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STRUCTURE REPORT

XCL Code: REW0406 **Date:** 13 July 2004

Compound: Bis(triphenylphosphine)(η^2–diphenylacetylene)platinum
Formula: $C_{50}H_{40}P_2Pt$

Supervisor: R. E. Wasylishen **Crystallographer:** R. McDonald

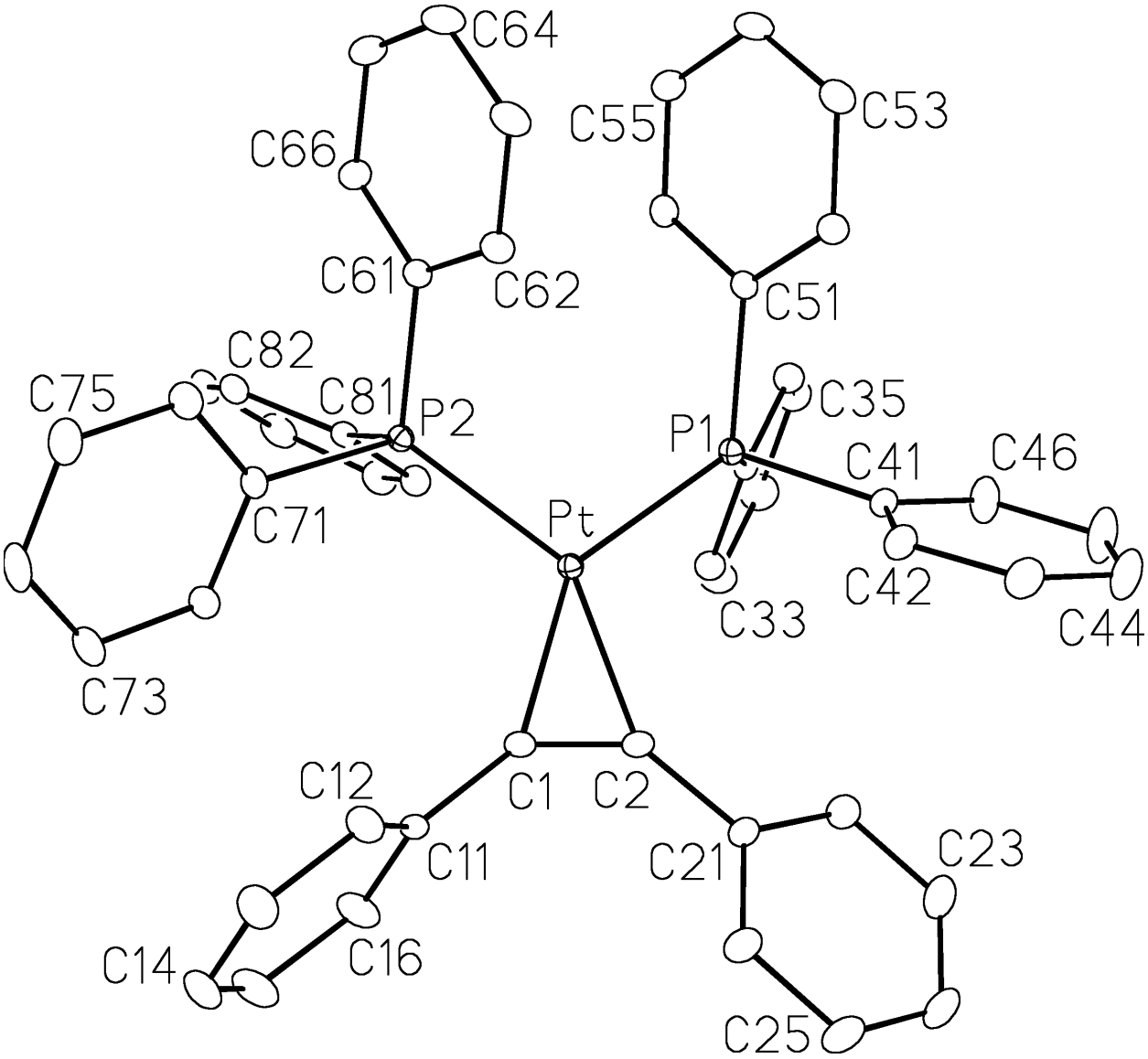
Figure Legends

Figure S1. Perspective view of one of the two crystallographically-independent molecules of bis(triphenylphosphine)(η^2–diphenylacetylene)platinum (molecule A) showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms are not shown.

Figure S2. Alternate view of molecule A showing the essentially planar arrangement of the atoms coordinated to platinum. Only the ipso carbons of the triphenylphosphine phenyl groups are shown.

Figure S3. View of the second crystallographically-independent molecules of bis-(triphenylphosphine)(η^2–diphenylacetylene)platinum (molecule B).

