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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G TO T H E P A P E R

Polyhedral metallaheteroborane chemistry. Synthesis, spectroscopy, structure and dynamics of the eleven-vertex rhodaazaborane [8,8-(PPh3)2-nido-8,7-RhNB9H11] and the platinacarbaborane [9-(OMe)-8,8-(PMe2Ph)2-nido-8,7-PtCB9H10]

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C o n t e n t s
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Table S1 - Crystal Data and Details of the Structure Determination
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Crystal Data

Formula	2(C36 H41 B9 N P2 Rh), C Cl2		
Formula Weight	791.29		
Crystal System	Triclinic		
Space group	P-1	(No. 2)	
a, b, c [Angstrom]	9.7567(12)	11.936(2)	17.698(2)
alpha, beta, gamma [deg]	93.138(9)	94.637(9)	105.790(9)
V [Ang**3]	1970.4(5)		
Z	2		
D(calc) [g/cm**3]	1.334		
Mu(MoKa) [/mm]	0.610		
F(000)	808		
Crystal Size [mm]	0.15 x	0.40 x	0.60

Data Collection

Temperature (K)	200		
Radiation [Angstrom]	MoKa	0.71069	
Theta Min-Max [Deg]	1.8,	25.0	
Dataset	-11: 11 ; -14: 14 ; -17: 21		
Tot., Uniq. Data, R(int)	8429,	6954,	0.040
Observed data [I > 2.0 sigma(I)]	5884		

Refinement

Nref, Npar	6954,	502	
R, wR2, S	0.0347,	0.0910,	1.03
w = 1/[\s^2^(Fo^2^)+(0.0520P)^2^+2.0822P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error	0.00,	0.00	
Min. and Max. Resd. Dens. [e/Ang^3]	-0.71,	1.16	

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	x	y	z	U(eq) [Ang^2]

Rh8	0.13776(2)	0.38317(2)	0.23326(1)	0.0166(1)
P1	0.11592(7)	0.26013(6)	0.13046(4)	0.0182(2)
P2	0.01645(7)	0.24246(6)	0.31611(4)	0.0180(2)
N7	0.1475(3)	0.5248(2)	0.32284(14)	0.0244(8)
C111	-0.0765(3)	0.1997(3)	0.10469(16)	0.0258(9)
C112	-0.1521(3)	0.2818(3)	0.08929(18)	0.0335(10)
C113	-0.2995(4)	0.2469(4)	0.0709(2)	0.0471(13)
C114	-0.3734(4)	0.1307(4)	0.0693(2)	0.0538(16)
C115	-0.3007(4)	0.0495(4)	0.0861(2)	0.0506(14)
C116	-0.1521(4)	0.0825(3)	0.10352(17)	0.0344(10)
C121	0.1999(3)	0.1432(2)	0.14564(16)	0.0218(8)
C122	0.1716(4)	0.0434(3)	0.09579(18)	0.0301(10)
C123	0.2410(4)	-0.0414(3)	0.1090(2)	0.0373(11)
C124	0.3433(4)	-0.0256(3)	0.1705(2)	0.0376(11)
C125	0.3767(3)	0.0750(3)	0.2186(2)	0.0342(10)
C126	0.3045(3)	0.1591(3)	0.20667(18)	0.0261(9)
C131	0.1872(3)	0.3087(2)	0.04106(16)	0.0218(8)
C132	0.3309(3)	0.3180(3)	0.03306(18)	0.0310(10)
C133	0.3914(4)	0.3574(3)	-0.03225(19)	0.0378(11)
C134	0.3093(4)	0.3862(3)	-0.09103(19)	0.0393(11)
C135	0.1670(4)	0.3762(4)	-0.0845(2)	0.0425(11)
C136	0.1055(3)	0.3377(3)	-0.01902(18)	0.0332(10)
C211	0.1211(3)	0.2425(2)	0.40654(16)	0.0231(9)
C212	0.0601(4)	0.1752(3)	0.46364(19)	0.0352(11)
C213	0.1386(4)	0.1783(3)	0.5329(2)	0.0430(11)
C214	0.2789(4)	0.2474(3)	0.5453(2)	0.0415(11)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	x	y	z	U(eq) [Ang^2]
C215	0.3405(4)	0.3132(3)	0.4893(2)	0.0384(11)
C216	0.2628(3)	0.3108(3)	0.41966(18)	0.0279(9)
C221	-0.0714(3)	0.0864(2)	0.29430(16)	0.0224(8)
C222	0.0158(4)	0.0128(3)	0.28538(19)	0.0321(10)
C223	-0.0431(5)	-0.1057(3)	0.2658(2)	0.0458(13)
C224	-0.1893(5)	-0.1517(3)	0.2558(2)	0.0486(13)
C225	-0.2767(4)	-0.0806(3)	0.2663(2)	0.0479(12)
C226	-0.2186(4)	0.0378(3)	0.2855(2)	0.0346(10)
C231	-0.1250(3)	0.3073(2)	0.34217(17)	0.0232(9)
C232	-0.2315(3)	0.3113(3)	0.28559(19)	0.0299(10)
C233	-0.3312(4)	0.3717(3)	0.3002(2)	0.0388(11)
C234	-0.3230(4)	0.4311(3)	0.3705(2)	0.0438(14)
C235	-0.2186(4)	0.4278(3)	0.4268(2)	0.0416(12)
C236	-0.1198(3)	0.3655(3)	0.41361(19)	0.0308(10)
B1	0.1897(4)	0.6754(3)	0.2170(2)	0.0256(10)
B2	0.1654(4)	0.6660(3)	0.3141(2)	0.0300(11)
B3	0.0727(4)	0.5462(3)	0.2434(2)	0.0237(10)
B4	0.1890(4)	0.5407(3)	0.16727(19)	0.0221(9)
B5	0.3546(4)	0.6472(3)	0.1973(2)	0.0255(10)
B6	0.3396(4)	0.7105(3)	0.2899(2)	0.0300(11)
B9	0.3396(4)	0.4968(3)	0.2009(2)	0.0242(10)
B10	0.4305(4)	0.6019(3)	0.2810(2)	0.0297(11)
B11	0.2986(4)	0.6021(3)	0.3529(2)	0.0309(11)
*C1S	0.5896(10)	0.1201(8)	0.4960(6)	0.054(2)
*Cl1S	0.4015(8)	0.0153(6)	0.4364(4)	0.145(2)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	x	y	z	U(eq) [Ang^2]
*Cl2S	0.3461(11)	-0.0610(9)	0.4878(6)	0.154(3)
*Cl3S	0.5393(11)	0.0854(9)	0.4426(6)	0.158(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	x	y	z	U(iso) [Ang^2]
H1	0.150(4)	0.739(3)	0.1857(19)	0.029(9)
H2	0.105(4)	0.708(3)	0.351(2)	0.036(10)
H3	-0.040(4)	0.520(3)	0.2345(18)	0.025(8)
H4	0.139(4)	0.530(3)	0.109(2)	0.034(9)
H5	0.425(4)	0.705(3)	0.161(2)	0.032(9)
H6	0.408(4)	0.801(4)	0.312(2)	0.050(11)
H7	0.090(4)	0.499(3)	0.357(2)	0.036(10)
H9	0.411(4)	0.447(3)	0.171(2)	0.042(10)
H10	0.545(4)	0.624(3)	0.2970(19)	0.029(9)
H11	0.327(4)	0.604(3)	0.414(2)	0.043(10)
H112	-0.10190	0.36240	0.09150	0.0400
H113	-0.34910	0.30320	0.05940	0.0560
H114	-0.47420	0.10640	0.05670	0.0640
H115	-0.35260	-0.03040	0.08590	0.0610
H116	-0.10340	0.02540	0.11440	0.0410
H122	0.10420	0.03350	0.05240	0.0360
H123	0.21850	-0.11060	0.07580	0.0450
H124	0.39060	-0.08420	0.17960	0.0450
H125	0.44900	0.08680	0.25990	0.0410
H126	0.32670	0.22770	0.24030	0.0310

