0020	-0.1730	0.3556	6.7
H(21)	0.0932	-0.1492	0.2356	6.0
H(22)	0.1078	-0.0969	0.1761	9.2
H(23)	0.1365	-0.2044	0.1438	6.7
H(24)	0.1708	-0.3363	0.1992	6.9
H(25)	0.1626	-0.3462	0.2707	6.7
H(26)	0.2396	0.1161	0.2752	8.7
H(27)	0.2891	0.1759	0.3493	4.4
H(28)	0.2717	0.1430	0.4192	3.8
H(29)	0.1893	-0.0406	0.2399	11.5
H(30)	0.1802	0.0595	0.2229	11.5
H(31)	0.1560	0.0097	0.2457	11.5
H(32)	0.2085	0.0654	0.4350	9.1
H(33)	0.2474	0.0119	0.4578	9.1
H(34)	0.2090	-0.0346	0.4209	9.1
H(35)	0.1096	-0.5382	0.4586	9.5
H(36)	0.1780	-0.5158	0.4727	11.9
H(37)	0.1993	-0.3644	0.5147	11.7
H(38)	0.0415	-0.3953	0.4299	3.8
H(39)	0.0408	-0.4554	0.3878	3.8
H(40)	0.0458	-0.3536	0.3860	3.8
H(41)	0.1785	-0.2097	0.4478	8.6

H(42)	0.1941	-0.2231	0.5027	8.6
H(43)	0.1534	-0.1783	0.4735	8.6
H(44)	0.0959	0.3797	0.5168	4.6
H(45)	0.1547	0.3391	0.5842	7.5
H(46)	0.1818	0.2024	0.5821	9.7
H(47)	0.0562	0.3373	0.4134	7.5
H(48)	0.0331	0.3279	0.4443	7.5
H(49)	0.0378	0.2459	0.4162	7.5
H(50)	0.1523	0.0228	0.5220	4.9
H(51)	0.1903	0.0757	0.5332	4.9
H(52)	0.1588	0.0627	0.4793	4.9
H(53)	-0.0083	0.0370	0.4394	5.0
H(54)	0.0202	0.0918	0.4260	5.0
H(55)	-0.0179	0.0547	0.3419	7.1
H(56)	-0.0473	0.0063	0.3564	7.1
H(57)	-0.0526	0.1406	0.3881	9.1
H(58)	-0.0322	0.1805	0.3584	9.1
H(59)	-0.1080	0.1138	0.3171	6.7
H(60)	-0.0972	0.2150	0.3208	6.7
H(61)	0.1001	-0.3906	0.3046	18.3
H(62)	0.0761	-0.3281	0.3220	18.3
H(63)	0.0612	-0.3230	0.2400	18.1
H(64)	0.0577	-0.4121	0.2641	18.1
H(65)	-0.0770	0.2049	0.2620	4.1
H(66)	-0.0675	0.1036	0.2728	4.1
H(68)	0.0222	-0.3424	0.2918	17.2
H(69)	0.1514	0.1702	0.2803	4.5
H(70)	0.1153	0.2320	0.2558	4.5
H(67)	0.0217	-0.2652	0.2575	17.2
H(333) ^d	0.210(4)	-0.200(3)	0.368(3)	14(1)
H(334) ^d	0.262(2)	-0.284(7)	0.424(3)	14(1)
H(335) ^d	0.252(2)	-0.433(7)	0.441(2)	14(1)
H(336) ^d	0.190(3)	-0.498(3)	0.402(3)	14(1)
H(337) ^d	0.138(2)	-0.414(8)	0.346(3)	14(1)

^a Estimated standard deviations are given in parentheses. ^b The Hg, Pt, and P atoms were assigned with anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos + 2U_{13}aa^*cc^*\cos + 2U_{23}bb^*cc^*\cos)$. Other non-H atoms were refined isotropically. ^c All hydrogen atoms were calculated with C-H = 0.95 Å and were not refined with the appropriate B_{iso} . ^d Treated as a phenyl rigid group.

Table S2-3. Final Anisotropic Thermal Parameters for **6a**^{a,b}

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg(1)	0.046(2)	0.066(2)	0.0355(13)	-0.012(2)	0.0008(11)	0.012(1)
Pt(1)	0.036(1)	0.0363(13)	0.0359(13)	-0.005(2)	0.0083(10)	0.0012(13)
Pt(2)	0.052(2)	0.050(1)	0.0327(13)	-0.004(2)	0.0157(11)	0.0125(13)
Pt(3)	0.050(2)	0.040(1)	0.039(2)	-0.008(1)	0.0108(13)	0.0023(13)
P(1)	0.018(10)	0.077(12)	0.061(12)	-0.021(9)	-0.023(8)	0.056(10)
P(2)	0.057(10)	0.026(9)	0.037(8)	0.001(8)	0.019(7)	0.008(7)
P(3)	0.083(13)	0.047(10)	0.050(11)	-0.015(10)	0.038(10)	-0.012(8)

^a Estimated standard deviations are given in parentheses. ^b Parameters have the form $\exp(-2^2(U_{11}h^2a^*2 + \dots + 2U_{12}hka^*b^*\cos + \dots))$

Table S2-4. Bond Lengths for Non-hydrogen Atoms of **6a**^a

atom	atom	distance	atom	atom	distance
Hg(1)	Hg(1)*	2.826(2)	Hg(1)	Pt(1)	2.937(3)
Hg(1)	Pt(2)	2.858(3)	Hg(1)	Pt(3)	2.980(3)

Pt(1)	Pt(2)	2.643(4)	Pt(1)	Pt(3)	2.647(3)
Pt(1)	P(1)	2.25(2)	Pt(1)	C(1)	2.18(6)
Pt(1)	C(3)	1.98(5)	Pt(2)	Pt(3)	2.627(4)
Pt(2)	P(2)	2.22(2)	Pt(2)	C(1)	2.26(5)
Pt(2)	C(2)	2.03(6)	Pt(3)	P(3)	2.20(2)
Pt(3)	C(2)	2.11(7)	Pt(3)	C(3)	1.92(5)
P(1)	C(41)	1.92(6)	P(1)	C(111)	1.71(4)
P(1)	C(121)	1.71(6)	P(2)	C(42)	1.81(5)
P(2)	C(211)	1.85(4)	P(2)	C(221)	1.80(5)
P(3)	C(47)	1.81(9)	P(3)	C(311)	1.79(5)
P(3)	C(327)	1.70(6)	N(1)	C(1)	1.14(7)
N(1)	C(11)	1.33(7)	N(2)	C(2)	1.22(7)
N(2)	C(21)	1.43(8)	N(3)	C(3)	1.12(7)
N(3)	C(31)	1.58(7)	C(11)	C(12)	1.54(9)
C(11)	C(16)	1.42(7)	C(12)	C(13)	1.24(7)
C(12)	C(17)	1.70(6)	C(13)	C(14)	1.41(6)
C(14)	C(15)	1.38(9)	C(15)	C(16)	1.50(8)
C(16)	C(18)	1.42(7)	C(21)	C(22)	1.5(1)
C(21)	C(26)	1.3(1)	C(22)	C(23)	1.34(9)
C(22)	C(27)	1.40(7)	C(23)	C(24)	1.5(1)
C(24)	C(25)	1.5(1)	C(25)	C(26)	1.3(1)
C(26)	C(28)	1.54(9)	C(31)	C(32)	1.37(9)
C(31)	C(36)	1.48(6)	C(32)	C(33)	1.24(9)
C(32)	C(37)	1.60(7)	C(33)	C(34)	1.45(6)
C(34)	C(35)	1.50(8)	C(35)	C(36)	1.30(7)
C(36)	C(38)	1.71(9)	C(41)	P(1)	1.92(6)
C(41)	C(46)*	1.56(5)	C(42)	C(43)	1.62(6)
C(43)	C(44)	1.38(8)	C(44)	C(43)	1.38(8)
C(44)	C(45)	1.55(6)	C(45)	C(44)	1.55(6)
C(45)	C(46)	1.53(8)	C(46)	C(41)*	1.56(5)
C(47)	C(48)	1.1(1)	C(48)	C(49)	1.5(1)
C(49)	C(49)*	1.3(1)	C(111)	C(112)	1.40(6)
C(111)	C(116)	1.41(8)	C(112)	C(113)	1.53(6)
C(113)	C(114)	1.2(1)	C(114)	C(115)	1.38(9)
C(115)	C(116)	1.47(6)	C(121)	C(122)	1.31(7)
C(121)	C(126)	1.61(8)	C(122)	C(123)	1.49(9)
C(123)	C(124)	1.52(8)	C(124)	C(125)	1.29(7)
C(125)	C(124)	1.29(7)	C(125)	C(126)	1.40(9)
C(126)	C(125)	1.40(9)	C(211)	C(212)	1.57(6)
C(211)	C(216)	1.42(6)	C(212)	C(213)	1.39(6)
C(213)	C(214)	1.37(8)	C(214)	C(215)	1.29(7)
C(215)	C(216)	1.32(5)	C(221)	C(222)	1.25(9)
C(221)	C(226)	1.29(7)	C(222)	C(223)	1.38(8)
C(223)	C(224)	1.30(9)	C(224)	C(225)	1.3(1)
C(225)	C(226)	1.62(8)	C(226)	C(221)	1.29(7)
C(226)	C(225)	1.62(8)	C(311)	C(312)	1.38(6)
C(311)	C(316)	1.29(8)	C(312)	C(313)	1.3(1)
C(313)	C(314)	1.4(1)	C(314)	C(315)	1.53(7)
C(315)	C(316)	1.43(9)	C(327)	C(328)	1.40(9)
C(327)	C(332)	1.4(1)	C(328)	C(329)	1.40(8)
C(329)	C(330)	1.4(1)	C(330)	C(331)	1.40(9)
C(331)	C(332)	1.40(8)			

^a Estimated standard deviations are given in parentheses.