Figure S4. Alternate view of molecule B, showing only the ipso carbons of the triphenylphosphine phenyl rings.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C33
C44
C73
C12
C1
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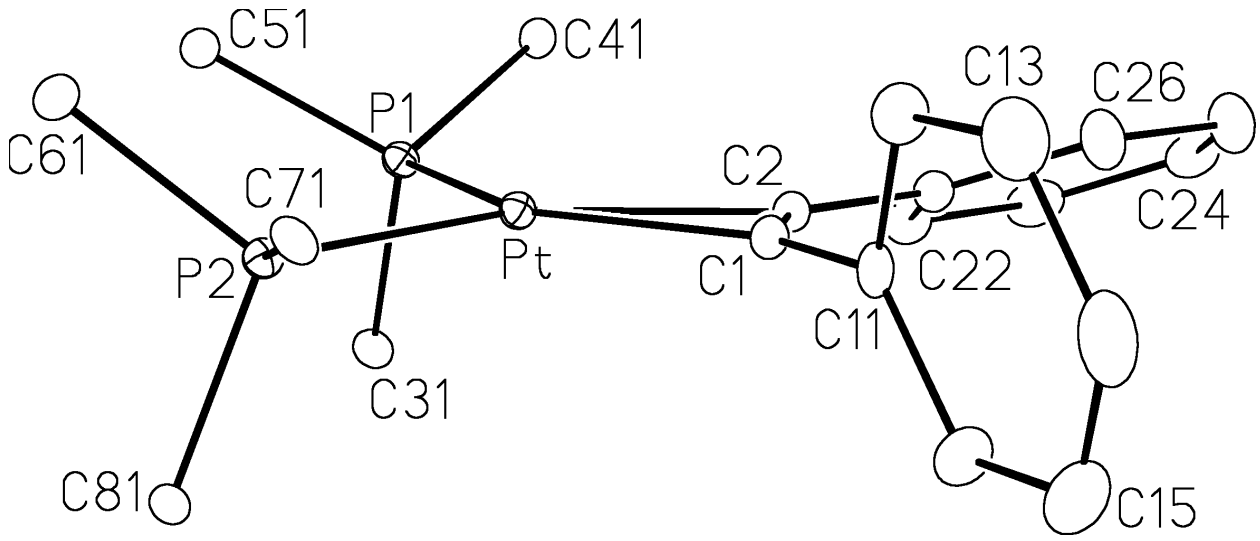
C16
C25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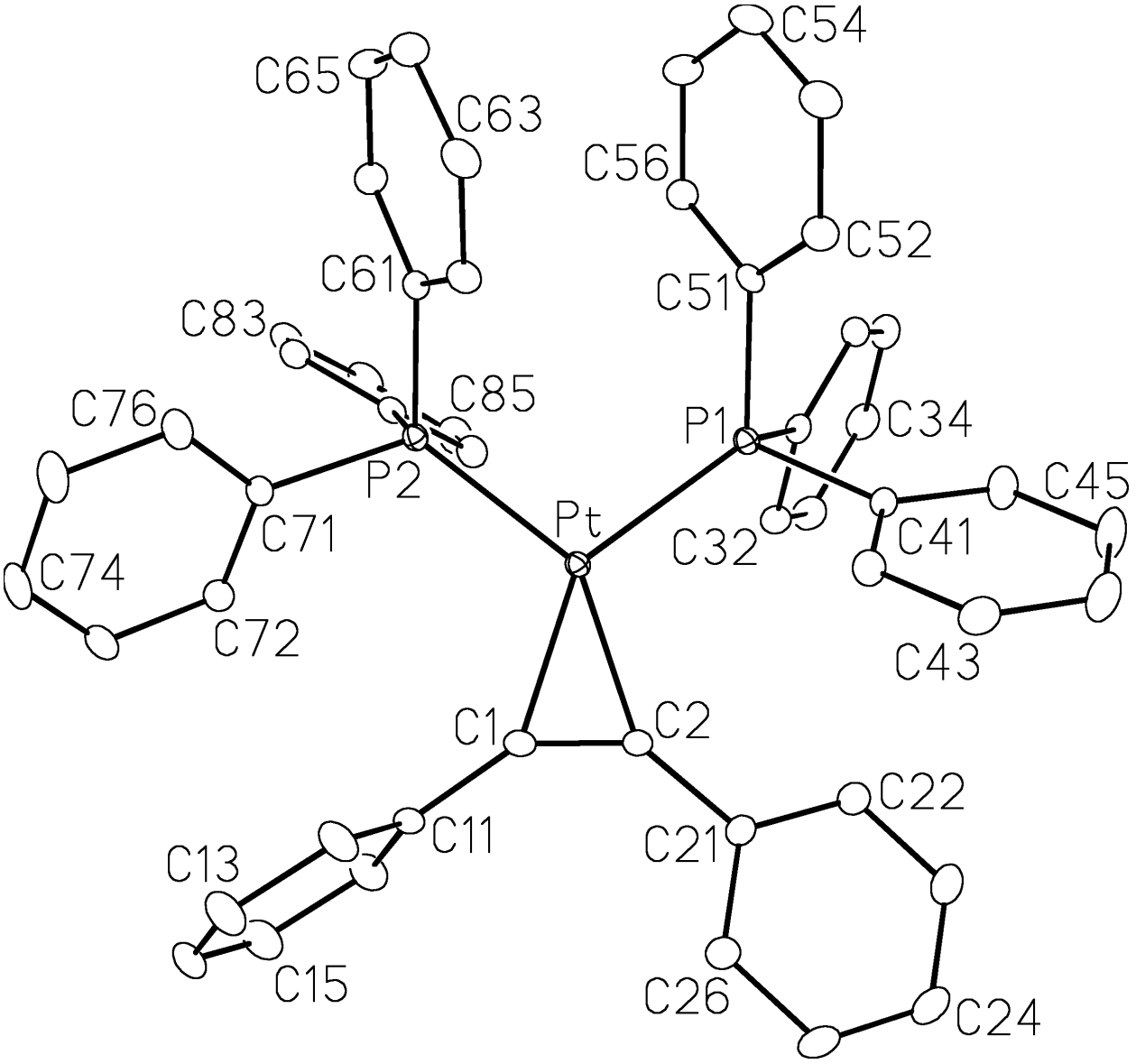
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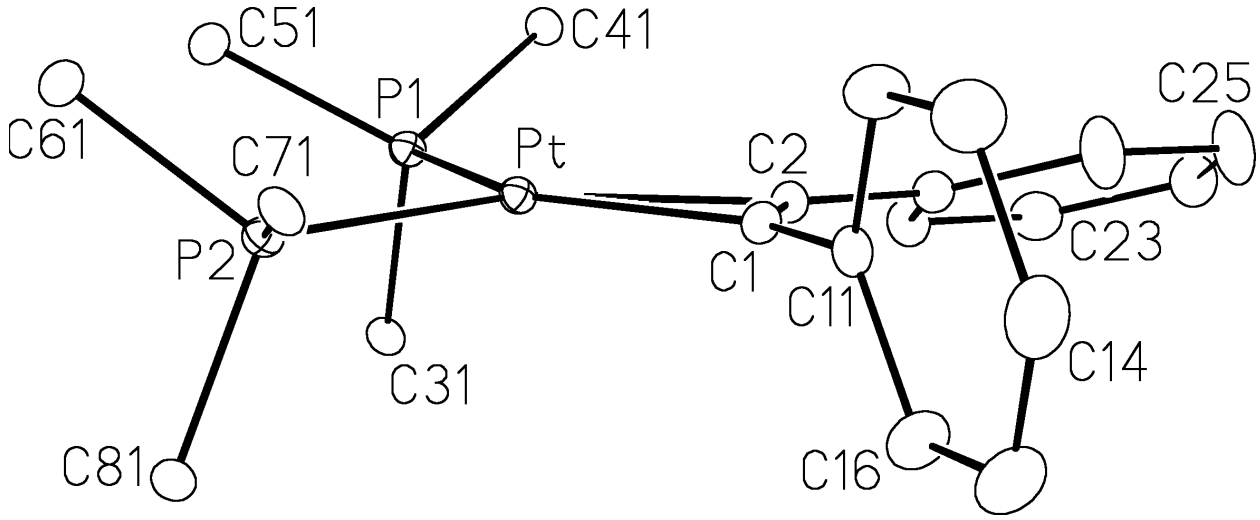
C24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P1
C25
C71
Pt
C2
P2
C1
C23
C11
C31
C14
C81
C16

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Table S1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{50}H_{40}P_2Pt$
formula weight	897.85
crystal dimensions (mm)	0.40 × 0.21 × 0.17
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	13.3195 (8)
b (Å)	16.6524 (9)
c (Å)	18.3044 (10)
α (deg)	81.1006 (10)
β (deg)	87.0241 (10)
γ (deg)	77.9296 (10)
V (Å^3)	3921.6 (4)
Z	4
ρ_{calcd} (g cm^{-3})	1.521
μ (mm^{-1})	3.694
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (15 s exposures)
data collection 2θ limit (deg)	52.84
total data collected	29292 ($-16 \le h \le 16$, $-20 \le k \le 20$, $-22 \le l \le 21$)
independent reflections	15941 (R_{int} = 0.0232)
number of observed reflections (*NO*)	13809 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	Patterson search/structure expansion (*DIRDIF–99*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.5724–0.3196
data/restraints/parameters	15941 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 955
goodness-of-fit (S)[e]	1.018 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0233
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.0584
largest difference peak and hole	1.067 and –0.450 e Å^{-3}

[a]Obtained from least-squares refinement of 6714 reflections with $4.50° < 2\theta < 52.76°$.

(continued)

Table S1. Crystallographic Experimental Details (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Garcia-Granda, S.; Israel, R.; Gould, R. O.; Smits, J. M. M. (1999). The *DIRDIF-99* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0278P)^2 + 1.0983P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

(a) bis(triphenylphosphine)(η²–diphenylacetylene)platinum, molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Pt	0.115503(8)	0.321379(6)	0.393740(5)	0.01761(3)*
P1	0.10767(5)	0.23974(4)	0.50587(4)	0.01931(14)*
P2	0.23611(5)	0.39820(4)	0.40518(4)	0.01873(14)*
C1	0.0568(2)	0.34878(17)	0.28902(15)	0.0226(6)*
C2	0.0179(2)	0.28945(18)	0.32535(16)	0.0241(6)*
C11	0.0571(2)	0.40131(18)	0.21737(15)	0.0251(6)*
C12	0.0047(3)	0.4834(2)	0.20809(18)	0.0358(7)*
C13	0.0044(3)	0.5336(2)	0.1410(2)	0.0478(9)*
C14	0.0573(3)	0.5030(3)	0.0815(2)	0.0532(11)*
C15	0.1096(3)	0.4218(3)	0.0890(2)	0.0565(11)*
C16	0.1093(3)	0.3703(2)	0.15617(18)	0.0419(8)*
C21	-0.0567(2)	0.23982(18)	0.31450(17)	0.0265(6)*
C22	-0.0580(3)	0.16282(19)	0.35615(18)	0.0332(7)*
C23	-0.1302(3)	0.1176(2)	0.3432(2)	0.0427(9)*
C24	-0.2018(3)	0.1492(2)	0.2880(2)	0.0440(9)*
C25	-0.2007(3)	0.2246(3)	0.2465(2)	0.0484(9)*
C26	-0.1292(3)	0.2702(2)	0.2593(2)	0.0401(8)*
C31	0.1976(2)	0.13874(16)	0.51275(16)	0.0232(6)*
C32	0.2247(2)	0.10459(18)	0.44835(17)	0.0283(7)*
C33	0.2928(3)	0.0290(2)	0.4492(2)	0.0388(8)*
C34	0.3347(3)	-0.0130(2)	0.5155(2)	0.0419(9)*
C35	0.3091(3)	0.02020(19)	0.58042(19)	0.0356(8)*
C36	0.2409(2)	0.09586(18)	0.57910(17)	0.0290(7)*
C41	-0.0171(2)	0.21033(17)	0.52454(16)	0.0237(6)*
C42	-0.1050(2)	0.26882(18)	0.50283(18)	0.0291(7)*
C43	-0.2018(3)	0.2517(2)	0.5194(2)	0.0388(8)*
C44	-0.2118(3)	0.1753(2)	0.5566(2)	0.0516(10)*
C45	-0.1255(3)	0.1169(2)	0.5778(3)	0.0580(12)*
C46	-0.0283(3)	0.1341(2)	0.5624(2)	0.0410(9)*
C51	0.1265(2)	0.27514(16)	0.59318(15)	0.0214(6)*
C52	0.0449(2)	0.29806(18)	0.64149(16)	0.0281(6)*
C53	0.0612(3)	0.3280(2)	0.70581(18)	0.0352(7)*
C54	0.1583(3)	0.33403(19)	0.72264(17)	0.0338(7)*
C55	0.2408(2)	0.31080(18)	0.67516(17)	0.0293(7)*
C56	0.2247(2)	0.28214(17)	0.61084(16)	0.0253(6)*
C61	0.2347(2)	0.44264(16)	0.49087(15)	0.0223(6)*
C62	0.1385(2)	0.46822(17)	0.52224(16)	0.0255(6)*
C63	0.1270(3)	0.50971(18)	0.58345(17)	0.0324(7)*
C64	0.2123(3)	0.52356(19)	0.61484(18)	0.0371(8)*