H132	0.38810	0.29700	0.07290	0.0370
H133	0.48980	0.36450	-0.03640	0.0450
H134	0.35070	0.41290	-0.13580	0.0470
H135	0.11020	0.39580	-0.12510	0.0510
H136	0.00710	0.33110	-0.01530	0.0400
H212	-0.03570	0.12700	0.45500	0.0420

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	x	y	z	U(iso) [Ang^2]
H213	0.09620	0.13310	0.57190	0.0520
H214	0.33280	0.24930	0.59280	0.0500
H215	0.43670	0.36050	0.49820	0.0460
H216	0.30620	0.35570	0.38090	0.0330
H222	0.11680	0.04400	0.29280	0.0380
H223	0.01750	-0.15500	0.25940	0.0550
H224	-0.22980	-0.23260	0.24160	0.0580
H225	-0.37770	-0.11290	0.26040	0.0570
H226	-0.28000	0.08620	0.29270	0.0420
H232	-0.23590	0.27250	0.23680	0.0360
H233	-0.40500	0.37220	0.26190	0.0470
H234	-0.38950	0.47420	0.38000	0.0530
H235	-0.21380	0.46830	0.47510	0.0500
H236	-0.04910	0.36260	0.45310	0.0370
H910	0.374(4)	0.498(3)	0.282(2)	0.041(10)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Rh8	0.0171(1)	0.0155(1)	0.0163(1)	0.0016(1)	0.0021(1)	0.0026(1)
P1	0.0151(3)	0.0209(4)	0.0174(4)	0.0004(3)	0.0007(3)	0.0034(3)
P2	0.0161(3)	0.0185(4)	0.0185(4)	0.0023(3)	0.0022(3)	0.0029(3)
N7	0.0327(14)	0.0186(12)	0.0208(13)	0.0014(10)	0.0088(11)	0.0036(11)
C111	0.0171(14)	0.0393(18)	0.0167(14)	-0.0033(12)	0.0016(11)	0.0015(13)
C112	0.0225(16)	0.048(2)	0.0294(17)	-0.0036(15)	-0.0002(13)	0.0111(14)
C113	0.0235(18)	0.080(3)	0.039(2)	-0.001(2)	0.0013(15)	0.0182(19)
C114	0.0198(17)	0.099(4)	0.034(2)	0.004(2)	0.0004(15)	0.003(2)
C115	0.035(2)	0.064(3)	0.032(2)	0.0019(18)	0.0047(16)	-0.0211(19)
C116	0.0309(17)	0.0419(19)	0.0206(16)	0.0014(14)	0.0010(13)	-0.0055(15)
C121	0.0235(14)	0.0228(15)	0.0211(14)	0.0049(11)	0.0076(11)	0.0077(12)
C122	0.0401(18)	0.0251(16)	0.0248(16)	0.0008(13)	0.0063(14)	0.0078(14)
C123	0.047(2)	0.0248(17)	0.043(2)	0.0029(14)	0.0165(17)	0.0112(15)
C124	0.0379(19)	0.0315(18)	0.053(2)	0.0186(16)	0.0194(17)	0.0184(15)
C125	0.0254(16)	0.0410(19)	0.0399(19)	0.0163(15)	0.0053(14)	0.0124(14)
C126	0.0228(15)	0.0275(16)	0.0275(16)	0.0026(12)	0.0042(12)	0.0054(12)
C131	0.0218(14)	0.0222(14)	0.0196(14)	0.0012(11)	0.0029(11)	0.0032(11)
C132	0.0230(15)	0.046(2)	0.0257(16)	0.0060(14)	0.0029(12)	0.0118(14)
C133	0.0277(17)	0.055(2)	0.0303(18)	0.0059(16)	0.0091(14)	0.0087(16)
C134	0.038(2)	0.051(2)	0.0245(17)	0.0084(15)	0.0095(14)	0.0019(16)
C135	0.043(2)	0.058(2)	0.0265(18)	0.0150(17)	-0.0010(15)	0.0129(18)
C136	0.0254(16)	0.048(2)	0.0278(17)	0.0090(15)	0.0013(13)	0.0123(15)
C211	0.0242(15)	0.0225(15)	0.0233(15)	0.0021(12)	0.0003(12)	0.0082(12)
C212	0.0337(18)	0.042(2)	0.0289(17)	0.0096(15)	0.0030(14)	0.0074(15)
C213	0.057(2)	0.048(2)	0.0255(18)	0.0101(16)	0.0029(16)	0.0162(19)
C214	0.056(2)	0.042(2)	0.0261(17)	-0.0024(15)	-0.0138(16)	0.0189(18)