Table S2-5. Bond Angles for Non-hydrogen Atoms of **6a**^a

atom	atom	atom	angle	atom	atom	atom	angle
Hg(1)*	Hg(1)	Pt(1)	154.8(1)	Hg(1)*	Hg(1)	Pt(2)	138.0(1)
Hg(1)*	Hg(1)	Pt(3)	150.5(1)	Pt(1)	Hg(1)	Pt(2)	54.25(7)
Pt(1)	Hg(1)	Pt(3)	53.14(6)	Pt(2)	Hg(1)	Pt(3)	53.43(8)
Pt(2)	Pt(1)	Hg(1)	61.36(8)	Pt(2)	Pt(1)	Pt(3)	59.6(1)
Pt(2)	Pt(1)	C(3)	105(1)	Pt(2)	Pt(1)	P(1)	145.1(5)

Pt(2)	Pt(1)	C(1)	54(1)	Pt(3)	Pt(1)	Hg(1)	64.28(8)
Pt(3)	Pt(1)	C(3)	46(1)	Pt(3)	Pt(1)	P(1)	153.7(5)
Pt(3)	Pt(1)	C(1)	114(1)	P(1)	Pt(1)	Hg(1)	114.1(3)
P(1)	Pt(1)	C(3)	109(1)	P(1)	Pt(1)	C(1)	91(1)
C(1)	Pt(1)	Hg(1)	89(1)	C(1)	Pt(1)	C(3)	155(1)
C(3)	Pt(1)	Hg(1)	91(1)	Pt(3)	Pt(2)	Hg(1)	65.67(8)
Pt(3)	Pt(2)	Pt(1)	60.29(9)	Pt(3)	Pt(2)	C(1)	111(1)
Pt(3)	Pt(2)	P(2)	151.0(3)	Pt(3)	Pt(2)	C(2)	51(2)
P(2)	Pt(2)	Hg(1)	119.9(3)	P(2)	Pt(2)	Pt(1)	148.7(3)
P(2)	Pt(2)	C(1)	96(1)	P(2)	Pt(2)	C(2)	100(2)
C(1)	Pt(2)	Hg(1)	89(1)	C(1)	Pt(2)	Pt(1)	51(1)
C(1)	Pt(2)	C(2)	153(2)	C(2)	Pt(2)	Hg(1)	99(1)
C(2)	Pt(2)	Pt(1)	110(2)	P(3)	Pt(3)	Hg(1)	117.0(4)
P(3)	Pt(3)	Pt(1)	149.3(5)	P(3)	Pt(3)	Pt(2)	149.4(5)
P(3)	Pt(3)	C(3)	102(1)	P(3)	Pt(3)	C(2)	103(1)
C(2)	Pt(3)	Hg(1)	93(1)	C(2)	Pt(3)	Pt(1)	107(1)
C(2)	Pt(3)	Pt(2)	49(1)	C(2)	Pt(3)	C(3)	147(1)
C(3)	Pt(3)	Hg(1)	91(1)	C(3)	Pt(3)	Pt(1)	48(1)
C(3)	Pt(3)	Pt(2)	107(1)	C(41)	P(1)	Pt(1)	108(1)
C(41)	P(1)	C(111)	103(2)	C(41)	P(1)	C(121)	102(2)
C(111)	P(1)	Pt(1)	114(1)	C(111)	P(1)	C(121)	103(2)
C(121)	P(1)	Pt(1)	122(2)	C(42)	P(2)	Pt(2)	112(1)
C(42)	P(2)	C(211)	99(2)	C(42)	P(2)	C(221)	105(2)
C(211)	P(2)	Pt(2)	111(1)	C(211)	P(2)	C(221)	108(2)
C(221)	P(2)	Pt(2)	118(2)	C(47)	P(3)	Pt(3)	114(3)
C(47)	P(3)	C(311)	100(3)	C(47)	P(3)	C(327)	113(3)
C(311)	P(3)	Pt(3)	117(1)	C(311)	P(3)	C(327)	92(2)
C(327)	P(3)	Pt(3)	116(2)	C(1)	N(1)	C(11)	167(5)
C(2)	N(2)	C(21)	147(6)	C(3)	N(3)	C(31)	133(4)
Pt(1)	C(1)	Pt(2)	73(1)	Pt(1)	C(1)	N(1)	131(4)
Pt(2)	C(1)	N(1)	118(4)	Pt(2)	C(2)	Pt(3)	78(2)
Pt(2)	C(2)	N(2)	143(5)	Pt(3)	C(2)	N(2)	137(5)
Pt(1)	C(3)	Pt(3)	85(1)	Pt(1)	C(3)	N(3)	142(3)
Pt(3)	C(3)	N(3)	132(3)				
C(12)	C(11)	N(1)	125(4)	C(12)	C(11)	C(16)	117(4)
C(16)	C(11)	N(1)	116(5)	C(13)	C(12)	C(11)	125(4)
C(13)	C(12)	C(17)	121(4)	C(17)	C(12)	C(11)	112(4)
C(14)	C(13)	C(12)	121(5)	C(15)	C(14)	C(13)	116(4)
C(16)	C(15)	C(14)	127(4)	C(18)	C(16)	C(11)	123(4)
C(18)	C(16)	C(15)	125(3)	C(22)	C(21)	N(2)	117(5)
C(22)	C(21)	C(26)	130(6)	C(26)	C(21)	N(2)	112(6)
C(23)	C(22)	C(21)	106(5)	C(23)	C(22)	C(27)	141(6)
C(27)	C(22)	C(21)	112(5)	C(24)	C(23)	C(22)	124(6)
C(25)	C(24)	C(23)	113(6)	C(26)	C(25)	C(24)	115(6)
C(28)	C(26)	C(21)	127(6)	C(28)	C(26)	C(25)	110(6)
C(32)	C(31)	N(3)	123(3)	C(32)	C(31)	C(36)	108(4)
C(36)	C(31)	N(3)	127(4)	C(33)	C(32)	C(31)	124(5)
C(33)	C(32)	C(37)	120(5)	C(37)	C(32)	C(31)	114(5)
C(34)	C(33)	C(32)	131(6)	C(35)	C(34)	C(33)	106(4)
C(36)	C(35)	C(34)	119(4)	C(38)	C(36)	C(31)	111(4)
C(38)	C(36)	C(35)	119(4)	P(1)	C(41)	C(46)*	112(3)
C(43)	C(42)	P(2)	118(3)	C(44)	C(43)	C(42)	111(4)
C(43)	C(44)	C(45)	123(4)	C(44)	C(45)	C(46)	108(4)
C(41)*	C(46)	C(45)	109(4)	C(48)	C(47)	P(3)	138(9)
C(49)	C(48)	C(47)	128(11)	C(49)*	C(49)	C(48)	158(9)
C(112)	C(111)	P(1)	115(3)	C(112)	C(111)	C(116)	116(3)
C(116)	C(111)	P(1)	127(3)	C(113)	C(112)	C(111)	123(4)
C(114)	C(113)	C(112)	114(5)	C(115)	C(114)	C(113)	127(5)
C(116)	C(115)	C(114)	121(5)	C(122)	C(121)	P(1)	134(4)
C(122)	C(121)	C(126)	112(5)	C(126)	C(121)	P(1)	112(3)
C(123)	C(122)	C(121)	129(5)	C(124)	C(123)	C(122)	108(4)
C(125)	C(124)	C(123)	129(4)	C(124)	C(125)	C(126)	115(5)

C(125)	C(126)	C(121)	122(4)	C(212)	C(211)	P(2)	110(2)
C(212)	C(211)	C(216)	122(3)	C(216)	C(211)	P(2)	126(2)
C(213)	C(212)	C(211)	109(3)	C(214)	C(213)	C(212)	123(4)
C(215)	C(214)	C(213)	121(4)	C(216)	C(215)	C(214)	126(5)
C(222)	C(221)	P(2)	122(3)	C(222)	C(221)	C(226)	124(4)
C(226)	C(221)	P(2)	112(4)	C(223)	C(222)	C(221)	130(5)
C(224)	C(223)	C(222)	112(6)	C(225)	C(224)	C(223)	121(6)
C(226)	C(225)	C(224)	123(5)	C(221)	C(226)	C(225)	106(5)
C(312)	C(311)	P(3)	121(4)	C(312)	C(311)	C(316)	108(4)
C(316)	C(311)	P(3)	128(3)	C(313)	C(312)	C(311)	131(5)
C(314)	C(313)	C(312)	116(5)	C(315)	C(314)	C(313)	116(5)
C(316)	C(315)	C(314)	113(5)	C(328)	C(327)	P(3)	131(5)
C(328)	C(327)	C(332)	120(4)	C(332)	C(327)	P(3)	106(4)
C(329)	C(328)	C(327)	119(5)	C(330)	C(329)	C(328)	119(5)
C(331)	C(330)	C(329)	120(4)	C(332)	C(331)	C(330)	120(5)

^a Estimated deviations are given in parentheses.