Table S2. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C65	0.3092(3)	0.4957(2)	0.58578(18)	0.0366(8)*
C66	0.3209(2)	0.45616(18)	0.52345(17)	0.0285(7)*
C71	0.2363(2)	0.49134(17)	0.33637(15)	0.0219(6)*
C72	0.2456(2)	0.48137(19)	0.26193(16)	0.0271(6)*
C73	0.2445(2)	0.5497(2)	0.20707(18)	0.0347(7)*
C74	0.2369(2)	0.6273(2)	0.22638(19)	0.0368(8)*
C75	0.2296(3)	0.63806(19)	0.2997(2)	0.0379(8)*
C76	0.2284(2)	0.57062(18)	0.35469(18)	0.0312(7)*
C81	0.3674(2)	0.34023(17)	0.39258(15)	0.0204(6)*
C82	0.4525(2)	0.37767(19)	0.38081(16)	0.0267(6)*
C83	0.5507(2)	0.3298(2)	0.37426(17)	0.0330(7)*
C84	0.5645(3)	0.2445(2)	0.37658(17)	0.0359(8)*
C85	0.4802(3)	0.2076(2)	0.38520(18)	0.0349(7)*
C86	0.3823(2)	0.25463(18)	0.39355(17)	0.0275(6)*

(b) bis(triphenylphosphine)(η^2*–diphenylacetylene)platinum, molecule B*

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Pt	0.602444(8)	0.180958(6)	-0.109130(5)	0.01817(3)*
P1	0.45408(5)	0.26000(4)	-0.06886(4)	0.01979(14)*
P2	0.55187(5)	0.10473(4)	-0.18847(4)	0.01991(14)*
C1	0.7591(2)	0.15555(17)	-0.10248(16)	0.0240(6)*
C2	0.7231(2)	0.21413(17)	-0.06471(16)	0.0227(6)*
C11	0.8524(2)	0.10202(18)	-0.12684(16)	0.0255(6)*
C12	0.8823(3)	0.0209(2)	-0.0927(2)	0.0387(8)*
C13	0.9682(3)	-0.0311(2)	-0.1178(2)	0.0486(10)*
C14	1.0249(3)	-0.0031(2)	-0.1772(2)	0.0448(9)*
C15	0.9977(3)	0.0778(2)	-0.2111(2)	0.0487(9)*
C16	0.9116(3)	0.1308(2)	-0.1865(2)	0.0404(8)*
C21	0.7596(2)	0.26646(18)	-0.01892(16)	0.0263(6)*
C22	0.7010(3)	0.34212(19)	-0.00444(18)	0.0323(7)*
C23	0.7399(3)	0.3905(2)	0.03759(19)	0.0392(8)*
C24	0.8375(3)	0.3644(2)	0.0653(2)	0.0427(9)*
C25	0.8963(3)	0.2898(3)	0.0518(2)	0.0534(10)*
C26	0.8573(3)	0.2410(2)	0.0098(2)	0.0456(9)*
C31	0.4171(2)	0.36209(17)	-0.12580(16)	0.0235(6)*
C32	0.4946(2)	0.39769(18)	-0.16346(17)	0.0280(7)*
C33	0.4714(3)	0.47429(19)	-0.20740(18)	0.0351(7)*
C34	0.3708(3)	0.51644(19)	-0.21517(18)	0.0357(8)*
C35	0.2931(3)	0.48134(18)	-0.17921(18)	0.0337(7)*
C36	0.3155(2)	0.40506(17)	-0.13423(16)	0.0267(6)*

Table S2. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C41	0.4660(2)	0.28575(17)	0.02364(15)	0.0233(6)*
C42	0.5254(2)	0.22699(19)	0.07515(17)	0.0299(7)*
C43	0.5324(3)	0.2418(2)	0.14694(18)	0.0375(8)*
C44	0.4818(3)	0.3163(2)	0.1676(2)	0.0489(10)*
C45	0.4251(3)	0.3750(2)	0.1173(2)	0.0536(11)*
C46	0.4166(3)	0.3605(2)	0.04509(19)	0.0398(8)*
C51	0.3318(2)	0.22508(16)	-0.05724(16)	0.0235(6)*
C52	0.2894(3)	0.2033(2)	0.01179(19)	0.0354(7)*
C53	0.1962(3)	0.1763(2)	0.0182(2)	0.0473(9)*
C54	0.1460(3)	0.1720(2)	-0.0439(2)	0.0447(9)*
C55	0.1877(2)	0.19354(19)	-0.1133(2)	0.0369(8)*
C56	0.2799(2)	0.21889(17)	-0.12006(17)	0.0269(6)*
C61	0.4379(2)	0.06137(17)	-0.16267(16)	0.0235(6)*
C62	0.4266(2)	0.03171(18)	-0.08821(17)	0.0288(7)*
C63	0.3480(3)	-0.00884(19)	-0.0627(2)	0.0365(8)*
C64	0.2781(3)	-0.0184(2)	-0.1122(2)	0.0428(9)*
C65	0.2863(3)	0.0136(2)	-0.1856(2)	0.0456(9)*
C66	0.3655(2)	0.0525(2)	-0.21118(18)	0.0352(7)*
C71	0.6423(2)	0.01154(17)	-0.21049(15)	0.0230(6)*
C72	0.7367(2)	0.02070(19)	-0.24280(17)	0.0299(7)*
C73	0.8084(3)	-0.0470(2)	-0.26032(18)	0.0370(8)*
C74	0.7870(3)	-0.1253(2)	-0.24611(18)	0.0383(8)*
C75	0.6932(3)	-0.1358(2)	-0.2153(2)	0.0432(9)*
C76	0.6209(3)	-0.06783(18)	-0.19676(18)	0.0342(7)*
C81	0.5310(2)	0.16235(17)	-0.28189(15)	0.0230(6)*
C82	0.5142(2)	0.12485(19)	-0.34226(16)	0.0276(6)*
C83	0.4980(2)	0.1716(2)	-0.41202(17)	0.0340(7)*
C84	0.5028(3)	0.2540(2)	-0.42260(18)	0.0378(8)*
C85	0.5229(3)	0.2914(2)	-0.36406(19)	0.0396(8)*
C86	0.5359(2)	0.24625(19)	-0.29402(17)	0.0311(7)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table S3. Selected Interatomic Distances (Å)

(a) Molecule A

Atom1	Atom2	Distance
Pt	P1	2.2903(7)
Pt	P2	2.2888(7)
Pt	C1	2.057(3)
Pt	C2	2.050(3)
P1	C31	1.841(3)
P1	C41	1.829(3)
P1	C51	1.833(3)
P2	C61	1.833(3)
P2	C71	1.841(3)
P2	C81	1.834(3)
C1	C2	1.289(4)
C1	C11	1.460(4)
C2	C21	1.458(4)
C11	C12	1.387(4)
C11	C16	1.398(4)
C12	C13	1.374(5)
C13	C14	1.372(6)
C14	C15	1.375(6)
C15	C16	1.387(5)
C21	C22	1.390(4)
C21	C26	1.395(5)
C22	C23	1.389(5)
C23	C24	1.390(5)
C24	C25	1.367(5)
C25	C26	1.385(5)
C31	C32	1.386(4)
C31	C36	1.396(4)
C32	C33	1.388(4)
C33	C34	1.385(5)
C34	C35	1.384(5)
C35	C36	1.388(4)
C41	C42	1.390(4)
C41	C46	1.383(4)
C42	C43	1.386(4)
C43	C44	1.375(5)
C44	C45	1.371(5)
C45	C46	1.390(5)
C51	C52	1.393(4)
C51	C56	1.396(4)