Table S4 - (An)isotropic Displacement Parameters (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C215	0.0363(19)	0.0354(19)	0.038(2)	-0.0044(15)	-0.0137(15)	0.0073(15)
C216	0.0261(16)	0.0266(16)	0.0290(16)	0.0009(13)	-0.0023(13)	0.0059(13)
C221	0.0246(15)	0.0206(14)	0.0202(14)	0.0032(11)	0.0051(12)	0.0021(12)
C222	0.0353(18)	0.0258(16)	0.0371(18)	0.0083(14)	0.0160(14)	0.0071(14)
C223	0.072(3)	0.0265(18)	0.046(2)	0.0086(16)	0.027(2)	0.0183(18)
C224	0.072(3)	0.0218(17)	0.041(2)	0.0000(15)	0.0115(19)	-0.0065(18)
C225	0.039(2)	0.037(2)	0.053(2)	0.0051(17)	-0.0024(18)	-0.0124(17)
C226	0.0264(16)	0.0319(18)	0.0407(19)	0.0040(15)	0.0017(14)	0.0002(14)
C231	0.0178(14)	0.0231(15)	0.0288(16)	0.0060(12)	0.0073(12)	0.0038(11)
C232	0.0250(16)	0.0352(18)	0.0308(17)	0.0058(14)	0.0044(13)	0.0097(13)
C233	0.0252(17)	0.040(2)	0.055(2)	0.0133(17)	0.0051(16)	0.0134(15)
C234	0.0350(19)	0.046(2)	0.060(3)	0.0094(18)	0.0195(18)	0.0221(17)
C235	0.047(2)	0.042(2)	0.042(2)	-0.0003(16)	0.0200(17)	0.0189(17)
C236	0.0309(17)	0.0331(17)	0.0296(17)	0.0027(14)	0.0078(13)	0.0095(14)
B1	0.0284(18)	0.0210(17)	0.0290(18)	0.0047(14)	0.0078(14)	0.0077(14)
B2	0.037(2)	0.0185(17)	0.034(2)	-0.0002(14)	0.0115(16)	0.0052(14)
B3	0.0219(17)	0.0218(16)	0.0292(18)	0.0032(13)	0.0083(14)	0.0073(13)
B4	0.0227(16)	0.0213(16)	0.0223(17)	0.0037(13)	0.0044(13)	0.0051(13)
B5	0.0256(17)	0.0201(16)	0.0292(18)	0.0029(14)	0.0066(14)	0.0024(13)
B6	0.037(2)	0.0197(17)	0.0299(19)	-0.0008(14)	0.0041(16)	0.0027(15)
B9	0.0201(16)	0.0228(17)	0.0278(18)	0.0021(14)	0.0024(13)	0.0030(13)
B10	0.0225(18)	0.0261(18)	0.036(2)	0.0000(15)	-0.0033(15)	0.0016(14)
B11	0.039(2)	0.0233(18)	0.0266(19)	-0.0025(14)	-0.0008(15)	0.0043(15)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Rh8	-P1	2.2331(8)	C125	-C126	1.390(5)
Rh8	-P2	2.4166(8)	C131	-C132	1.395(4)
Rh8	-N7	2.231(2)	C131	-C136	1.393(4)
Rh8	-B3	2.208(4)	C132	-C133	1.387(5)
Rh8	-B4	2.230(3)	C133	-C134	1.377(5)
Rh8	-B9	2.204(4)	C134	-C135	1.376(6)
Cl2S	-Cl3S_a	1.687(15)	C135	-C136	1.391(5)
P1	-C111	1.828(3)	C211	-C216	1.394(4)
P1	-C131	1.839(3)	C211	-C212	1.395(4)
P1	-C121	1.822(3)	C112	-H112	0.9500
P2	-C211	1.827(3)	C212	-C213	1.385(5)
P2	-C231	1.833(3)	C113	-H113	0.9500
P2	-C221	1.831(2)	C213	-C214	1.385(5)
N7	-B2	1.664(4)	C214	-C215	1.373(5)
N7	-B3	1.597(4)	C114	-H114	0.9500
N7	-B11	1.545(5)	C215	-C216	1.389(5)
N7	-H7	0.87(4)	C115	-H115	0.9500
C111	-C112	1.403(5)	C116	-H116	0.9500
C111	-C116	1.391(5)	C221	-C226	1.387(5)
C112	-C113	1.390(5)	C221	-C222	1.391(5)
C113	-C114	1.376(6)	C122	-H122	0.9500
C114	-C115	1.379(6)	C222	-C223	1.387(5)
C115	-C116	1.399(6)	C123	-H123	0.9500
C121	-C122	1.393(4)	C223	-C224	1.375(7)
C121	-C126	1.392(4)	C124	-H124	0.9500
C122	-C123	1.382(5)	C224	-C225	1.373(6)
C123	-C124	1.384(5)	C225	-C226	1.384(5)
C124	-C125	1.380(5)	C125	-H125	0.9500