Table S3-1. Crystallographic and Experimental Data for 11·3.5C₆H₆

formula	C ₁₁₁ H ₁₁₇ P ₆ Pt ₂ Hg
formula weight	2227.76
color	orange
size, mm	0.20 x 0.15 x 0.10
cryst. system	triclinic
space group	P1- (No. 2)
no. refs used for cell determination	8833 (6 < 2 < 55 °)
lattice const.	a = 14.8858(8) Å b = 15.2745(7) Å c = 23.2773(9) Å = 93.889(1) ° = 101.819(2) ° = 111.113(2) ° V = 4774.2(4) Å ³
Z	2
D _{calc.} , g cm ⁻³	1.550
F(000)	2218
μ (Mo Kα), cm ⁻¹	46.68
diffractometer	An empirical absorption correction was applied (multi-scan spherical method). Rigaku/MSM Mercury CCD (50 kV 190 mA)
radiation	Mo Kα (λ = 0.71069 Å)
monochromator	graphite
temp, °C	-120
2θ range, °	6 < 2θ < 55
detector aperture, mm	70 x 70
data images	2160
oscillation range (ω = 45, φ = 90), °	-62 -118
exposure rate, °sec ⁻¹	128
detector swing angle, °	28
detector position, mm	59.9
solution	Heavy Atom methods (DIRDIF94 Patty)
refinement	full-matrix least-squares (teXsan) All non-H atoms were refined with anisotropic temperature factors.
hydrogen atoms	All H atoms were calcd with C-H = 0.95 Å, and were not refined.
function minimized	$w(F_o^2 - F_c^2)^2$
weighting scheme	$w = 1 / \sigma^2(F_o^2)$
anomalous dispersion	all non-hydrogen atoms
no. unique reflections	13523
R _{int}	0.021
no. obsd. unique reflections	12555 (I > 2σ(I))
no. variables	1082
data / param ratio	11.60
R ^a	0.033
wR ² ^b	0.066
GOF ^c	1.00
ρ _{max.} , eÅ ⁻³	1.18, -1.29

^a $R = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR^2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ ($w = 1 / \sigma^2(F_o^2)$). ^c $GOF = [\sum w(F_o^2 - F_c^2)^2 / (N_o - N_p)]^{1/2}$ ($N_o = \text{no. data}$, $N_p = \text{no. variables}$).

Table S3-2. Final Positional Parameters and B_{eq} for 11-3.5C₆H₆^{a,b,c}

atom	x	y	z	B_{eq}
Hg(1)	0.17846(2)	0.21077(2)	0.24909(1)	1.887(5)
Pt(1)	0.06316(2)	0.30847(2)	0.19911(1)	1.429(5)
Pt(2)	0.29384(2)	0.11338(2)	0.29998(1)	1.632(5)
P(1)	0.1672(1)	0.4158(1)	0.15493(7)	1.56(3)
P(2)	0.4250(1)	0.2390(1)	0.35913(7)	1.67(3)
P(3)	0.0350(1)	0.3725(1)	0.28174(7)	1.63(3)
P(4)	0.1819(1)	0.0165(1)	0.34528(7)	1.69(3)
P(5)	-0.0690(1)	0.1891(1)	0.13727(7)	1.54(3)
P(6)	0.3146(1)	0.0554(1)	0.21236(7)	1.73(3)
C(11)	0.2941(4)	0.4947(4)	0.1948(3)	1.9(1)
C(12)	0.3623(4)	0.4462(4)	0.2066(2)	1.9(1)
C(13)	0.4630(4)	0.5045(4)	0.2518(3)	2.1(1)
C(14)	0.5379(4)	0.4573(4)	0.2614(3)	2.2(1)
C(15)	0.4981(4)	0.3583(4)	0.2779(3)	2.4(1)
C(16)	0.4617(4)	0.3571(4)	0.3350(3)	1.8(1)
C(21)	-0.0037(4)	0.3068(4)	0.3418(3)	1.9(1)
C(22)	0.0740(4)	0.2763(4)	0.3792(3)	2.2(1)
C(23)	0.0295(4)	0.2081(4)	0.4198(3)	2.2(1)
C(24)	0.1047(5)	0.1833(4)	0.4634(3)	2.4(1)
C(25)	0.1709(4)	0.1480(4)	0.4333(3)	2.2(1)
C(26)	0.1089(4)	0.0639(4)	0.3844(3)	2.0(1)
C(31)	-0.0583(4)	0.0960(4)	0.0876(2)	1.8(1)
C(32)	-0.0250(4)	0.0244(4)	0.1189(3)	2.1(1)
C(33)	-0.0015(4)	-0.0395(4)	0.0759(3)	2.1(1)
C(34)	0.0307(4)	-0.1134(4)	0.1040(3)	2.2(1)
C(35)	0.1206(4)	-0.0721(4)	0.1584(3)	2.0(1)
C(36)	0.2082(4)	0.0076(4)	0.1463(3)	2.1(1)
C(111)	0.1161(4)	0.5047(4)	0.1331(3)	1.8(1)
C(112)	0.1527(4)	0.5954(4)	0.1659(3)	2.4(1)
C(113)	0.1056(5)	0.6580(4)	0.1512(3)	2.8(2)
C(114)	0.0235(5)	0.6315(5)	0.1041(3)	3.0(2)
C(115)	-0.0130(5)	0.5418(5)	0.0714(3)	2.7(2)
C(116)	0.0329(4)	0.4794(4)	0.0858(3)	2.1(1)
C(121)	0.1918(4)	0.3769(4)	0.0852(2)	1.9(1)
C(122)	0.2209(5)	0.4377(5)	0.0451(3)	2.7(2)
C(123)	0.2421(5)	0.4068(5)	-0.0060(3)	3.3(2)
C(124)	0.2384(5)	0.3162(6)	-0.0166(3)	3.3(2)
C(125)	0.2121(5)	0.2555(5)	0.0235(3)	3.1(2)
C(126)	0.1863(4)	0.2848(4)	0.0737(3)	2.2(1)
C(211)	0.5456(4)	0.2252(4)	0.3713(3)	2.0(1)
C(212)	0.5511(5)	0.1441(4)	0.3426(3)	2.4(1)
C(213)	0.6426(5)	0.1373(5)	0.3460(3)	3.0(2)
C(214)	0.7285(5)	0.2100(5)	0.3780(3)	3.2(2)
C(215)	0.7247(5)	0.2893(5)	0.4072(3)	3.0(2)
C(216)	0.6331(5)	0.2962(4)	0.4041(3)	2.6(1)
C(221)	0.4264(4)	0.2743(4)	0.4365(3)	2.1(1)
C(222)	0.4444(5)	0.2199(5)	0.4795(3)	2.6(1)
C(223)	0.4389(5)	0.2406(6)	0.5372(3)	3.8(2)
C(224)	0.4156(6)	0.3162(6)	0.5532(3)	4.5(2)
C(225)	0.3965(6)	0.3702(6)	0.5110(4)	4.4(2)
C(226)	0.4015(5)	0.3504(5)	0.4532(3)	3.2(2)
C(311)	-0.0673(4)	0.4136(4)	0.2600(2)	1.7(1)
C(312)	-0.1522(5)	0.3843(5)	0.2808(3)	3.2(2)
C(313)	-0.2290(5)	0.4148(6)	0.2598(4)	4.1(2)
C(314)	-0.2212(5)	0.4756(5)	0.2185(3)	2.9(2)
C(315)	-0.1381(5)	0.5051(4)	0.1974(3)	2.7(1)
C(316)	-0.0624(5)	0.4744(4)	0.2181(3)	2.4(1)
C(321)	0.1347(4)	0.4796(4)	0.3276(3)	2.1(1)
C(322)	0.2315(4)	0.4835(4)	0.3397(3)	2.4(1)
C(323)	0.3086(5)	0.5589(5)	0.3772(3)	3.4(2)