(b) Molecule B

Atom1	Atom2	Distance
Pt	P1	2.2895(7)
Pt	P2	2.2812(7)
Pt	C1	2.047(3)
Pt	C2	2.048(3)
P1	C31	1.837(3)
P1	C41	1.832(3)
P1	C51	1.832(3)
P2	C61	1.824(3)
P2	C71	1.839(3)
P2	C81	1.831(3)
C1	C2	1.280(4)
C1	C11	1.463(4)
C2	C21	1.464(4)
C11	C12	1.383(4)
C11	C16	1.396(4)
C12	C13	1.388(5)
C13	C14	1.368(5)
C14	C15	1.376(5)
C15	C16	1.395(5)
C21	C22	1.392(4)
C21	C26	1.386(5)
C22	C23	1.384(4)
C23	C24	1.379(5)
C24	C25	1.373(5)
C25	C26	1.391(5)
C31	C32	1.396(4)
C31	C36	1.397(4)
C32	C33	1.383(4)
C33	C34	1.380(5)
C34	C35	1.382(5)
C35	C36	1.387(4)
C41	C42	1.393(4)
C41	C46	1.385(4)
C42	C43	1.385(4)
C43	C44	1.379(5)
C44	C45	1.363(5)
C45	C46	1.395(5)
C51	C52	1.385(4)
C51	C56	1.400(4)

Table S3. Selected Interatomic Distances (continued)

(a) Molecule A

Atom1	Atom2	Distance
C52	C53	1.391(4)
C53	C54	1.374(5)
C54	C55	1.392(5)
C55	C56	1.379(4)
C61	C62	1.387(4)
C61	C66	1.395(4)
C62	C63	1.391(4)
C63	C64	1.376(5)
C64	C65	1.385(5)
C65	C66	1.390(4)
C71	C72	1.394(4)
C71	C76	1.393(4)
C72	C73	1.394(4)
C73	C74	1.374(5)
C74	C75	1.378(5)
C75	C76	1.389(4)
C81	C82	1.396(4)
C81	C86	1.395(4)
C82	C83	1.392(4)
C83	C84	1.389(5)
C84	C85	1.380(5)
C85	C86	1.387(4)

(b) Molecule B

Atom1	Atom2	Distance
C52	C53	1.400(5)
C53	C54	1.367(5)
C54	C55	1.386(5)
C55	C56	1.373(4)
C61	C62	1.388(4)
C61	C66	1.389(4)
C62	C63	1.384(4)
C63	C64	1.382(5)
C64	C65	1.375(5)
C65	C66	1.376(5)
C71	C72	1.389(4)
C71	C76	1.392(4)
C72	C73	1.383(4)
C73	C74	1.375(5)
C74	C75	1.377(5)
C75	C76	1.397(4)
C81	C82	1.399(4)
C81	C86	1.395(4)
C82	C83	1.391(4)
C83	C84	1.371(5)
C84	C85	1.383(5)
C85	C86	1.382(4)

Table S4. Selected Interatomic Angles (deg)

(a) Molecule A				*(b) Molecule B*			
Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P1	Pt	P2	105.83(3)	P1	Pt	P2	105.42(3)
P1	Pt	C1	143.48(8)	P1	Pt	C1	144.14(8)
P1	Pt	C2	106.93(8)	P1	Pt	C2	107.74(8)
P2	Pt	C1	110.68(8)	P2	Pt	C1	110.43(8)
P2	Pt	C2	147.11(8)	P2	Pt	C2	146.64(8)
C1	Pt	C2	36.58(11)	C1	Pt	C2	36.43(11)
Pt	P1	C31	113.53(10)	Pt	P1	C31	113.46(10)
Pt	P1	C41	112.71(10)	Pt	P1	C41	112.30(10)
Pt	P1	C51	122.21(9)	Pt	P1	C51	123.16(9)
C31	P1	C41	102.88(13)	C31	P1	C41	103.35(13)
C31	P1	C51	102.56(13)	C31	P1	C51	101.91(13)
C41	P1	C51	100.52(13)	C41	P1	C51	100.17(13)
Pt	P2	C61	117.75(10)	Pt	P2	C61	117.56(10)
Pt	P2	C71	117.46(9)	Pt	P2	C71	118.39(9)
Pt	P2	C81	112.30(9)	Pt	P2	C81	112.41(10)
C61	P2	C71	100.25(13)	C61	P2	C71	100.19(13)
C61	P2	C81	106.46(13)	C61	P2	C81	106.57(13)
C71	P2	C81	100.52(12)	C71	P2	C81	99.45(13)
Pt	C1	C2	71.43(18)	Pt	C1	C2	71.86(18)
Pt	C1	C11	145.3(2)	Pt	C1	C11	142.9(2)
C2	C1	C11	143.3(3)	C2	C1	C11	145.2(3)
Pt	C2	C1	71.99(18)	Pt	C2	C1	71.71(18)
Pt	C2	C21	149.3(2)	Pt	C2	C21	148.8(2)
C1	C2	C21	138.6(3)	C1	C2	C21	139.5(3)
C1	C11	C12	120.8(3)	C1	C11	C12	120.7(3)
C1	C11	C16	121.0(3)	C1	C11	C16	120.8(3)
C12	C11	C16	118.2(3)	C12	C11	C16	118.5(3)
C11	C12	C13	121.4(3)	C11	C12	C13	120.8(3)
C12	C13	C14	120.0(4)	C12	C13	C14	120.5(3)
C13	C14	C15	119.9(3)	C13	C14	C15	119.7(3)
C14	C15	C16	120.6(4)	C14	C15	C16	120.4(3)
C11	C16	C15	119.9(3)	C11	C16	C15	120.1(3)
C2	C21	C22	122.8(3)	C2	C21	C22	122.6(3)
C2	C21	C26	118.8(3)	C2	C21	C26	119.0(3)
C22	C21	C26	118.3(3)	C22	C21	C26	118.4(3)
C21	C22	C23	120.6(3)	C21	C22	C23	120.5(3)
C22	C23	C24	120.0(3)	C22	C23	C24	120.3(3)
C23	C24	C25	119.9(3)	C23	C24	C25	120.0(3)
C24	C25	C26	120.4(4)	C24	C25	C26	119.8(3)

Table S4. Selected Interatomic Angles (continued)

(a) Molecule A				*(b) Molecule B*			
Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C21	C26	C25	120.8(3)	C21	C26	C25	121.0(3)
P1	C31	C32	117.9(2)	P1	C31	C32	118.1(2)
P1	C31	C36	123.3(2)	P1	C31	C36	123.4(2)
C32	C31	C36	118.7(3)	C32	C31	C36	118.5(3)
C31	C32	C33	121.1(3)	C31	C32	C33	120.8(3)
C32	C33	C34	119.4(3)	C32	C33	C34	120.3(3)
C33	C34	C35	120.4(3)	C33	C34	C35	119.6(3)
C34	C35	C36	119.8(3)	C34	C35	C36	120.6(3)
C31	C36	C35	120.5(3)	C31	C36	C35	120.2(3)
P1	C41	C42	118.4(2)	P1	C41	C42	118.7(2)
P1	C41	C46	123.1(2)	P1	C41	C46	122.8(2)
C42	C41	C46	118.4(3)	C42	C41	C46	118.5(3)
C41	C42	C43	120.9(3)	C41	C42	C43	120.8(3)
C42	C43	C44	120.0(3)	C42	C43	C44	119.9(3)
C43	C44	C45	119.5(3)	C43	C44	C45	119.9(3)
C44	C45	C46	120.8(3)	C44	C45	C46	120.8(3)
C41	C46	C45	120.3(3)	C41	C46	C45	120.1(3)
P1	C51	C52	121.9(2)	P1	C51	C52	122.2(2)
P1	C51	C56	119.3(2)	P1	C51	C56	119.2(2)
C52	C51	C56	118.8(3)	C52	C51	C56	118.6(3)
C51	C52	C53	120.4(3)	C51	C52	C53	120.4(3)
C52	C53	C54	120.1(3)	C52	C53	C54	120.0(3)
C53	C54	C55	120.1(3)	C53	C54	C55	120.1(3)
C54	C55	C56	119.9(3)	C54	C55	C56	120.2(3)
C51	C56	C55	120.6(3)	C51	C56	C55	120.7(3)
P2	C61	C62	115.7(2)	P2	C61	C62	116.0(2)
P2	C61	C66	125.2(2)	P2	C61	C66	125.7(2)
C62	C61	C66	119.0(3)	C62	C61	C66	118.3(3)
C61	C62	C63	120.9(3)	C61	C62	C63	121.4(3)
C62	C63	C64	119.7(3)	C62	C63	C64	119.2(3)
C63	C64	C65	120.0(3)	C63	C64	C65	119.8(3)
C64	C65	C66	120.5(3)	C64	C65	C66	120.9(3)
C61	C66	C65	119.8(3)	C61	C66	C65	120.3(3)
P2	C71	C72	117.8(2)	P2	C71	C72	118.4(2)
P2	C71	C76	123.7(2)	P2	C71	C76	123.4(2)
C72	C71	C76	118.6(3)	C72	C71	C76	118.2(3)
C71	C72	C73	120.6(3)	C71	C72	C73	121.3(3)
C72	C73	C74	119.9(3)	C72	C73	C74	120.2(3)
C73	C74	C75	120.3(3)	C73	C74	C75	119.6(3)