Table S5 - Bond Distances (Angstrom) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C126	-H126	0.9500	B1	-B4	1.788(5)
C231	-C232	1.396(4)	B1	-B5	1.788(6)
C231	-C236	1.399(4)	B1	-B6	1.812(5)
C132	-H132	0.9500	B1	-B2	1.759(5)
C232	-C233	1.391(5)	B2	-B3	1.829(5)
C233	-C234	1.383(5)	B2	-B6	1.734(6)
C133	-H133	0.9500	B2	-B11	1.787(5)
C234	-C235	1.376(5)	B3	-B4	1.840(5)
C134	-H134	0.9500	B4	-B5	1.783(5)
C235	-C236	1.394(5)	B4	-B9	1.761(6)
C135	-H135	0.9500	B5	-B9	1.766(5)
C136	-H136	0.9500	B5	-B10	1.779(5)
C212	-H212	0.9500	B5	-B6	1.800(5)
C213	-H213	0.9500	B6	-B11	1.739(5)
C214	-H214	0.9500	B6	-B10	1.766(5)
C215	-H215	0.9500	B9	-B10	1.835(5)
C216	-H216	0.9500	B10	-B11	1.882(5)
C222	-H222	0.9500	B1	-H1	1.10(4)
C223	-H223	0.9500	B2	-H2	1.10(4)
C224	-H224	0.9500	B3	-H3	1.05(4)
C225	-H225	0.9500	B4	-H4	1.09(4)
C226	-H226	0.9500	B5	-H5	1.11(4)
C232	-H232	0.9500	B6	-H6	1.13(5)
C233	-H233	0.9500	B9	-H9	1.17(4)
C234	-H234	0.9500	B9	-H910	1.45(4)
C235	-H235	0.9500	B10	-H910	1.21(3)
C236	-H236	0.9500	B10	-H10	1.09(4)
B1	-B3	1.763(5)	B11	-H11	1.09(4)

Table S6 - Bond Angles (Degrees)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

P1	-Rh8	-P2	97.64(3)	Rh8	-N7	-B3	68.16(15)
P1	-Rh8	-N7	170.61(7)	Rh8	-N7	-B11	116.2(2)
P1	-Rh8	-B3	128.54(9)	B2	-N7	-B3	68.2(2)
P1	-Rh8	-B4	93.31(9)	B2	-N7	-B11	67.6(2)
P1	-Rh8	-B9	91.57(9)	B3	-N7	-B11	120.3(2)
P2	-Rh8	-N7	88.82(7)	B2	-N7	-H7	111(2)
P2	-Rh8	-B3	111.61(10)	B3	-N7	-H7	116(3)
P2	-Rh8	-B4	159.80(10)	B11	-N7	-H7	116(2)
P2	-Rh8	-B9	148.90(10)	Rh8	-N7	-H7	111(2)
N7	-Rh8	-B3	42.17(11)	P1	-C111	-C116	125.5(3)
N7	-Rh8	-B4	78.57(11)	P1	-C111	-C112	115.5(3)
N7	-Rh8	-B9	86.29(12)	C112	-C111	-C116	118.9(3)
B3	-Rh8	-B4	48.99(14)	C111	-C112	-C113	120.9(3)
B3	-Rh8	-B9	84.48(14)	C112	-C113	-C114	119.9(4)
B4	-Rh8	-B9	46.78(14)	C113	-C114	-C115	119.8(4)
Rh8	-P1	-C111	105.70(10)	C114	-C115	-C116	121.3(4)
Rh8	-P1	-C121	113.78(9)	C111	-C116	-C115	119.3(3)
Rh8	-P1	-C131	122.33(8)	P1	-C121	-C122	122.8(2)
C111	-P1	-C121	110.38(14)	P1	-C121	-C126	118.1(2)
C111	-P1	-C131	104.33(13)	C122	-C121	-C126	119.0(3)
C121	-P1	-C131	99.78(13)	C121	-C122	-C123	120.5(3)
Rh8	-P2	-C211	113.82(9)	C122	-C123	-C124	120.1(3)
Rh8	-P2	-C221	128.66(10)	C123	-C124	-C125	120.1(3)
Rh8	-P2	-C231	100.62(9)	C124	-C125	-C126	120.0(3)
C211	-P2	-C221	101.56(12)	C121	-C126	-C125	120.3(3)
C211	-P2	-C231	104.04(13)	P1	-C131	-C132	118.5(2)
C221	-P2	-C231	105.61(13)	P1	-C131	-C136	123.4(2)
Rh8	-N7	-B2	129.17(18)	C132	-C131	-C136	118.1(3)

Table S6 - Bond Angles (Degrees) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C131	-C132	-C133	120.9(3)	C221	-C222	-C223	120.8(4)
C132	-C133	-C134	120.2(4)	C222	-C223	-C224	119.9(4)
C133	-C134	-C135	119.6(3)	C122	-C123	-H123	120.00
C134	-C135	-C136	120.6(3)	C124	-C123	-H123	120.00
C131	-C136	-C135	120.5(3)	C123	-C124	-H124	120.00
P2	-C211	-C212	120.6(2)	C223	-C224	-C225	120.0(3)
P2	-C211	-C216	120.4(2)	C125	-C124	-H124	120.00
C212	-C211	-C216	119.1(3)	C224	-C225	-C226	120.4(4)
C211	-C212	-C213	120.3(3)	C126	-C125	-H125	120.00
C111	-C112	-H112	120.00	C124	-C125	-H125	120.00
C113	-C112	-H112	120.00	C125	-C126	-H126	120.00
C112	-C113	-H113	120.00	C121	-C126	-H126	120.00
C212	-C213	-C214	119.9(3)	C221	-C226	-C225	120.6(3)
C114	-C113	-H113	120.00	P2	-C231	-C236	122.3(2)
C113	-C114	-H114	120.00	C232	-C231	-C236	118.9(3)
C115	-C114	-H114	120.00	P2	-C231	-C232	118.3(2)
C213	-C214	-C215	120.3(3)	C231	-C232	-C233	120.5(3)
C214	-C215	-C216	120.3(3)	C131	-C132	-H132	120.00
C114	-C115	-H115	119.00	C133	-C132	-H132	120.00
C116	-C115	-H115	119.00	C232	-C233	-C234	120.1(3)
C211	-C216	-C215	120.1(3)	C134	-C133	-H133	120.00
C111	-C116	-H116	120.00	C132	-C133	-H133	120.00
C115	-C116	-H116	120.00	C233	-C234	-C235	120.0(4)
P2	-C221	-C226	124.1(2)	C135	-C134	-H134	120.00
C222	-C221	-C226	118.4(3)	C133	-C134	-H134	120.00
P2	-C221	-C222	117.5(2)	C134	-C135	-H135	120.00
C121	-C122	-H122	120.00	C234	-C235	-C236	120.6(3)