C(324)	0.2908(5)	0.6347(5)	0.4006(3)	3.8(2)
C(325)	0.1955(6)	0.6330(5)	0.3886(4)	4.4(2)
C(326)	0.1188(5)	0.5564(5)	0.3523(3)	3.5(2)
C(411)	0.2371(4)	-0.0386(4)	0.4034(3)	1.9(1)
C(412)	0.3357(5)	-0.0283(4)	0.4108(3)	2.3(1)
C(413)	0.3783(5)	-0.0716(5)	0.4522(3)	2.7(1)
C(414)	0.3232(5)	-0.1264(4)	0.4870(3)	2.8(2)
C(415)	0.2251(5)	-0.1369(5)	0.4804(3)	2.7(1)
C(416)	0.1822(4)	-0.0940(4)	0.4387(3)	2.3(1)
C(421)	0.0767(4)	-0.0893(4)	0.3017(3)	1.8(1)
C(422)	-0.0083(5)	-0.0809(4)	0.2693(3)	2.3(1)
C(423)	-0.0874(5)	-0.1572(5)	0.2345(3)	2.8(2)
C(424)	-0.0817(5)	-0.2454(5)	0.2309(3)	3.3(2)
C(425)	0.0021(5)	-0.2558(5)	0.2616(3)	3.1(2)
C(426)	0.0806(5)	-0.1792(4)	0.2963(3)	2.5(1)
C(511)	-0.1385(4)	0.2377(4)	0.0829(3)	1.6(1)
C(512)	-0.1406(5)	0.2265(4)	0.0225(3)	2.5(1)
C(513)	-0.1924(5)	0.2664(5)	-0.0173(3)	2.9(1)
C(514)	-0.2412(5)	0.3191(5)	0.0029(3)	3.0(2)
C(515)	-0.2377(5)	0.3328(5)	0.0628(3)	3.0(2)
C(516)	-0.1871(4)	0.2924(4)	0.1014(3)	2.1(1)
C(521)	-0.1695(4)	0.1129(4)	0.1679(2)	1.7(1)
C(522)	-0.2674(4)	0.0704(4)	0.1346(3)	2.2(1)
C(523)	-0.3405(4)	0.0110(4)	0.1583(3)	2.4(1)
C(524)	-0.3166(5)	-0.0084(4)	0.2154(3)	2.7(2)
C(525)	-0.2195(5)	0.0314(4)	0.2483(3)	2.5(1)
C(526)	-0.1466(4)	0.0921(4)	0.2253(3)	2.1(1)
C(611)	0.3512(4)	-0.0482(4)	0.2145(3)	2.0(1)
C(612)	0.3837(5)	-0.0803(5)	0.1680(3)	2.9(2)
C(613)	0.4043(5)	-0.1610(5)	0.1691(3)	3.3(2)
C(614)	0.3933(5)	-0.2121(5)	0.2157(4)	3.6(2)
C(615)	0.3613(5)	-0.1813(5)	0.2617(3)	3.3(2)
C(616)	0.3403(5)	-0.1000(4)	0.2608(3)	2.6(1)
C(621)	0.4064(5)	0.1371(4)	0.1783(3)	2.1(1)
C(622)	0.3791(5)	0.1974(5)	0.1426(3)	2.7(1)
C(623)	0.4471(5)	0.2649(5)	0.1196(3)	3.1(2)
C(624)	0.5449(6)	0.2737(5)	0.1330(3)	3.7(2)
C(625)	0.5733(5)	0.2150(5)	0.1682(3)	3.4(2)
C(626)	0.5056(5)	0.1463(5)	0.1904(3)	2.8(2)
C(711)	0.1501(9)	0.3822(7)	0.6136(4)	5.9(3)
C(712)	0.0486(7)	0.3545(6)	0.5904(4)	5.1(3)
C(713)	0.0178(7)	0.3822(7)	0.5381(5)	5.6(3)
C(714)	0.0836(7)	0.4336(6)	0.5084(4)	4.7(2)
C(715)	0.1838(7)	0.4596(6)	0.5310(4)	5.2(2)
C(716)	0.2165(7)	0.4348(7)	0.5838(5)	5.9(3)
C(721)	0.1871(6)	0.1466(7)	0.6270(4)	5.0(2)
C(722)	0.1969(6)	0.0732(6)	0.5943(4)	4.6(2)
C(723)	0.2836(7)	0.0596(6)	0.6074(3)	4.3(2)
C(724)	0.3614(6)	0.1177(6)	0.6534(3)	4.0(2)
C(725)	0.3517(6)	0.1908(6)	0.6855(3)	4.3(2)
C(726)	0.2652(7)	0.2050(6)	0.6722(4)	5.1(2)
C(731)	0.3792(7)	0.3404(9)	0.8479(4)	5.8(3)
C(732)	0.3720(7)	0.2556(8)	0.8620(5)	5.9(3)
C(733)	0.4247(8)	0.2474(8)	0.9145(5)	6.2(3)
C(734)	0.4891(8)	0.327(1)	0.9538(4)	7.3(3)
C(735)	0.4977(7)	0.4148(8)	0.9368(5)	6.7(3)
C(736)	0.4408(8)	0.4208(7)	0.8850(5)	6.2(3)
C(741)	0.4537(6)	0.0470(6)	0.0281(3)	4.0(2)
C(742)	0.4133(5)	-0.0501(6)	0.0145(3)	4.0(2)
C(743)	0.4598(6)	-0.0967(5)	-0.0126(3)	3.9(2)
H(1)	0.3195	0.5439	0.1720	2.3
H(2)	0.2927	0.5243	0.2321	2.3
H(3)	0.3295	0.3884	0.2209	2.2

H(4)	0.3751	0.4284	0.1694	2.2
H(5)	0.4925	0.5643	0.2386	2.5
H(6)	0.4500	0.5177	0.2894	2.5
H(7)	0.5580	0.4522	0.2247	2.6
H(8)	0.5948	0.4959	0.2915	2.6
H(9)	0.4443	0.3172	0.2462	2.8
H(10)	0.5496	0.3336	0.2835	2.8
H(11)	0.4060	0.3760	0.3282	2.2
H(12)	0.5137	0.4031	0.3659	2.2
H(13)	-0.0215	0.3459	0.3675	2.4
H(14)	-0.0617	0.2509	0.3243	2.4
H(15)	0.1013	0.2466	0.3538	2.9
H(16)	0.1276	0.3314	0.4033	2.9
H(17)	-0.0049	0.2354	0.4413	2.7
H(18)	-0.0186	0.1504	0.3953	2.7
H(19)	0.1455	0.2385	0.4923	2.9
H(20)	0.0701	0.1344	0.4839	2.9
H(21)	0.2114	0.1994	0.4165	2.8
H(22)	0.2145	0.1308	0.4624	2.8
H(23)	0.0655	0.0823	0.3561	2.5
H(24)	0.0684	0.0138	0.4021	2.5
H(25)	-0.1213	0.0617	0.0601	2.2
H(26)	-0.0111	0.1254	0.0651	2.2
H(27)	0.0326	0.0570	0.1509	2.5
H(28)	-0.0768	-0.0148	0.1359	2.5
H(29)	-0.0591	-0.0708	0.0436	2.5
H(30)	0.0509	-0.0002	0.0597	2.5
H(31)	-0.0246	-0.1560	0.1163	2.7
H(32)	0.0467	-0.1483	0.0750	2.7
H(33)	0.1010	-0.0491	0.1908	2.5
H(34)	0.1421	-0.1224	0.1699	2.5
H(35)	0.1869	0.0573	0.1348	2.4
H(36)	0.2284	-0.0159	0.1141	2.4
H(37)	0.2108	0.6145	0.1992	3.0
H(38)	0.1309	0.7209	0.1749	3.4
H(39)	-0.0084	0.6749	0.0939	3.8
H(40)	-0.0718	0.5217	0.0387	3.2
H(41)	0.0072	0.4170	0.0621	2.5
H(42)	0.2262	0.5028	0.0527	3.3
H(43)	0.2611	0.4498	-0.0343	4.1
H(44)	0.2529	0.2954	-0.0524	3.9
H(45)	0.2125	0.1918	0.0174	3.7
H(46)	0.1644	0.2411	0.1006	2.5
H(47)	-0.1578	0.3426	0.3109	4.1
H(48)	-0.2884	0.3929	0.2743	4.9
H(49)	-0.2732	0.4974	0.2045	3.4
H(50)	-0.1316	0.5472	0.1678	3.2
H(51)	-0.0033	0.4971	0.2030	2.9
H(52)	0.2448	0.4318	0.3218	3.0
H(53)	0.3743	0.5579	0.3874	4.0
H(54)	0.3450	0.6900	0.4249	4.5
H(55)	0.1813	0.6846	0.4057	5.2
H(56)	0.0517	0.5548	0.3440	4.1
H(57)	-0.1045	0.1912	0.0080	3.2
H(58)	-0.1946	0.2567	-0.0589	3.5
H(59)	-0.2783	0.3460	-0.0245	3.7
H(60)	-0.2688	0.3723	0.0783	3.6
H(61)	-0.1852	0.3027	0.1431	2.7
H(62)	-0.2840	0.0831	0.0949	2.6
H(63)	-0.4074	-0.0170	0.1337	3.0
H(64)	-0.3692	-0.0502	0.2313	3.2
H(65)	-0.2026	0.0172	0.2878	2.9
H(66)	-0.0793	0.1206	0.2491	2.5