Table S4. Selected Interatomic Angles (continued)

(a) Molecule A				*(b) Molecule B*			
Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C74	C75	C76	120.2(3)	C74	C75	C76	120.4(3)
C71	C76	C75	120.5(3)	C71	C76	C75	120.3(3)
P2	C81	C82	123.3(2)	P2	C81	C82	122.6(2)
P2	C81	C86	118.1(2)	P2	C81	C86	118.8(2)
C82	C81	C86	118.6(3)	C82	C81	C86	118.6(3)
C81	C82	C83	120.5(3)	C81	C82	C83	120.3(3)
C82	C83	C84	120.1(3)	C82	C83	C84	120.0(3)
C83	C84	C85	119.5(3)	C83	C84	C85	120.4(3)
C84	C85	C86	120.7(3)	C84	C85	C86	120.1(3)
C81	C86	C85	120.5(3)	C81	C86	C85	120.5(3)

Table S5. Torsional Angles (deg)

(a) Molecule A

Atom1	Atom2	Atom3	Atom4	Angle
P2	Pt	P1	C31	-89.88(10)
P2	Pt	P1	C41	153.65(10)
P2	Pt	P1	C51	33.81(11)
C1	Pt	P1	C31	88.86(17)
C1	Pt	P1	C41	-27.61(17)
C1	Pt	P1	C51	-147.45(17)
C2	Pt	P1	C31	87.05(13)
C2	Pt	P1	C41	-29.43(13)
C2	Pt	P1	C51	-149.27(14)
P1	Pt	P2	C61	-42.57(10)
P1	Pt	P2	C71	-162.56(10)
P1	Pt	P2	C81	81.62(10)
C1	Pt	P2	C61	138.23(13)
C1	Pt	P2	C71	18.24(13)
C1	Pt	P2	C81	-97.58(12)
C2	Pt	P2	C61	142.86(17)
C2	Pt	P2	C71	22.86(18)
C2	Pt	P2	C81	-92.96(17)
P1	Pt	C1	C2	-2.9(3)
P1	Pt	C1	C11	177.2(3)
P2	Pt	C1	C2	175.79(15)
P2	Pt	C1	C11	-4.0(4)
C2	Pt	C1	C11	-179.8(5)
P1	Pt	C2	C1	178.19(16)
P1	Pt	C2	C21	2.0(4)
P2	Pt	C2	C1	-7.3(3)
P2	Pt	C2	C21	176.6(3)
C1	Pt	C2	C21	-176.2(5)
Pt	P1	C31	C32	-28.7(3)
Pt	P1	C31	C36	150.2(2)
C41	P1	C31	C32	93.4(2)
C41	P1	C31	C36	-87.7(3)
C51	P1	C31	C32	-162.5(2)
C51	P1	C31	C36	16.4(3)
Pt	P1	C41	C42	-38.5(3)
Pt	P1	C41	C46	144.8(3)
C31	P1	C41	C42	-161.1(2)
C31	P1	C41	C46	22.1(3)
C51	P1	C41	C42	93.2(3)

(b) Molecule B

Atom1	Atom2	Atom3	Atom4	Angle
P2	Pt	P1	C31	-91.26(10)
P2	Pt	P1	C41	151.99(10)
P2	Pt	P1	C51	32.27(12)
C1	Pt	P1	C31	86.92(17)
C1	Pt	P1	C41	-29.83(17)
C1	Pt	P1	C51	-149.55(17)
C2	Pt	P1	C31	84.98(13)
C2	Pt	P1	C41	-31.77(13)
C2	Pt	P1	C51	-151.50(14)
P1	Pt	P2	C61	-40.87(11)
P1	Pt	P2	C71	-161.46(11)
P1	Pt	P2	C81	83.41(10)
C1	Pt	P2	C61	140.27(13)
C1	Pt	P2	C71	19.68(14)
C1	Pt	P2	C81	-95.45(13)
C2	Pt	P2	C61	145.66(17)
C2	Pt	P2	C71	25.07(18)
C2	Pt	P2	C81	-90.07(17)
P1	Pt	C1	C2	-3.1(3)
P1	Pt	C1	C11	176.6(3)
P2	Pt	C1	C2	175.01(15)
P2	Pt	C1	C11	-5.2(4)
C2	Pt	C1	C11	179.7(5)
P1	Pt	C2	C1	178.08(16)
P1	Pt	C2	C21	-1.1(4)
P2	Pt	C2	C1	-8.5(3)
P2	Pt	C2	C21	172.3(3)
C1	Pt	C2	C21	-179.2(5)
Pt	P1	C31	C32	-27.6(3)
Pt	P1	C31	C36	151.3(2)
C41	P1	C31	C32	94.3(2)
C41	P1	C31	C36	-86.8(3)
C51	P1	C31	C32	-162.1(2)
C51	P1	C31	C36	16.8(3)
Pt	P1	C41	C42	-35.8(3)
Pt	P1	C41	C46	145.7(3)
C31	P1	C41	C42	-158.4(2)
C31	P1	C41	C46	23.1(3)
C51	P1	C41	C42	96.6(2)

Table S5. Torsional Angles (continued)

(a) Molecule A

Atom1	Atom2	Atom3	Atom4	Angle
C51	P1	C41	C46	-83.5(3)
Pt	P1	C51	C52	105.9(2)
Pt	P1	C51	C56	-71.9(2)
C31	P1	C51	C52	-125.5(2)
C31	P1	C51	C56	56.7(2)
C41	P1	C51	C52	-19.7(3)
C41	P1	C51	C56	162.6(2)
Pt	P2	C61	C62	-35.0(2)
Pt	P2	C61	C66	148.6(2)
C71	P2	C61	C62	93.7(2)
C71	P2	C61	C66	-82.7(3)
C81	P2	C61	C62	-162.0(2)
C81	P2	C61	C66	21.6(3)
Pt	P2	C71	C72	-56.2(2)
Pt	P2	C71	C76	124.3(2)
C61	P2	C71	C72	175.0(2)
C61	P2	C71	C76	-4.6(3)
C81	P2	C71	C72	65.9(2)
C81	P2	C71	C76	-113.6(3)
Pt	P2	C81	C82	165.5(2)
Pt	P2	C81	C86	-13.3(2)
C61	P2	C81	C82	-64.2(3)
C61	P2	C81	C86	117.0(2)
C71	P2	C81	C82	39.9(3)
C71	P2	C81	C86	-138.9(2)
Pt	C1	C2	C21	177.0(4)
C11	C1	C2	Pt	179.8(5)
C11	C1	C2	C21	-3.1(7)
Pt	C1	C11	C12	-76.1(5)
Pt	C1	C11	C16	104.5(4)
C2	C1	C11	C12	104.2(5)
C2	C1	C11	C16	-75.3(6)
Pt	C2	C21	C22	-26.8(6)
Pt	C2	C21	C26	154.1(3)
C1	C2	C21	C22	158.8(4)
C1	C2	C21	C26	-20.4(6)
C1	C11	C12	C13	179.9(3)
C16	C11	C12	C13	-0.6(5)
C1	C11	C16	C15	-179.0(3)

(b) Molecule B

Atom1	Atom2	Atom3	Atom4	Angle
C51	P1	C41	C46	-81.9(3)
Pt	P1	C51	C52	108.3(2)
Pt	P1	C51	C56	-70.7(2)
C31	P1	C51	C52	-123.1(3)
C31	P1	C51	C56	57.9(2)
C41	P1	C51	C52	-17.0(3)
C41	P1	C51	C56	164.0(2)
Pt	P2	C61	C62	-38.4(2)
Pt	P2	C61	C66	144.6(2)
C71	P2	C61	C62	91.3(2)
C71	P2	C61	C66	-85.7(3)
C81	P2	C61	C62	-165.6(2)
C81	P2	C61	C66	17.4(3)
Pt	P2	C71	C72	-59.5(2)
Pt	P2	C71	C76	120.8(2)
C61	P2	C71	C72	171.4(2)
C61	P2	C71	C76	-8.3(3)
C81	P2	C71	C72	62.5(2)
C81	P2	C71	C76	-117.2(3)
Pt	P2	C81	C82	170.5(2)
Pt	P2	C81	C86	-7.0(3)
C61	P2	C81	C82	-59.3(3)
C61	P2	C81	C86	123.2(2)
C71	P2	C81	C82	44.4(3)
C71	P2	C81	C86	-133.1(2)
Pt	C1	C2	C21	179.3(4)
C11	C1	C2	Pt	-179.7(5)
C11	C1	C2	C21	-0.4(8)
Pt	C1	C11	C12	-78.4(4)
Pt	C1	C11	C16	99.7(4)
C2	C1	C11	C12	101.2(5)
C2	C1	C11	C16	-80.8(6)
Pt	C2	C21	C22	-22.0(6)
Pt	C2	C21	C26	159.6(3)
C1	C2	C21	C22	159.2(4)
C1	C2	C21	C26	-19.2(6)
C1	C11	C12	C13	177.1(3)
C16	C11	C12	C13	-1.1(5)
C1	C11	C16	C15	-177.1(3)