C123	-C122	-H122	120.00	C136	-C135	-H135	120.00

Table S6 - Bond Angles (Degrees) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C231	-C236	-C235	119.9(3)	C233	-C234	-H234	120.00
C131	-C136	-H136	120.00	C234	-C235	-H235	120.00
C135	-C136	-H136	120.00	C236	-C235	-H235	120.00
C211	-C212	-H212	120.00	C231	-C236	-H236	120.00
C213	-C212	-H212	120.00	C235	-C236	-H236	120.00
C212	-C213	-H213	120.00	B2	-B1	-B3	62.6(2)
C214	-C213	-H213	120.00	B2	-B1	-B4	114.5(2)
C213	-C214	-H214	120.00	B2	-B1	-B5	110.8(3)
C215	-C214	-H214	120.00	B2	-B1	-B6	58.1(2)
C214	-C215	-H215	120.00	B3	-B1	-B4	62.4(2)
C216	-C215	-H215	120.00	B3	-B1	-B5	109.0(3)
C211	-C216	-H216	120.00	B3	-B1	-B6	104.6(2)
C215	-C216	-H216	120.00	B4	-B1	-B5	59.8(2)
C221	-C222	-H222	120.00	B4	-B1	-B6	106.9(3)
C223	-C222	-H222	120.00	B5	-B1	-B6	60.0(2)
C224	-C223	-H223	120.00	N7	-B2	-B1	101.2(2)
C222	-C223	-H223	120.00	N7	-B2	-B3	54.16(18)
C225	-C224	-H224	120.00	N7	-B2	-B6	100.5(3)
C223	-C224	-H224	120.00	N7	-B2	-B11	53.04(19)
C224	-C225	-H225	120.00	B1	-B2	-B6	62.5(2)
C226	-C225	-H225	120.00	B1	-B2	-B11	105.8(3)
C225	-C226	-H226	120.00	B3	-B2	-B6	105.1(3)
C221	-C226	-H226	120.00	B3	-B2	-B11	97.8(2)
C231	-C232	-H232	120.00	B6	-B2	-B11	59.2(2)
C233	-C232	-H232	120.00	B1	-B2	-B3	58.8(2)
C232	-C233	-H233	120.00	Rh8	-B3	-N7	69.68(16)

C234	-C233	-H233	120.00	Rh8	-B3	-B1	118.4(2)
C235	-C234	-H234	120.00	Rh8	-B3	-B4	66.14(16)

Table S6 - Bond Angles (Degrees) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

N7	-B3	-B1	103.8(3)	B1	-B6	-B10	108.0(2)
Rh8	-B3	-B2	121.4(2)	B1	-B6	-B2	59.5(2)
N7	-B3	-B4	110.3(3)	B2	-B6	-B5	111.4(3)
B1	-B3	-B2	58.62(19)	B2	-B6	-B10	116.9(3)
B1	-B3	-B4	59.5(2)	B1	-B6	-B11	105.6(3)
B2	-B3	-B4	108.8(3)	B5	-B6	-B10	59.8(2)
N7	-B3	-B2	57.63(18)	B5	-B6	-B11	110.1(2)
Rh8	-B4	-B1	116.1(2)	B10	-B6	-B11	64.9(2)
Rh8	-B4	-B3	64.88(15)	B2	-B6	-B11	62.0(2)
Rh8	-B4	-B9	65.85(16)	Rh8	-B9	-B5	117.9(2)
B1	-B4	-B3	58.1(2)	Rh8	-B9	-B10	110.0(2)
B1	-B4	-B5	60.1(2)	Rh8	-B9	-B4	67.37(17)
B1	-B4	-B9	110.1(3)	B4	-B9	-B10	106.2(2)
B3	-B4	-B5	105.8(2)	B5	-B9	-B10	59.16(19)
B3	-B4	-B9	110.9(2)	B4	-B9	-B5	60.7(2)
B5	-B4	-B9	59.8(2)	B5	-B10	-B6	61.1(2)
Rh8	-B4	-B5	115.9(2)	B5	-B10	-B9	58.50(19)
B1	-B5	-B6	60.6(2)	B6	-B10	-B9	108.6(3)
B1	-B5	-B9	109.9(3)	B6	-B10	-B11	56.9(2)
B1	-B5	-B10	108.5(3)	B5	-B10	-B11	104.8(3)
B4	-B5	-B6	107.6(3)	B9	-B10	-B11	108.1(3)
B4	-B5	-B9	59.5(2)	N7	-B11	-B6	105.2(3)
B4	-B5	-B10	107.7(2)	N7	-B11	-B10	111.3(2)
B1	-B5	-B4	60.1(2)	N7	-B11	-B2	59.4(2)
B6	-B5	-B10	59.1(2)	B2	-B11	-B10	108.7(2)

B9	-B5	-B10	62.3(2)	B6	-B11	-B10	58.2(2)
B6	-B5	-B9	110.1(2)	B2	-B11	-B6	58.9(2)
B1	-B6	-B5	59.3(2)	B2	-B1	-H1	119.1(19)