H(67)	0.4908	0.0928	0.3198	3.2
H(68)	0.6456	0.0807	0.3261	3.6
H(69)	0.7927	0.2058	0.3804	3.7
H(70)	0.7858	0.3406	0.4302	3.7
H(71)	0.6293	0.3514	0.4248	3.4
H(72)	0.4627	0.1678	0.4684	3.2
H(73)	0.4505	0.1988	0.5661	4.7
H(74)	0.4139	0.3324	0.5934	5.3
H(75)	0.3788	0.4229	0.5220	5.2
H(76)	0.3878	0.3892	0.4243	4.1
H(77)	0.3750	0.0084	0.3858	2.9
H(78)	0.4463	-0.0639	0.4565	3.2
H(79)	0.3531	-0.1560	0.5160	3.3
H(80)	0.1865	-0.1747	0.5051	3.2
H(81)	0.1133	-0.1029	0.4337	2.8
H(82)	0.3947	-0.0437	0.1357	3.6
H(83)	0.4241	-0.1838	0.1361	4.0
H(84)	0.4080	-0.2687	0.2155	4.4
H(85)	0.3547	-0.2153	0.2954	4.1
H(86)	0.3167	-0.0799	0.2928	3.2
H(87)	0.3100	0.1925	0.1337	3.2
H(88)	0.4266	0.3042	0.0932	3.6
H(89)	0.5934	0.3214	0.1183	4.6
H(90)	0.6417	0.2216	0.1775	4.0
H(91)	0.5271	0.1047	0.2148	3.4
H(92)	-0.0119	-0.0186	0.2713	2.7
H(93)	-0.1455	-0.1488	0.2132	3.4
H(94)	-0.1369	-0.3000	0.2069	4.0
H(95)	0.0057	-0.3183	0.2585	3.7
H(96)	0.1391	-0.1884	0.3168	3.0
H(97)	0.1737	0.3628	0.6509	7.2
H(98)	-0.0008	0.3170	0.6111	6.0
H(99)	-0.0532	0.3648	0.5209	6.7
H(100)	0.0611	0.4531	0.4717	6.1
H(101)	0.2298	0.4938	0.5079	6.1
H(102)	0.2884	0.4566	0.6010	7.0
H(103)	0.1242	0.1568	0.6180	6.0
H(104)	0.1417	0.0321	0.5629	5.6
H(105)	0.2911	0.0093	0.5834	5.1
H(106)	0.4224	0.1064	0.6638	4.9
H(107)	0.4062	0.2319	0.7174	5.1
H(108)	0.2588	0.2571	0.6949	6.1
H(109)	0.3370	0.3443	0.8104	6.6
H(110)	0.3285	0.2001	0.8338	7.5
H(111)	0.4161	0.1830	0.9240	7.2
H(112)	0.5267	0.3241	0.9924	8.9
H(113)	0.5458	0.4735	0.9624	8.0
H(114)	0.4466	0.4841	0.8745	7.3
H(115)	0.3503	-0.0862	0.0240	4.7
H(116)	0.4216	0.0804	0.0470	4.9
H(117)	0.4320	-0.1646	-0.0223	4.7

^a Estimated standard deviations are given in parentheses. ^b All non-H atoms were assigned with anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8^2/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos + 2U_{13}aa^*cc^*\cos + 2U_{23}bb^*cc^*\cos)$. ^c All hydrogen were calculated with C-H = 0.95 Å, and were not refined with the appropriate B_{iso} .

Table S3-3. Final Anisotropic Thermal Parameters for 11.3.5C₆H₆^{a,b}

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg(1)	0.0240(1)	0.0253(1)	0.0266(1)	0.01459(9)	0.00444(9)	0.00678(9)

Pt(1)	0.0173(1)	0.0179(1)	0.0201(1)	0.00774(10)	0.00452(9)	0.00362(9)
Pt(2)	0.0210(1)	0.0220(1)	0.0215(1)	0.0101(1)	0.0060(1)	0.0056(1)
P(1)	0.0179(8)	0.0189(8)	0.0229(8)	0.0069(6)	0.0054(6)	0.0057(6)
P(2)	0.0194(8)	0.0227(8)	0.0224(8)	0.0089(7)	0.0049(6)	0.0058(6)
P(3)	0.0191(8)	0.0208(8)	0.0231(8)	0.0081(6)	0.0069(6)	0.0017(6)
P(4)	0.0215(8)	0.0232(8)	0.0220(8)	0.0103(7)	0.0063(6)	0.0061(6)
P(5)	0.0191(8)	0.0198(8)	0.0202(8)	0.0081(6)	0.0047(6)	0.0044(6)
P(6)	0.0240(8)	0.0244(8)	0.0217(8)	0.0133(7)	0.0072(6)	0.0040(6)
C(11)	0.020(3)	0.016(3)	0.036(4)	0.012(2)	0.001(3)	0.006(3)
C(12)	0.013(3)	0.026(3)	0.013(3)	-0.017(2)	0.009(2)	-0.009(2)
C(13)	0.026(3)	0.026(3)	0.029(3)	0.008(3)	0.008(3)	0.012(3)
C(14)	0.021(3)	0.030(3)	0.030(3)	0.008(3)	0.004(3)	0.007(3)
C(15)	0.026(3)	0.030(4)	0.041(4)	0.011(3)	0.023(3)	0.007(3)
C(16)	0.022(3)	0.024(3)	0.027(3)	0.012(3)	0.007(3)	0.007(3)
C(21)	0.026(3)	0.025(3)	0.027(3)	0.014(3)	0.012(3)	0.007(3)
C(22)	0.032(4)	0.030(3)	0.026(3)	0.017(3)	0.010(3)	0.001(3)
C(23)	0.034(4)	0.030(3)	0.027(3)	0.018(3)	0.014(3)	0.007(3)
C(24)	0.041(4)	0.031(4)	0.023(3)	0.016(3)	0.010(3)	0.007(3)
C(25)	0.028(3)	0.030(4)	0.027(3)	0.014(3)	0.004(3)	0.001(3)
C(26)	0.027(3)	0.030(3)	0.030(3)	0.017(3)	0.014(3)	0.007(3)
C(31)	0.020(3)	0.022(3)	0.026(3)	0.009(2)	0.004(2)	0.003(3)
C(32)	0.030(3)	0.024(3)	0.027(3)	0.015(3)	0.005(3)	0.004(3)
C(33)	0.030(3)	0.025(3)	0.024(3)	0.013(3)	0.004(3)	-0.005(3)
C(34)	0.032(3)	0.029(3)	0.024(3)	0.015(3)	0.003(3)	-0.003(3)
C(35)	0.031(3)	0.023(3)	0.025(3)	0.013(3)	0.005(3)	0.003(3)
C(36)	0.029(3)	0.036(4)	0.025(3)	0.019(3)	0.012(3)	0.010(3)
C(111)	0.020(3)	0.021(3)	0.034(3)	0.012(3)	0.010(3)	0.011(3)
C(112)	0.029(3)	0.022(3)	0.039(4)	0.008(3)	0.008(3)	0.008(3)
C(113)	0.039(4)	0.030(4)	0.048(4)	0.022(3)	0.016(3)	0.008(3)
C(114)	0.044(4)	0.036(4)	0.061(5)	0.030(3)	0.030(4)	0.033(4)
C(115)	0.034(4)	0.039(4)	0.041(4)	0.022(3)	0.012(3)	0.019(3)
C(116)	0.020(3)	0.030(3)	0.034(4)	0.012(3)	0.010(3)	0.016(3)
C(121)	0.019(3)	0.032(3)	0.022(3)	0.013(3)	0.003(2)	0.003(3)
C(122)	0.036(4)	0.046(4)	0.033(4)	0.025(3)	0.015(3)	0.015(3)
C(123)	0.035(4)	0.062(5)	0.037(4)	0.022(4)	0.016(3)	0.020(4)
C(124)	0.036(4)	0.067(5)	0.026(4)	0.022(4)	0.012(3)	-0.002(4)
C(125)	0.035(4)	0.033(4)	0.046(4)	0.014(3)	0.009(3)	-0.015(3)
C(126)	0.025(3)	0.029(3)	0.032(4)	0.011(3)	0.008(3)	0.006(3)
C(211)	0.025(3)	0.031(3)	0.025(3)	0.013(3)	0.007(3)	0.016(3)
C(212)	0.035(4)	0.035(4)	0.022(3)	0.016(3)	0.004(3)	0.007(3)
C(213)	0.041(4)	0.052(4)	0.039(4)	0.034(4)	0.014(3)	0.018(3)
C(214)	0.032(4)	0.059(5)	0.043(4)	0.025(4)	0.017(3)	0.029(4)
C(215)	0.023(3)	0.046(4)	0.045(4)	0.012(3)	0.008(3)	0.025(3)
C(216)	0.030(4)	0.033(4)	0.037(4)	0.015(3)	0.003(3)	0.011(3)
C(221)	0.019(3)	0.033(4)	0.020(3)	0.003(3)	0.002(2)	-0.001(3)
C(222)	0.026(3)	0.038(4)	0.029(4)	0.005(3)	0.004(3)	0.006(3)
C(223)	0.037(4)	0.071(6)	0.021(4)	0.005(4)	0.005(3)	0.009(4)
C(224)	0.045(5)	0.080(6)	0.025(4)	0.001(4)	0.015(3)	-0.009(4)
C(225)	0.058(5)	0.059(5)	0.049(5)	0.017(4)	0.026(4)	-0.005(4)
C(226)	0.043(4)	0.043(4)	0.040(4)	0.017(4)	0.017(3)	0.002(3)
C(311)	0.023(3)	0.021(3)	0.022(3)	0.010(3)	0.006(2)	0.001(2)
C(312)	0.031(4)	0.060(5)	0.045(4)	0.023(4)	0.018(3)	0.028(4)
C(313)	0.022(4)	0.078(6)	0.070(6)	0.025(4)	0.025(4)	0.034(5)
C(314)	0.027(4)	0.040(4)	0.048(4)	0.022(3)	0.005(3)	0.006(3)
C(315)	0.034(4)	0.034(4)	0.043(4)	0.020(3)	0.014(3)	0.015(3)
C(316)	0.031(4)	0.024(3)	0.043(4)	0.015(3)	0.013(3)	0.006(3)
C(321)	0.022(3)	0.028(3)	0.029(3)	0.008(3)	0.007(3)	0.001(3)
C(322)	0.025(3)	0.030(4)	0.036(4)	0.009(3)	0.008(3)	-0.001(3)
C(323)	0.028(4)	0.047(5)	0.047(4)	0.010(3)	0.005(3)	-0.005(4)
C(324)	0.034(4)	0.039(4)	0.055(5)	0.002(3)	0.002(4)	-0.013(4)
C(325)	0.046(5)	0.043(5)	0.068(6)	0.017(4)	0.001(4)	-0.029(4)
C(326)	0.026(4)	0.038(4)	0.060(5)	0.013(3)	0.003(3)	-0.021(4)
C(411)	0.029(3)	0.017(3)	0.026(3)	0.010(3)	0.007(3)	0.002(2)