Table S5. Torsional Angles (continued)

(a) Molecule A

Atom1	Atom2	Atom3	Atom4	Angle
C12	C11	C16	C15	1.5(5)
C11	C12	C13	C14	-0.4(6)
C12	C13	C14	C15	0.7(6)
C13	C14	C15	C16	0.2(6)
C14	C15	C16	C11	-1.3(6)
C2	C21	C22	C23	-179.4(3)
C26	C21	C22	C23	-0.3(5)
C2	C21	C26	C25	179.2(3)
C22	C21	C26	C25	0.0(5)
C21	C22	C23	C24	0.2(5)
C22	C23	C24	C25	0.2(5)
C23	C24	C25	C26	-0.5(6)
C24	C25	C26	C21	0.4(6)
P1	C31	C32	C33	179.5(2)
C36	C31	C32	C33	0.5(5)
P1	C31	C36	C35	-179.4(2)
C32	C31	C36	C35	-0.5(5)
C31	C32	C33	C34	-0.3(5)
C32	C33	C34	C35	0.0(6)
C33	C34	C35	C36	0.0(5)
C34	C35	C36	C31	0.2(5)
P1	C41	C42	C43	-176.1(3)
C46	C41	C42	C43	0.8(5)
P1	C41	C46	C45	177.0(3)
C42	C41	C46	C45	0.3(5)
C41	C42	C43	C44	-1.3(5)
C42	C43	C44	C45	0.9(6)
C43	C44	C45	C46	0.2(7)
C44	C45	C46	C41	-0.8(7)
P1	C51	C52	C53	-177.3(2)
C56	C51	C52	C53	0.5(4)
P1	C51	C56	C55	178.2(2)
C52	C51	C56	C55	0.4(4)
C51	C52	C53	C54	-0.9(5)
C52	C53	C54	C55	0.4(5)
C53	C54	C55	C56	0.4(5)
C54	C55	C56	C51	-0.8(4)
P2	C61	C62	C63	-174.1(2)
C66	C61	C62	C63	2.5(4)

(b) Molecule B

Atom1	Atom2	Atom3	Atom4	Angle
C12	C11	C16	C15	1.0(5)
C11	C12	C13	C14	-0.2(6)
C12	C13	C14	C15	1.4(6)
C13	C14	C15	C16	-1.4(6)
C14	C15	C16	C11	0.2(6)
C2	C21	C22	C23	-178.3(3)
C26	C21	C22	C23	0.1(5)
C2	C21	C26	C25	178.2(3)
C22	C21	C26	C25	-0.2(6)
C21	C22	C23	C24	0.3(5)
C22	C23	C24	C25	-0.5(6)
C23	C24	C25	C26	0.4(6)
C24	C25	C26	C21	0.0(6)
P1	C31	C32	C33	179.8(2)
C36	C31	C32	C33	0.8(4)
P1	C31	C36	C35	-178.9(2)
C32	C31	C36	C35	0.0(4)
C31	C32	C33	C34	-0.6(5)
C32	C33	C34	C35	-0.5(5)
C33	C34	C35	C36	1.4(5)
C34	C35	C36	C31	-1.1(5)
P1	C41	C42	C43	-176.6(3)
C46	C41	C42	C43	1.9(5)
P1	C41	C46	C45	177.3(3)
C42	C41	C46	C45	-1.2(5)
C41	C42	C43	C44	-1.3(5)
C42	C43	C44	C45	0.0(6)
C43	C44	C45	C46	0.7(7)
C44	C45	C46	C41	-0.1(6)
P1	C51	C52	C53	-179.4(3)
C56	C51	C52	C53	-0.4(5)
P1	C51	C56	C55	-179.5(2)
C52	C51	C56	C55	1.4(4)
C51	C52	C53	C54	-0.6(5)
C52	C53	C54	C55	0.7(6)
C53	C54	C55	C56	0.3(5)
C54	C55	C56	C51	-1.4(5)
P2	C61	C62	C63	-174.6(2)
C66	C61	C62	C63	2.7(4)

Table S5. Torsional Angles (continued)

(a) Molecule A

Atom1	Atom2	Atom3	Atom4	Angle
P2	C61	C66	C65	175.5(2)
C62	C61	C66	C65	-0.8(4)
C61	C62	C63	C64	-1.9(4)
C62	C63	C64	C65	-0.4(5)
C63	C64	C65	C66	2.2(5)
C64	C65	C66	C61	-1.5(5)
P2	C71	C72	C73	178.9(2)
C76	C71	C72	C73	-1.5(4)
P2	C71	C76	C75	179.7(2)
C72	C71	C76	C75	0.1(5)
C71	C72	C73	C74	1.7(5)
C72	C73	C74	C75	-0.5(5)
C73	C74	C75	C76	-0.8(5)
C74	C75	C76	C71	1.0(5)
P2	C81	C82	C83	177.7(2)
C86	C81	C82	C83	-3.5(4)
P2	C81	C86	C85	-179.2(2)
C82	C81	C86	C85	1.9(4)
C81	C82	C83	C84	2.5(5)
C82	C83	C84	C85	0.2(5)
C83	C84	C85	C86	-1.8(5)
C84	C85	C86	C81	0.7(5)

(b) Molecule B

Atom1	Atom2	Atom3	Atom4	Angle
P2	C61	C66	C65	175.5(3)
C62	C61	C66	C65	-1.4(5)
C61	C62	C63	C64	-1.4(5)
C62	C63	C64	C65	-1.1(5)
C63	C64	C65	C66	2.3(5)
C64	C65	C66	C61	-1.1(5)
P2	C71	C72	C73	179.6(2)
C76	C71	C72	C73	-0.7(5)
P2	C71	C76	C75	179.7(3)
C72	C71	C76	C75	0.0(5)
C71	C72	C73	C74	0.2(5)
C72	C73	C74	C75	0.9(5)
C73	C74	C75	C76	-1.6(5)
C74	C75	C76	C71	1.2(5)
P2	C81	C82	C83	179.5(2)
C86	C81	C82	C83	-3.0(4)
P2	C81	C86	C85	178.6(2)
C82	C81	C86	C85	1.0(5)
C81	C82	C83	C84	2.8(5)
C82	C83	C84	C85	-0.5(5)
C83	C84	C85	C86	-1.6(5)
C84	C85	C86	C81	1.3(5)

Table S6. Least-Squares Planes

(a) bis(triphenylphosphine)(η²–diphenylacetylene)platinum, molecule A

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1A	-7.633(6)	10.427(6)	6.924(10)	5.174(6)				
					Pt	0.0217(7)	P1	0.0065(7)
					P2	-0.0187(6)	C1	0.0305(18)
					C2	-0.0400(18)		
					C11	0.080(4)	C21	-0.063(4)

(b) bis(triphenylphosphine)(η²–diphenylacetylene)platinum, molecule B

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1B	2.184(8)	10.560(6)	-12.161(6)	4.581(4)				
					Pt	-0.0274(7)	P1	-0.0065(7)
					P2	0.0221(6)	C1	-0.0344(18)
					C2	0.0462(18)		
					C11	-0.100(4)	C21	0.122(4)

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table S7. Anisotropic Displacement Parameters (U_{ij}, Å^2)