Table S6 - Bond Angles (Degrees) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B3	-B1	-H1	122(2)	B5	-B6	-H6	121.6(19)
B4	-B1	-H1	118.6(18)	B10	-B6	-H6	116(2)
B5	-B1	-H1	120(2)	B11	-B6	-H6	119.2(19)
B6	-B1	-H1	125.6(19)	Rh8	-B9	-H9	114.4(18)
N7	-B2	-H2	116.4(18)	Rh8	-B9	-H910	79.3(15)
B1	-B2	-H2	131.0(19)	B4	-B9	-H9	132.5(18)
B3	-B2	-H2	121(2)	B4	-B9	-H910	119.1(16)
B6	-B2	-H2	132(2)	B5	-B9	-H9	125.1(18)
B11	-B2	-H2	121.5(19)	B5	-B9	-H910	97.6(14)
Rh8	-B3	-H3	105.4(19)	B10	-B9	-H9	115.7(18)
N7	-B3	-H3	118.5(18)	B10	-B9	-H910	41.4(14)
B1	-B3	-H3	127.3(19)	H9	-B9	-H910	107(2)
B2	-B3	-H3	120.5(19)	B5	-B10	-H10	123.0(18)
B4	-B3	-H3	123.4(18)	B5	-B10	-H910	106.8(17)
Rh8	-B4	-H4	116.4(18)	B6	-B10	-H10	119.8(19)
B1	-B4	-H4	113.3(19)	B6	-B10	-H910	124.1(19)
B3	-B4	-H4	117(2)	B9	-B10	-H10	123.2(18)
B5	-B4	-H4	122(2)	B9	-B10	-H910	51.9(17)
B9	-B4	-H4	127(2)	B11	-B10	-H10	122.2(18)
B1	-B5	-H5	119(2)	B11	-B10	-H910	78.9(18)
B4	-B5	-H5	126.9(19)	H10	-B10	-H910	112(3)
B6	-B5	-H5	116.2(18)	N7	-B11	-H11	116(2)
B9	-B5	-H5	124.1(19)	B2	-B11	-H11	123(2)
B10	-B5	-H5	120(2)	B6	-B11	-H11	131.2(19)

B1	-B6	-H6	127(2)	B10	-B11	-H11	123(2)
B2	-B6	-H6	118(2)				

Table S7 - Torsion Angles (Degrees)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

P2	-Rh8	-P1	-C111	61.24(11)
P2	-Rh8	-P1	-C121	-60.04(10)
P2	-Rh8	-P1	-C131	-179.94(12)
B3	-Rh8	-P1	-C111	-64.35(17)
B3	-Rh8	-P1	-C121	174.39(16)
B3	-Rh8	-P1	-C131	54.48(18)
B4	-Rh8	-P1	-C111	-101.75(15)
B4	-Rh8	-P1	-C121	136.98(14)
B4	-Rh8	-P1	-C131	17.08(16)
B9	-Rh8	-P1	-C111	-148.54(15)
B9	-Rh8	-P1	-C121	90.19(14)
B9	-Rh8	-P1	-C131	-29.72(15)
P1	-Rh8	-P2	-C211	126.41(10)
P1	-Rh8	-P2	-C221	-2.90(13)
P1	-Rh8	-P2	-C231	-122.94(10)
N7	-Rh8	-P2	-C211	-60.42(12)
N7	-Rh8	-P2	-C221	170.27(15)
N7	-Rh8	-P2	-C231	50.22(12)
B3	-Rh8	-P2	-C211	-96.76(14)
B3	-Rh8	-P2	-C221	133.93(16)
B3	-Rh8	-P2	-C231	13.89(14)
B4	-Rh8	-P2	-C211	-111.4(3)
B4	-Rh8	-P2	-C221	119.3(3)
B4	-Rh8	-P2	-C231	-0.7(3)
B9	-Rh8	-P2	-C211	20.4(2)

B9	-Rh8	-P2	-C221	-108.9(2)
B9	-Rh8	-P2	-C231	131.0(2)
P1	-Rh8	-B4	-B1	169.4(2)

Table S7 - Torsion Angles (Degrees) (continued)
For [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

P2	-Rh8	-B4	-B1	46.5(4)
N7	-Rh8	-B4	-B1	-5.8(2)
B3	-Rh8	-B4	-B1	28.4(2)
B9	-Rh8	-B4	-B1	-101.5(3)
P1	-Rh8	-B4	-B3	140.97(15)
P2	-Rh8	-B4	-B3	18.1(4)
N7	-Rh8	-B4	-B3	-34.28(16)
B9	-Rh8	-B4	-B3	-130.0(2)
P1	-Rh8	-B4	-B5	-122.9(2)
P2	-Rh8	-B4	-B5	114.2(3)
N7	-Rh8	-B4	-B5	61.9(2)
B3	-Rh8	-B4	-B5	96.1(3)
B9	-Rh8	-B4	-B5	-33.9(2)
P1	-Rh8	-B4	-B9	-89.05(15)
P2	-Rh8	-B4	-B9	148.1(2)
N7	-Rh8	-B4	-B9	95.70(17)
B3	-Rh8	-B4	-B9	130.0(2)
P1	-Rh8	-B9	-B4	93.06(15)
P2	-Rh8	-B9	-B4	-159.30(15)
N7	-Rh8	-B9	-B4	-77.79(16)
P2	-Rh8	-N7	-B2	-157.5(3)
B3	-Rh8	-N7	-B2	-32.6(3)
P1	-Rh8	-B3	-N7	-178.17(11)
P2	-Rh8	-B3	-N7	61.94(17)

B4	-Rh8	-B3	-N7	-124.7(2)
B9	-Rh8	-B3	-N7	-90.56(18)
P1	-Rh8	-B3	-B1	-83.0(3)
P2	-Rh8	-B3	-B1	157.1(2)

Table S7 - Torsion Angles (Degrees) (continued)
for[8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

N7	-Rh8	-B3	-B1	95.1(3)
B4	-Rh8	-B3	-B1	-29.6(2)
B9	-Rh8	-B3	-B1	4.6(2)
P1	-Rh8	-B3	-B2	-151.70(19)
P2	-Rh8	-N7	-B3	-124.85(17)
B4	-Rh8	-N7	-B3	39.28(19)
B9	-Rh8	-N7	-B3	85.88(19)
P2	-Rh8	-B3	-B2	88.4(2)
N7	-Rh8	-B3	-B2	26.5(2)
B4	-Rh8	-N7	-B2	6.6(3)
B9	-Rh8	-N7	-B2	53.3(3)
B4	-Rh8	-B9	-B10	99.8(3)
P2	-Rh8	-B9	-B5	-124.4(2)
N7	-Rh8	-B9	-B5	-42.9(2)
P2	-Rh8	-N7	-B11	121.0(2)
B3	-Rh8	-N7	-B11	-114.1(3)
B4	-Rh8	-N7	-B11	-74.9(2)
B9	-Rh8	-N7	-B11	-28.3(2)
P1	-Rh8	-B9	-B5	128.0(2)
B3	-Rh8	-B9	-B10	64.3(2)
B4	-Rh8	-B3	-B2	-98.2(3)
B3	-Rh8	-B9	-B5	-0.6(2)
B4	-Rh8	-B9	-B5	34.9(2)