C(412)	0.032(4)	0.033(4)	0.025(3)	0.013(3)	0.007(3)	0.008(3)
C(413)	0.029(4)	0.040(4)	0.032(4)	0.016(3)	-0.001(3)	0.004(3)
C(414)	0.045(4)	0.031(4)	0.029(4)	0.017(3)	0.001(3)	0.007(3)
C(415)	0.042(4)	0.035(4)	0.029(3)	0.014(3)	0.010(3)	0.016(3)
C(416)	0.029(3)	0.035(4)	0.027(3)	0.013(3)	0.010(3)	0.011(3)
C(421)	0.025(3)	0.022(3)	0.025(3)	0.008(3)	0.008(3)	0.010(2)
C(422)	0.034(4)	0.029(3)	0.027(3)	0.016(3)	0.009(3)	-0.005(3)
C(423)	0.027(4)	0.040(4)	0.037(4)	0.012(3)	0.006(3)	0.004(3)
C(424)	0.034(4)	0.040(4)	0.040(4)	0.006(3)	0.004(3)	-0.008(3)
C(425)	0.044(4)	0.028(4)	0.047(4)	0.016(3)	0.011(3)	0.004(3)
C(426)	0.035(4)	0.030(4)	0.029(4)	0.011(3)	0.007(3)	0.005(3)
C(511)	0.016(3)	0.018(3)	0.027(3)	0.004(2)	0.007(2)	0.007(2)
C(512)	0.033(4)	0.030(4)	0.028(3)	0.009(3)	0.006(3)	0.007(3)
C(513)	0.036(4)	0.039(4)	0.028(4)	0.007(3)	0.003(3)	0.017(3)
C(514)	0.025(3)	0.036(4)	0.050(5)	0.007(3)	0.002(3)	0.025(3)
C(515)	0.027(4)	0.033(4)	0.059(5)	0.012(3)	0.013(3)	0.019(3)
C(516)	0.023(3)	0.025(3)	0.034(4)	0.008(3)	0.006(3)	0.014(3)
C(521)	0.026(3)	0.019(3)	0.022(3)	0.012(3)	0.008(2)	0.003(2)
C(522)	0.020(3)	0.030(3)	0.027(3)	0.006(3)	0.000(3)	0.005(3)
C(523)	0.023(3)	0.023(3)	0.040(4)	0.002(3)	0.006(3)	0.005(3)
C(524)	0.039(4)	0.029(4)	0.044(4)	0.011(3)	0.027(3)	0.014(3)
C(525)	0.039(4)	0.037(4)	0.022(3)	0.016(3)	0.013(3)	0.008(3)
C(526)	0.025(3)	0.026(3)	0.027(3)	0.009(3)	0.006(3)	0.005(3)
C(611)	0.017(3)	0.024(3)	0.035(4)	0.008(3)	0.004(3)	0.001(3)
C(612)	0.036(4)	0.034(4)	0.039(4)	0.013(3)	0.013(3)	0.001(3)
C(613)	0.034(4)	0.033(4)	0.060(5)	0.016(3)	0.013(4)	-0.009(4)
C(614)	0.034(4)	0.020(4)	0.079(6)	0.014(3)	0.000(4)	-0.006(4)
C(615)	0.042(4)	0.025(4)	0.054(5)	0.017(3)	-0.003(3)	0.008(3)
C(616)	0.035(4)	0.034(4)	0.035(4)	0.017(3)	0.008(3)	0.009(3)
C(621)	0.033(4)	0.026(3)	0.024(3)	0.013(3)	0.010(3)	0.001(3)
C(622)	0.035(4)	0.039(4)	0.033(4)	0.017(3)	0.014(3)	0.006(3)
C(623)	0.049(4)	0.035(4)	0.039(4)	0.016(3)	0.022(3)	0.011(3)
C(624)	0.050(5)	0.043(4)	0.051(5)	0.009(4)	0.039(4)	0.007(4)
C(625)	0.033(4)	0.045(4)	0.052(5)	0.009(3)	0.023(4)	0.000(4)
C(626)	0.034(4)	0.043(4)	0.033(4)	0.018(3)	0.008(3)	0.001(3)
C(711)	0.111(9)	0.082(7)	0.052(6)	0.065(7)	0.015(6)	0.010(5)
C(712)	0.075(7)	0.057(6)	0.079(7)	0.037(5)	0.037(6)	0.010(5)
C(713)	0.056(6)	0.066(6)	0.091(8)	0.025(5)	0.021(6)	-0.003(6)
C(714)	0.078(7)	0.048(5)	0.047(5)	0.030(5)	-0.007(5)	-0.011(4)
C(715)	0.077(7)	0.043(5)	0.066(6)	0.011(5)	0.020(5)	-0.005(4)
C(716)	0.062(6)	0.089(8)	0.070(7)	0.033(6)	0.008(5)	-0.001(6)
C(721)	0.058(6)	0.085(7)	0.056(6)	0.036(5)	0.013(5)	0.030(5)
C(722)	0.056(5)	0.058(6)	0.047(5)	0.011(5)	-0.003(4)	0.018(4)
C(723)	0.076(6)	0.051(5)	0.039(5)	0.023(5)	0.022(4)	0.013(4)
C(724)	0.052(5)	0.059(5)	0.046(5)	0.018(4)	0.017(4)	0.028(4)
C(725)	0.063(6)	0.056(5)	0.039(4)	0.014(4)	0.010(4)	0.014(4)
C(726)	0.089(7)	0.071(6)	0.047(5)	0.047(6)	0.014(5)	0.015(5)
C(731)	0.071(7)	0.107(9)	0.046(5)	0.045(7)	0.006(5)	0.004(6)
C(732)	0.060(6)	0.079(7)	0.077(7)	0.028(6)	0.013(5)	-0.028(6)
C(733)	0.090(8)	0.089(8)	0.091(8)	0.064(7)	0.037(7)	0.022(7)
C(734)	0.073(7)	0.18(1)	0.052(6)	0.087(9)	0.001(5)	0.007(8)
C(735)	0.044(6)	0.089(8)	0.095(9)	0.005(6)	0.008(6)	-0.024(7)
C(736)	0.081(7)	0.080(7)	0.072(7)	0.016(6)	0.036(6)	0.027(6)
C(741)	0.051(5)	0.055(5)	0.038(4)	0.017(4)	0.003(4)	0.000(4)
C(742)	0.039(4)	0.060(5)	0.030(4)	-0.003(4)	0.002(3)	0.004(4)
C(743)	0.064(5)	0.032(4)	0.036(4)	0.009(4)	-0.003(4)	0.001(3)