(a) bis(triphenylphosphine)(η^2–diphenylacetylene)platinum, molecule A

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	0.01837(6)	0.01662(6)	0.01724(6)	-0.00142(4)	-0.00154(4)	-0.00273(4)
P1	0.0190(4)	0.0185(3)	0.0196(4)	-0.0010(3)	-0.0009(3)	-0.0031(3)
P2	0.0195(4)	0.0173(3)	0.0186(3)	-0.0013(3)	-0.0010(3)	-0.0029(3)
C1	0.0238(15)	0.0244(14)	0.0199(14)	-0.0047(11)	-0.0035(11)	-0.0035(11)
C2	0.0214(15)	0.0285(15)	0.0230(15)	-0.0078(12)	-0.0029(12)	-0.0033(12)
C11	0.0258(15)	0.0339(16)	0.0184(14)	-0.0015(12)	-0.0049(12)	-0.0131(12)
C12	0.041(2)	0.0375(18)	0.0275(17)	0.0001(14)	-0.0022(14)	-0.0070(15)
C13	0.058(2)	0.042(2)	0.040(2)	0.0114(16)	-0.0110(18)	-0.0126(18)
C14	0.058(3)	0.073(3)	0.0276(19)	0.0211(18)	-0.0143(18)	-0.027(2)
C15	0.061(3)	0.086(3)	0.0227(19)	-0.0071(19)	0.0055(18)	-0.016(2)
C16	0.049(2)	0.049(2)	0.0234(17)	-0.0044(15)	-0.0004(15)	-0.0012(17)
C21	0.0228(15)	0.0314(16)	0.0283(16)	-0.0104(13)	0.0009(12)	-0.0081(12)
C22	0.0365(18)	0.0299(16)	0.0352(18)	-0.0094(14)	0.0011(14)	-0.0087(14)
C23	0.046(2)	0.0339(18)	0.056(2)	-0.0186(17)	0.0142(18)	-0.0206(16)
C24	0.0328(19)	0.054(2)	0.058(2)	-0.0341(19)	0.0109(17)	-0.0223(17)
C25	0.034(2)	0.066(3)	0.052(2)	-0.017(2)	-0.0086(17)	-0.0186(18)
C26	0.0354(19)	0.047(2)	0.041(2)	-0.0046(16)	-0.0093(16)	-0.0156(16)
C31	0.0214(15)	0.0190(13)	0.0286(16)	-0.0004(11)	0.0001(12)	-0.0052(11)
C32	0.0308(17)	0.0246(15)	0.0291(16)	-0.0044(12)	-0.0020(13)	-0.0039(12)
C33	0.046(2)	0.0287(17)	0.040(2)	-0.0136(14)	0.0005(16)	0.0022(15)
C34	0.042(2)	0.0244(16)	0.054(2)	-0.0074(15)	-0.0056(17)	0.0075(14)
C35	0.0384(19)	0.0248(16)	0.0394(19)	0.0051(14)	-0.0123(15)	-0.0011(13)
C36	0.0314(17)	0.0248(15)	0.0294(16)	-0.0015(12)	-0.0032(13)	-0.0041(12)
C41	0.0238(15)	0.0250(14)	0.0244(15)	-0.0045(11)	-0.0006(12)	-0.0087(12)
C42	0.0251(16)	0.0258(15)	0.0364(17)	-0.0035(13)	-0.0038(13)	-0.0053(12)
C43	0.0251(17)	0.0420(19)	0.049(2)	-0.0073(16)	-0.0045(15)	-0.0037(14)
C44	0.0293(19)	0.057(2)	0.071(3)	-0.001(2)	0.0035(18)	-0.0214(18)
C45	0.045(2)	0.048(2)	0.079(3)	0.019(2)	0.001(2)	-0.0250(19)
C46	0.0289(18)	0.0334(18)	0.054(2)	0.0144(16)	-0.0012(16)	-0.0069(14)
C51	0.0255(15)	0.0184(13)	0.0191(14)	0.0009(11)	-0.0012(11)	-0.0043(11)
C52	0.0242(16)	0.0334(16)	0.0274(16)	-0.0068(13)	-0.0002(12)	-0.0056(12)
C53	0.0348(19)	0.0420(19)	0.0291(17)	-0.0104(14)	0.0057(14)	-0.0065(15)
C54	0.047(2)	0.0334(17)	0.0216(16)	-0.0051(13)	-0.0077(14)	-0.0063(15)
C55	0.0298(17)	0.0287(16)	0.0283(16)	0.0010(12)	-0.0114(13)	-0.0044(13)
C56	0.0239(15)	0.0224(14)	0.0267(15)	0.0031(12)	-0.0026(12)	-0.0026(11)
C61	0.0303(16)	0.0156(13)	0.0200(14)	-0.0003(11)	-0.0019(12)	-0.0034(11)
C62	0.0278(16)	0.0215(14)	0.0245(15)	-0.0019(11)	-0.0032(12)	0.0005(12)
C63	0.0413(19)	0.0267(16)	0.0245(16)	-0.0042(12)	0.0008(14)	0.0033(13)
C64	0.058(2)	0.0264(16)	0.0268(17)	-0.0112(13)	-0.0044(16)	-0.0025(15)

Table S7. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C65	0.046(2)	0.0373(18)	0.0319(18)	-0.0091(14)	-0.0074(15)	-0.0151(15)
C66	0.0312(17)	0.0275(15)	0.0283(16)	-0.0071(12)	-0.0012(13)	-0.0071(13)
C71	0.0161(14)	0.0237(14)	0.0235(15)	0.0033(11)	-0.0025(11)	-0.0031(11)
C72	0.0253(16)	0.0288(15)	0.0256(16)	0.0006(12)	-0.0020(12)	-0.0045(12)
C73	0.0317(18)	0.0405(19)	0.0268(17)	0.0086(14)	0.0003(13)	-0.0062(14)
C74	0.0297(18)	0.0307(17)	0.042(2)	0.0132(14)	0.0069(15)	-0.0043(13)
C75	0.040(2)	0.0218(15)	0.048(2)	0.0031(14)	0.0024(16)	-0.0037(13)
C76	0.0365(18)	0.0239(15)	0.0305(17)	-0.0006(13)	0.0010(14)	-0.0030(13)
C81	0.0171(14)	0.0240(14)	0.0184(14)	-0.0013(11)	-0.0019(11)	-0.0013(11)
C82	0.0258(16)	0.0305(16)	0.0220(15)	0.0001(12)	-0.0007(12)	-0.0047(12)
C83	0.0214(16)	0.048(2)	0.0268(16)	0.0022(14)	0.0032(13)	-0.0078(14)
C84	0.0267(17)	0.0436(19)	0.0290(17)	-0.0027(14)	0.0021(13)	0.0093(14)
C85	0.0362(19)	0.0276(16)	0.0357(18)	-0.0040(13)	0.0009(14)	0.0043(14)
C86	0.0241(16)	0.0272(15)	0.0289(16)	-0.0017(12)	-0.0018(13)	-0.0018(12)

(b) bis(triphenylphosphine)(η^2–diphenylacetylene)platinum, molecule B

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	0.01735(6)	0.01827(6)	0.01818(6)	-0.00241(4)	-0.00061(4)	-0.00211(4)
P1	0.0194(4)	0.0197(3)	0.0193(4)	-0.0026(3)	-0.0003(3)	-0.0021(3)
P2	0.0199(4)	0.0209(3)	0.0183(3)	-0.0033(3)	0.0004(3)	-0.0027(3)
C1	0.0199(14)	0.0255(15)	0.0262(15)	0.0001(12)	-0.0014(12)	-0.0065(11)
C2	0.0197(14)	0.0230(14)	0.0253(15)	-0.0020(11)	-0.0026(11)	-0.0046(11)
C11	0.0191(15)	0.0304(15)	0.0272(16)	-0.0054(12)	-0.0031(12)	-0.0038(12)
C12	0.0310(18)	0.0363(18)	0.041(2)	0.0029(15)	0.0067(15)	0.0020(14)
C13	0.038(2)	0.0361(19)	0.063(3)	-0.0018(18)	0.0018(18)	0.0076(16)
C14	0.0261(18)	0.049(2)	0.058(2)	-0.0216(18)	0.0054(17)	0.0040(15)
C15	0.035(2)	0.059(2)	0.051(2)	-0.0104(19)	0.0175(17)	-0.0094(17)
C16	0.0336(19)	0.0363(18)	0.048(2)	-0.0012(16)	0.0070(16)	-0.0060(15)
C21	0.0283(16)	0.0284(15)	0.0239(15)	-0.0051(12)	-0.0002(12)	-0.0090(12)
C22	0.0323(18)	0.0292(16)	0.0355(18)	-0.0057(13)	-0.0047(14)	-0.0050(13)
C23	0.051(2)	0.0319(17)	0.0376(19)	-0.0111(15)	0.0005(16)	-0.0113(16)
C24	0.050(2)	0.049(2)	0.037(2)	-0.0130(16)	-0.0054(17)	-0.0231(18)
C25	0.041(2)	0.063(3)	0.063(3)	-0.025(2)	-0.0220(19)	-0.0074(19)
C26	0.0323(19)	0.049(2)	0.058(2)	-0.0250(18)	-0.0127(17)	0.0011(16)
C31	0.0285(16)	0.0209(14)	0.0210(14)	-0.0039(11)	-0.0034(12)	-0.0039(11)
C32	0.0275(16)	0.0245(15)	0.0319(17)	-0.0016(12)	-0.0037(13)	-0.0061(12)
C33	0.045(2)	0.0287(16)	0.0324(18)	0.0032(13)	-0.0002(15)	-0.0152(15)
C34	0.051(2)	0.0228(15)	0.0304(17)	0.0049(13)	-0.0104(15)	-0.0059(14)
C35	0.0391(19)	0.0252(16)	0.0340(18)	-0.0045(13)	-0.0093(15)	0.0017(13)
C36	0.0266(16)	0.0238(15)	0.0291(16)	-0.0046(12)	-0.0016(13)	-0.0031(12)