P1	-Rh8	-B9	-B10	-167.1(2)
B3	-Rh8	-B9	-B4	-35.51(17)
N7	-Rh8	-B9	-B10	22.0(2)
P1	-Rh8	-B3	-B4	-53.5(2)
P2	-Rh8	-B3	-B4	-173.38(14)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B9	-Rh8	-B3	-B2	-64.1(3)
B9	-Rh8	-B3	-B4	34.13(17)
P2	-Rh8	-B9	-B10	-59.5(3)
N7	-Rh8	-B3	-B4	124.7(2)
Rh8	-P1	-C111	-C116	-117.8(3)
C111	-P1	-C131	-C136	24.4(3)
C131	-P1	-C111	-C116	112.0(3)
C121	-P1	-C131	-C132	-42.0(2)
Rh8	-P1	-C111	-C112	58.4(2)
C111	-P1	-C131	-C132	-156.2(2)
C111	-P1	-C121	-C122	46.2(3)
C121	-P1	-C111	-C112	-178.1(2)
Rh8	-P1	-C131	-C132	84.4(2)
C111	-P1	-C121	-C126	-138.7(2)
C121	-P1	-C131	-C136	138.5(2)
Rh8	-P1	-C131	-C136	-95.1(2)
C131	-P1	-C111	-C112	-71.8(2)
Rh8	-P1	-C121	-C126	-20.1(3)
Rh8	-P1	-C121	-C122	164.8(2)
C121	-P1	-C111	-C116	5.6(3)
C131	-P1	-C121	-C122	-63.2(3)
C131	-P1	-C121	-C126	111.9(2)

C221	-P2	-C211	-C212	-45.0(3)
Rh8	-P2	-C211	-C212	173.1(2)
C231	-P2	-C211	-C212	64.6(3)
C211	-P2	-C231	-C236	13.3(3)
Rh8	-P2	-C211	-C216	-6.3(3)
C221	-P2	-C231	-C232	-68.5(2)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C221	-P2	-C211	-C216	135.7(2)
C211	-P2	-C231	-C232	-175.0(2)
Rh8	-P2	-C221	-C226	-106.5(3)
C221	-P2	-C231	-C236	119.8(2)
C211	-P2	-C221	-C222	-60.9(3)
C231	-P2	-C211	-C216	-114.8(2)
Rh8	-P2	-C221	-C222	72.9(3)
Rh8	-P2	-C231	-C232	67.0(2)
Rh8	-P2	-C231	-C236	-104.8(2)
C211	-P2	-C221	-C226	119.8(3)
C231	-P2	-C221	-C222	-169.2(2)
C231	-P2	-C221	-C226	11.4(3)
B11	-N7	-B2	-B3	138.8(3)
Rh8	-N7	-B2	-B6	-68.5(3)
B3	-N7	-B11	-B2	45.1(3)
B2	-N7	-B3	-B4	99.9(3)
B3	-N7	-B2	-B11	-138.8(3)
B11	-N7	-B3	-B4	55.1(3)
Rh8	-N7	-B3	-B2	-153.2(2)
B11	-N7	-B3	-B1	-7.1(4)
Rh8	-N7	-B11	-B6	85.6(3)

B2	-N7	-B11	-B6	-38.4(2)
B11	-N7	-B3	-B2	-44.8(3)
Rh8	-N7	-B3	-B4	-53.32(19)
B11	-N7	-B2	-B6	37.7(2)
B3	-N7	-B2	-B6	-101.1(3)
Rh8	-N7	-B2	-B11	-106.2(3)
B11	-N7	-B2	-B1	101.5(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Rh8	-N7	-B2	-B3	32.6(3)
B3	-N7	-B11	-B6	6.7(4)
B2	-N7	-B3	-B1	37.7(2)
B11	-N7	-B3	-Rh8	108.4(3)
Rh8	-N7	-B3	-B1	-115.5(2)
B2	-N7	-B3	-Rh8	153.2(2)
B2	-N7	-B11	-B10	-99.7(3)
B3	-N7	-B11	-B10	-54.6(4)
Rh8	-N7	-B11	-B10	24.3(3)
Rh8	-N7	-B11	-B2	124.0(2)
B3	-N7	-B2	-B1	-37.4(3)
Rh8	-N7	-B2	-B1	-4.8(4)
C212	-C211	-C216	-C215	-1.3(5)
C216	-C211	-C212	-C213	1.3(5)
P1	-C111	-C112	-H112	2.00
P2	-C211	-C216	-C215	178.1(3)
C116	-C111	-C112	-H112	178.00
C112	-C111	-C116	-H116	-179.00
P2	-C211	-C212	-C213	-178.1(3)
P1	-C111	-C116	-H116	-3.00

H112	-C112	-C113	-C114	-179.00
C111	-C112	-C113	-H113	-178.00
H112	-C112	-C113	-H113	2.00
C211	-C212	-C213	-C214	-0.8(5)
H113	-C113	-C114	-H114	0.00
C112	-C113	-C114	-H114	-180.00
H113	-C113	-C114	-C115	-180.00
C212	-C213	-C214	-C215	0.2(6)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