^a Estimated standard deviations are given in parentheses. ^b Parameters have the form $\exp(-2^2(U_{11}h^2a^2 + \dots + 2U_{12}hka^*b^*\cos + \dots))$

Table S3-4. Bond Lengths for Non-hydrogen Atoms of 11·3.5C₆H₆^a

atom	atom	distance	atom	atom	distance
Hg(1)	Pt(1)	2.7908(4)	C(11)	C(12)	1.452(8)
Hg(1)	Pt(2)	2.7952(4)	C(12)	C(13)	1.553(8)
Pt(1)	P(1)	2.279(2)	C(13)	C(14)	1.521(8)
Pt(1)	P(3)	2.281(2)	C(14)	C(15)	1.521(8)
Pt(1)	P(5)	2.273(2)	C(15)	C(16)	1.531(8)
Pt(2)	P(2)	2.287(2)	C(21)	C(22)	1.531(8)
Pt(2)	P(4)	2.288(2)	C(22)	C(23)	1.521(8)
Pt(2)	P(6)	2.291(2)	C(23)	C(24)	1.524(8)
P(1)	C(11)	1.836(6)	C(24)	C(25)	1.539(8)
P(1)	C(111)	1.834(6)	C(25)	C(26)	1.521(8)
P(1)	C(121)	1.841(6)	C(31)	C(32)	1.524(8)
P(2)	C(16)	1.850(6)	C(32)	C(33)	1.529(8)
P(2)	C(211)	1.849(6)	C(33)	C(34)	1.514(8)
P(2)	C(221)	1.838(6)	C(34)	C(35)	1.543(8)
P(3)	C(21)	1.844(6)	C(35)	C(36)	1.522(8)
P(3)	C(311)	1.841(6)	C(111)	C(112)	1.393(8)
P(3)	C(321)	1.839(6)	C(111)	C(116)	1.392(8)
P(4)	C(26)	1.848(6)	C(112)	C(113)	1.397(8)
P(4)	C(411)	1.847(6)	C(113)	C(114)	1.376(9)
P(4)	C(421)	1.842(6)	C(114)	C(115)	1.380(9)
P(5)	C(31)	1.845(6)	C(115)	C(116)	1.380(8)
P(5)	C(511)	1.835(6)	C(121)	C(122)	1.384(8)
P(5)	C(521)	1.843(6)	C(121)	C(126)	1.384(8)
P(6)	C(36)	1.850(6)	C(122)	C(123)	1.385(9)
P(6)	C(611)	1.851(6)	C(123)	C(124)	1.37(1)
P(6)	C(621)	1.844(6)	C(124)	C(125)	1.37(1)
C(125)	C(126)	1.396(8)	C(411)	C(416)	1.389(8)
C(211)	C(212)	1.405(8)	C(412)	C(413)	1.381(8)
C(211)	C(216)	1.385(8)	C(413)	C(414)	1.378(9)
C(212)	C(213)	1.388(8)	C(414)	C(415)	1.385(9)
C(213)	C(214)	1.38(1)	C(415)	C(416)	1.383(8)
C(214)	C(215)	1.37(1)	C(421)	C(422)	1.388(8)
C(215)	C(216)	1.394(9)	C(421)	C(426)	1.395(8)
C(221)	C(222)	1.388(8)	C(422)	C(423)	1.375(8)
C(221)	C(226)	1.396(9)	C(423)	C(424)	1.378(9)
C(222)	C(223)	1.385(9)	C(424)	C(425)	1.374(9)
C(223)	C(224)	1.37(1)	C(425)	C(426)	1.374(9)
C(224)	C(225)	1.37(1)	C(511)	C(512)	1.395(8)
C(225)	C(226)	1.38(1)	C(511)	C(516)	1.386(8)
C(311)	C(312)	1.381(8)	C(512)	C(513)	1.396(9)
C(311)	C(316)	1.387(8)	C(513)	C(514)	1.382(9)
C(312)	C(313)	1.396(9)	C(514)	C(515)	1.38(1)
C(313)	C(314)	1.375(9)	C(515)	C(516)	1.374(8)
C(314)	C(315)	1.360(9)	C(521)	C(522)	1.391(8)
C(315)	C(316)	1.381(8)	C(521)	C(526)	1.397(8)
C(321)	C(322)	1.388(8)	C(522)	C(523)	1.383(8)
C(321)	C(326)	1.388(8)	C(523)	C(524)	1.385(9)
C(322)	C(323)	1.381(9)	C(524)	C(525)	1.378(9)
C(323)	C(324)	1.38(1)	C(525)	C(526)	1.379(8)
C(324)	C(325)	1.38(1)	C(611)	C(612)	1.401(8)
C(325)	C(326)	1.377(9)	C(611)	C(616)	1.382(8)
C(411)	C(412)	1.392(8)	C(612)	C(613)	1.374(9)
C(613)	C(614)	1.38(1)	C(735)	C(736)	1.35(1)
C(614)	C(615)	1.38(1)	C(741)	C(742)	1.37(1)
C(615)	C(616)	1.385(8)	C(741)	C(743)*	1.37(1)
C(621)	C(622)	1.394(9)	C(742)	C(743)	1.36(1)
C(621)	C(626)	1.399(8)			
C(622)	C(623)	1.386(9)			

C(623)	C(624)	1.38(1)
C(624)	C(625)	1.37(1)
C(625)	C(626)	1.381(9)
C(711)	C(712)	1.39(1)
C(711)	C(716)	1.37(1)
C(712)	C(713)	1.36(1)
C(713)	C(714)	1.36(1)
C(714)	C(715)	1.37(1)
C(715)	C(716)	1.36(1)
C(721)	C(722)	1.38(1)
C(721)	C(726)	1.37(1)
C(722)	C(723)	1.36(1)
C(723)	C(724)	1.38(1)
C(724)	C(725)	1.37(1)
C(725)	C(726)	1.36(1)
C(731)	C(732)	1.33(1)
C(731)	C(736)	1.35(1)
C(732)	C(733)	1.35(1)
C(733)	C(734)	1.38(1)
C(734)	C(735)	1.39(2)

^a Estimated standard deviations are given in parentheses.