Table S7. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C41	0.0241(15)	0.0297(15)	0.0173(14)	-0.0065(11)	0.0013(11)	-0.0064(12)
C42	0.0332(17)	0.0295(16)	0.0256(16)	-0.0031(12)	-0.0017(13)	-0.0038(13)
C43	0.041(2)	0.0439(19)	0.0279(17)	0.0000(14)	-0.0087(15)	-0.0104(15)
C44	0.067(3)	0.055(2)	0.0273(19)	-0.0169(17)	-0.0062(18)	-0.011(2)
C45	0.072(3)	0.048(2)	0.040(2)	-0.0237(18)	-0.008(2)	0.006(2)
C46	0.049(2)	0.0365(18)	0.0300(18)	-0.0108(14)	-0.0079(16)	0.0061(15)
C51	0.0178(14)	0.0203(14)	0.0304(16)	-0.0043(12)	0.0024(12)	0.0002(11)
C52	0.0345(18)	0.0417(19)	0.0321(18)	-0.0057(14)	0.0046(14)	-0.0137(15)
C53	0.040(2)	0.060(2)	0.047(2)	-0.0117(18)	0.0151(17)	-0.0216(18)
C54	0.0265(18)	0.048(2)	0.062(3)	-0.0082(18)	0.0088(17)	-0.0148(16)
C55	0.0282(17)	0.0303(17)	0.052(2)	-0.0015(15)	-0.0093(15)	-0.0060(13)
C56	0.0254(16)	0.0244(15)	0.0293(16)	-0.0017(12)	-0.0040(13)	-0.0024(12)
C61	0.0217(15)	0.0210(14)	0.0284(16)	-0.0063(12)	0.0035(12)	-0.0045(11)
C62	0.0260(16)	0.0255(15)	0.0326(17)	-0.0006(12)	0.0009(13)	-0.0036(12)
C63	0.0343(19)	0.0282(16)	0.043(2)	0.0032(14)	0.0100(15)	-0.0051(14)
C64	0.036(2)	0.0373(19)	0.061(2)	-0.0127(17)	0.0142(17)	-0.0201(15)
C65	0.0314(19)	0.065(2)	0.051(2)	-0.028(2)	0.0056(16)	-0.0219(17)
C66	0.0320(18)	0.050(2)	0.0296(17)	-0.0174(15)	0.0049(14)	-0.0140(15)
C71	0.0232(15)	0.0271(15)	0.0173(14)	-0.0053(11)	-0.0040(11)	0.0002(11)
C72	0.0276(17)	0.0313(16)	0.0303(17)	-0.0069(13)	-0.0015(13)	-0.0031(13)
C73	0.0260(17)	0.048(2)	0.0345(18)	-0.0127(15)	0.0044(14)	0.0021(14)
C74	0.046(2)	0.0329(17)	0.0277(17)	-0.0081(14)	0.0021(15)	0.0124(15)
C75	0.059(2)	0.0238(16)	0.040(2)	-0.0024(14)	0.0128(17)	0.0020(15)
C76	0.0381(19)	0.0246(15)	0.0366(18)	-0.0032(13)	0.0091(15)	-0.0027(13)
C81	0.0189(14)	0.0281(15)	0.0199(14)	-0.0017(11)	0.0005(11)	-0.0013(11)
C82	0.0245(16)	0.0334(16)	0.0236(15)	-0.0041(12)	-0.0008(12)	-0.0029(12)
C83	0.0284(17)	0.050(2)	0.0206(16)	-0.0057(14)	-0.0008(13)	-0.0002(14)
C84	0.0324(18)	0.048(2)	0.0238(17)	0.0054(14)	-0.0020(14)	0.0058(15)
C85	0.045(2)	0.0293(17)	0.0367(19)	0.0078(14)	-0.0010(16)	-0.0003(15)
C86	0.0320(18)	0.0322(16)	0.0263(16)	-0.0018(13)	-0.0035(13)	-0.0012(13)

The form of the anisotropic displacement parameter is:

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

Table S8. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

(a) bis(triphenylphosphine)(η²–diphenylacetylene)platinum, molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H12	-0.0318	0.5053	0.2490	0.043
H13	-0.0324	0.5895	0.1358	0.057
H14	0.0577	0.5379	0.0353	0.064
H15	0.1463	0.4009	0.0478	0.068
H16	0.1445	0.3139	0.1606	0.050
H22	-0.0091	0.1409	0.3938	0.040
H23	-0.1306	0.0651	0.3721	0.051
H24	-0.2513	0.1184	0.2792	0.053
H25	-0.2493	0.2460	0.2085	0.058
H26	-0.1296	0.3227	0.2303	0.048
H32	0.1961	0.1334	0.4028	0.034
H33	0.3104	0.0061	0.4047	0.047
H34	0.3814	-0.0647	0.5164	0.050
H35	0.3381	-0.0087	0.6258	0.043
H36	0.2236	0.1186	0.6237	0.035
H42	-0.0988	0.3213	0.4762	0.035
H43	-0.2613	0.2927	0.5051	0.047
H44	-0.2780	0.1631	0.5675	0.062
H45	-0.1323	0.0641	0.6034	0.070
H46	0.0308	0.0932	0.5780	0.049
H52	-0.0223	0.2932	0.6304	0.034
H53	0.0050	0.3442	0.7382	0.042
H54	0.1693	0.3541	0.7668	0.041
H55	0.3080	0.3147	0.6870	0.035
H56	0.2810	0.2670	0.5783	0.030
H62	0.0796	0.4572	0.5016	0.031
H63	0.0605	0.5284	0.6035	0.039
H64	0.2047	0.5522	0.6564	0.045
H65	0.3680	0.5037	0.6086	0.044
H66	0.3875	0.4384	0.5031	0.034
H72	0.2527	0.4276	0.2485	0.033
H73	0.2490	0.5426	0.1564	0.042
H74	0.2368	0.6737	0.1890	0.044
H75	0.2252	0.6917	0.3128	0.045
H76	0.2222	0.5786	0.4051	0.037
H82	0.4433	0.4363	0.3772	0.032
H83	0.6085	0.3556	0.3682	0.040
H84	0.6315	0.2117	0.3723	0.043
H85	0.4892	0.1494	0.3854	0.042
H86	0.3250	0.2283	0.4000	0.033

Table S8. Derived Parameters for Hydrogen Atoms (continued)

(b) bis(triphenylphosphine)(η²–diphenylacetylene)platinum, molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H12	0.8436	0.0006	-0.0515	0.046
H13	0.9878	-0.0866	-0.0936	0.058
H14	1.0827	-0.0394	-0.1948	0.054
H15	1.0379	0.0976	-0.2517	0.058
H16	0.8932	0.1865	-0.2103	0.048
H22	0.6338	0.3607	-0.0235	0.039
H23	0.6991	0.4419	0.0473	0.047
H24	0.8641	0.3980	0.0938	0.051
H25	0.9634	0.2716	0.0712	0.064
H26	0.8982	0.1894	0.0006	0.055
H32	0.5641	0.3690	-0.1589	0.034
H33	0.5250	0.4980	-0.2323	0.042
H34	0.3551	0.5692	-0.2451	0.043
H35	0.2236	0.5097	-0.1854	0.040
H36	0.2615	0.3820	-0.1091	0.032
H42	0.5615	0.1761	0.0609	0.036
H43	0.5719	0.2008	0.1819	0.045
H44	0.4865	0.3266	0.2168	0.059
H45	0.3911	0.4264	0.1316	0.064
H46	0.3768	0.4019	0.0106	0.048
H52	0.3237	0.2068	0.0551	0.042
H53	0.1678	0.1609	0.0657	0.057
H54	0.0824	0.1541	-0.0395	0.054
H55	0.1525	0.1908	-0.1564	0.044
H56	0.3087	0.2324	-0.1678	0.032
H62	0.4738	0.0394	-0.0540	0.035
H63	0.3423	-0.0299	-0.0117	0.044
H64	0.2245	-0.0470	-0.0955	0.051
H65	0.2366	0.0087	-0.2192	0.055
H66	0.3707	0.0734	-0.2623	0.042
H72	0.7523	0.0745	-0.2531	0.036
H73	0.8726	-0.0393	-0.2822	0.044
H74	0.8366	-0.1718	-0.2575	0.046
H75	0.6776	-0.1896	-0.2066	0.052
H76	0.5569	-0.0758	-0.1747	0.041
H82	0.5139	0.0672	-0.3355	0.033
H83	0.4837	0.1464	-0.4524	0.041
H84	0.4921	0.2857	-0.4704	0.045
H85	0.5277	0.3482	-0.3720	0.047
H86	0.5483	0.2725	-0.2538	0.037