Table S3-5. Bond Angles for Non-hydrogen Atoms of 11·3.5C₆H₆^a

atom	atom	atom	angle	atom	atom	atom	angle
Pt(1)	Hg(1)	Pt(2)	179.58(2)	Pt(1)	P(3)	C(311)	109.7(2)
Hg(1)	Pt(1)	P(1)	102.76(4)	Pt(1)	P(3)	C(321)	118.1(2)
Hg(1)	Pt(1)	P(3)	101.13(4)	C(21)	P(3)	C(311)	100.2(3)
Hg(1)	Pt(1)	P(5)	101.72(4)	C(21)	P(3)	C(321)	98.6(3)
P(1)	Pt(1)	P(3)	114.64(6)	C(311)	P(3)	C(321)	102.2(3)
P(1)	Pt(1)	P(5)	116.37(6)	Pt(2)	P(4)	C(26)	120.4(2)
P(3)	Pt(1)	P(5)	116.64(5)	Pt(2)	P(4)	C(411)	113.9(2)
Hg(1)	Pt(2)	P(2)	99.14(4)	Pt(2)	P(4)	C(421)	120.4(2)
Hg(1)	Pt(2)	P(4)	97.81(4)	C(26)	P(4)	C(411)	101.5(3)
Hg(1)	Pt(2)	P(6)	95.84(4)	C(26)	P(4)	C(421)	96.7(3)
P(2)	Pt(2)	P(4)	117.30(6)	C(411)	P(4)	C(421)	100.2(3)
P(2)	Pt(2)	P(6)	117.49(6)	Pt(1)	P(5)	C(31)	123.9(2)
P(4)	Pt(2)	P(6)	120.07(6)	Pt(1)	P(5)	C(511)	110.4(2)
Pt(1)	P(1)	C(11)	122.4(2)	Pt(1)	P(5)	C(521)	119.3(2)
Pt(1)	P(1)	C(111)	109.7(2)	C(31)	P(5)	C(511)	100.2(3)
Pt(1)	P(1)	C(121)	120.2(2)	C(31)	P(5)	C(521)	98.5(3)
C(11)	P(1)	C(111)	99.7(3)	C(511)	P(5)	C(521)	100.7(3)
C(11)	P(1)	C(121)	99.5(3)	Pt(2)	P(6)	C(36)	119.9(2)
C(111)	P(1)	C(121)	101.8(3)	Pt(2)	P(6)	C(611)	115.5(2)
Pt(2)	P(2)	C(16)	119.5(2)	Pt(2)	P(6)	C(621)	117.9(2)
Pt(2)	P(2)	C(211)	114.6(2)	C(36)	P(6)	C(611)	98.7(3)
Pt(2)	P(2)	C(221)	120.7(2)	C(36)	P(6)	C(621)	98.8(3)
C(16)	P(2)	C(211)	99.2(3)	C(611)	P(6)	C(621)	102.7(3)
C(16)	P(2)	C(221)	99.3(3)	P(1)	C(11)	C(12)	113.6(4)
C(211)	P(2)	C(221)	99.5(3)	C(11)	C(12)	C(13)	115.2(5)
Pt(1)	P(3)	C(21)	124.6(2)	C(12)	C(13)	C(14)	115.8(5)
C(13)	C(14)	C(15)	114.2(5)	C(121)	C(122)	C(123)	121.0(6)
C(14)	C(15)	C(16)	112.8(5)	C(122)	C(123)	C(124)	120.5(6)
P(2)	C(16)	C(15)	112.7(4)	C(123)	C(124)	C(125)	119.3(6)
P(3)	C(21)	C(22)	115.5(4)	C(124)	C(125)	C(126)	120.5(6)
C(21)	C(22)	C(23)	111.4(5)	C(121)	C(126)	C(125)	120.3(6)
C(22)	C(23)	C(24)	114.4(5)	P(2)	C(211)	C(212)	119.6(5)
C(23)	C(24)	C(25)	113.2(5)	P(2)	C(211)	C(216)	122.0(5)
C(24)	C(25)	C(26)	111.3(5)	C(212)	C(211)	C(216)	118.2(6)
P(4)	C(26)	C(25)	114.6(4)	C(211)	C(212)	C(213)	120.3(6)
P(5)	C(31)	C(32)	115.0(4)	C(212)	C(213)	C(214)	120.1(6)
C(31)	C(32)	C(33)	111.3(5)	C(213)	C(214)	C(215)	120.5(6)

C(32)	C(33)	C(34)	114.1(5)	C(214)	C(215)	C(216)	119.6(6)
C(33)	C(34)	C(35)	114.2(5)	C(211)	C(216)	C(215)	121.2(6)
C(34)	C(35)	C(36)	113.0(5)	P(2)	C(221)	C(222)	120.0(5)
P(6)	C(36)	C(35)	111.9(4)	P(2)	C(221)	C(226)	122.1(5)
P(1)	C(111)	C(112)	121.8(5)	C(222)	C(221)	C(226)	117.7(6)
P(1)	C(111)	C(116)	119.7(5)	C(221)	C(222)	C(223)	121.5(7)
C(112)	C(111)	C(116)	118.2(5)	C(222)	C(223)	C(224)	120.2(7)
C(111)	C(112)	C(113)	120.1(6)	C(223)	C(224)	C(225)	119.0(7)
C(112)	C(113)	C(114)	120.6(6)	C(224)	C(225)	C(226)	121.4(8)
C(113)	C(114)	C(115)	119.6(6)	C(221)	C(226)	C(225)	120.2(7)
C(114)	C(115)	C(116)	120.1(6)	P(3)	C(311)	C(312)	124.0(5)
C(111)	C(116)	C(115)	121.4(6)	P(3)	C(311)	C(316)	119.0(4)
P(1)	C(121)	C(122)	122.6(5)	C(312)	C(311)	C(316)	116.9(6)
P(1)	C(121)	C(126)	119.0(5)	C(311)	C(312)	C(313)	120.6(6)
C(122)	C(121)	C(126)	118.3(6)	C(312)	C(313)	C(314)	120.7(6)
C(313)	C(314)	C(315)	119.4(6)	C(421)	C(426)	C(425)	120.8(6)
C(314)	C(315)	C(316)	119.7(6)	P(5)	C(511)	C(512)	122.6(4)
C(311)	C(316)	C(315)	122.5(6)	P(5)	C(511)	C(516)	120.2(5)
P(3)	C(321)	C(322)	118.5(5)	C(512)	C(511)	C(516)	117.1(5)
P(3)	C(321)	C(326)	123.8(5)	C(511)	C(512)	C(513)	121.0(6)
C(322)	C(321)	C(326)	117.6(6)	C(512)	C(513)	C(514)	120.0(6)
C(321)	C(322)	C(323)	121.4(6)	C(513)	C(514)	C(515)	119.7(6)
C(322)	C(323)	C(324)	119.7(6)	C(514)	C(515)	C(516)	119.6(6)
C(323)	C(324)	C(325)	120.0(6)	C(511)	C(516)	C(515)	122.7(6)
C(324)	C(325)	C(326)	119.7(6)	P(5)	C(521)	C(522)	122.2(4)
C(321)	C(326)	C(325)	121.5(6)	P(5)	C(521)	C(526)	119.5(4)
P(4)	C(411)	C(412)	119.5(5)	C(522)	C(521)	C(526)	118.2(5)
P(4)	C(411)	C(416)	122.2(5)	C(521)	C(522)	C(523)	120.8(6)
C(412)	C(411)	C(416)	118.2(6)	C(522)	C(523)	C(524)	120.2(6)
C(411)	C(412)	C(413)	121.1(6)	C(523)	C(524)	C(525)	119.5(6)
C(412)	C(413)	C(414)	120.2(6)	C(524)	C(525)	C(526)	120.5(6)
C(413)	C(414)	C(415)	119.4(6)	C(521)	C(526)	C(525)	120.7(6)
C(414)	C(415)	C(416)	120.4(6)	P(6)	C(611)	C(612)	121.6(5)
C(411)	C(416)	C(415)	120.7(6)	P(6)	C(611)	C(616)	120.1(5)
P(4)	C(421)	C(422)	120.5(5)	C(612)	C(611)	C(616)	118.2(6)
P(4)	C(421)	C(426)	122.4(5)	C(611)	C(612)	C(613)	120.2(6)
C(422)	C(421)	C(426)	116.9(6)	C(612)	C(613)	C(614)	121.1(7)
C(421)	C(422)	C(423)	122.6(6)	C(613)	C(614)	C(615)	119.2(6)
C(422)	C(423)	C(424)	118.9(6)	C(614)	C(615)	C(616)	120.0(7)
C(423)	C(424)	C(425)	119.9(6)	C(611)	C(616)	C(615)	121.3(6)
C(424)	C(425)	C(426)	120.7(6)	P(6)	C(621)	C(622)	119.6(5)
P(6)	C(621)	C(626)	122.5(5)	C(741)	C(742)	C(743)	120.4(7)
C(622)	C(621)	C(626)	117.8(6)	C(741)	C(743)	C(742)	120.5(7)
C(621)	C(622)	C(623)	121.8(6)				
C(622)	C(623)	C(624)	119.3(7)				
C(623)	C(624)	C(625)	119.8(6)				
C(624)	C(625)	C(626)	121.4(7)				
C(621)	C(626)	C(625)	119.9(6)				
C(712)	C(711)	C(716)	120.5(9)				
C(711)	C(712)	C(713)	117.9(9)				
C(712)	C(713)	C(714)	121.6(9)				
C(713)	C(714)	C(715)	120.4(9)				
C(714)	C(715)	C(716)	119.2(9)				
C(711)	C(716)	C(715)	120.5(9)				
C(722)	C(721)	C(726)	119.6(8)				
C(721)	C(722)	C(723)	119.7(8)				
C(722)	C(723)	C(724)	120.5(8)				
C(723)	C(724)	C(725)	119.7(8)				
C(724)	C(725)	C(726)	119.8(8)				
C(721)	C(726)	C(725)	120.7(8)				
C(732)	C(731)	C(736)	121(1)				

C(731)	C(732)	C(733)	121(1)
C(732)	C(733)	C(734)	120(1)
C(733)	C(734)	C(735)	117.3(9)
C(734)	C(735)	C(736)	121(1)
C(731)	C(736)	C(735)	119(1)
C(742)	C(741)	C(743)	119.1(7)

^a Estimated deviations are given in parentheses.