H114	-C114	-C115	-C116	179.00
C213	-C214	-C215	-C216	-0.2(6)
C113	-C114	-C115	-H115	179.00
H114	-C114	-C115	-H115	-1.00
H115	-C115	-C116	-C111	-179.00
H115	-C115	-C116	-H116	1.00
C114	-C115	-C116	-H116	-179.00
C214	-C215	-C216	-C211	0.7(5)
C226	-C221	-C222	-C223	2.0(5)
P2	-C221	-C222	-C223	-177.4(3)
P2	-C221	-C226	-C225	177.6(3)
C222	-C221	-C226	-C225	-1.7(5)
P1	-C121	-C122	-H122	-2.00
C126	-C121	-C122	-H122	-177.00
P1	-C121	-C126	-H126	3.00
C122	-C121	-C126	-H126	178.00
H122	-C122	-C123	-C124	178.00
C221	-C222	-C223	-C224	-0.7(5)
H122	-C122	-C123	-H123	-2.00

C121	-C122	-C123	-H123	178.00
H123	-C123	-C124	-H124	0.00
C222	-C223	-C224	-C225	-1.0(5)
H123	-C123	-C124	-C125	180.00
C122	-C123	-C124	-H124	180.00
C223	-C224	-C225	-C226	1.3(5)
C123	-C124	-C125	-H125	-178.00
H124	-C124	-C125	-H125	2.00
H124	-C124	-C125	-C126	-178.00

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C224	-C225	-C226	-C221	0.1(5)
H125	-C125	-C126	-C121	179.00
C124	-C125	-C126	-H126	179.00
H125	-C125	-C126	-H126	-1.00
C236	-C231	-C232	-C233	-0.3(5)
P2	-C231	-C232	-C233	-172.4(3)
C136	-C131	-C132	-H132	-179.00
P1	-C131	-C132	-H132	2.00
C232	-C231	-C236	-C235	-1.1(5)
P2	-C231	-C236	-C235	170.6(2)
C132	-C131	-C136	-H136	179.00
P1	-C131	-C136	-H136	-1.00
C231	-C232	-C233	-C234	1.8(5)
H132	-C132	-C133	-C134	179.00
C131	-C132	-C133	-H133	179.00
H132	-C132	-C133	-H133	-1.00
H133	-C133	-C134	-C135	-180.00
H133	-C133	-C134	-H134	0.00

C132	-C133	-C134	-H134	-180.00
C232	-C233	-C234	-C235	-1.8(5)
C133	-C134	-C135	-H135	-180.00
H134	-C134	-C135	-C136	-180.00
H134	-C134	-C135	-H135	0.00
C233	-C234	-C235	-C236	0.4(5)
H135	-C135	-C136	-H136	0.00
C234	-C235	-C236	-C231	1.1(5)
H135	-C135	-C136	-C131	-180.00
C134	-C135	-C136	-H136	-180.00

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B6	-B1	-B3	-N7	4.0(3)
B6	-B1	-B3	-B2	41.3(2)
B5	-B1	-B3	-B4	-38.8(2)
B6	-B1	-B3	-Rh8	-70.1(3)
B5	-B1	-B3	-B2	104.2(3)
B4	-B1	-B5	-B6	-136.3(2)
B2	-B1	-B4	-Rh8	5.5(4)
B3	-B1	-B5	-B9	6.1(3)
B5	-B1	-B3	-N7	66.9(3)
B4	-B1	-B3	-Rh8	31.6(2)
B3	-B1	-B5	-B6	-96.3(3)
B2	-B1	-B4	-B3	36.0(3)
B2	-B1	-B4	-B5	-100.7(3)
B4	-B1	-B5	-B9	-33.8(2)
B6	-B1	-B3	-B4	-101.7(3)
B6	-B1	-B5	-B10	36.0(2)
B4	-B1	-B3	-N7	105.7(3)

B3	-B1	-B5	-B4	40.0(2)
B2	-B1	-B3	-Rh8	-111.4(3)
B4	-B1	-B6	-B5	38.6(2)
B4	-B1	-B6	-B10	2.4(3)
B4	-B1	-B6	-B11	-65.8(3)
B5	-B1	-B3	-Rh8	-7.2(3)
B6	-B1	-B5	-B4	136.3(2)
B6	-B1	-B5	-B9	102.5(3)
B5	-B1	-B4	-B3	136.7(3)
B6	-B1	-B4	-B3	98.0(3)
B6	-B1	-B4	-B5	-38.7(2)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B2	-B1	-B6	-B5	147.4(3)
B4	-B1	-B5	-B10	-100.3(3)
B4	-B1	-B3	-B2	143.0(3)
B2	-B1	-B5	-B10	6.7(3)
B2	-B1	-B4	-B9	-66.7(4)
B3	-B1	-B2	-N7	35.1(2)
B3	-B1	-B6	-B10	67.5(3)
B3	-B1	-B6	-B11	-0.7(3)
B3	-B1	-B4	-Rh8	-30.5(2)
B3	-B1	-B5	-B10	-60.3(3)
B3	-B1	-B4	-B9	-102.7(3)
B5	-B1	-B4	-Rh8	106.2(3)
B3	-B1	-B2	-B11	89.6(3)
B5	-B1	-B4	-B9	34.0(2)
B6	-B1	-B4	-Rh8	67.5(3)
B6	-B1	-B4	-B9	-4.7(3)

B2	-B1	-B6	-B10	111.1(3)
B2	-B1	-B6	-B11	43.0(2)
B3	-B1	-B6	-B2	-43.7(2)
B2	-B1	-B3	-N7	-37.3(2)
B2	-B1	-B3	-B4	-143.0(3)
B6	-B1	-B2	-B11	-41.6(2)
B6	-B1	-B2	-N7	-96.1(3)
B5	-B1	-B6	-B10	-36.2(2)
B3	-B1	-B4	-B5	-136.7(3)
B2	-B1	-B5	-B4	107.0(3)
B3	-B1	-B2	-B6	131.2(3)
B2	-B1	-B5	-B9	73.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B4	-B1	-B2	-N7	-0.8(4)
B4	-B1	-B2	-B3	-35.9(3)
B5	-B1	-B2	-B6	30.0(2)
B5	-B1	-B6	-B11	-104.4(3)
B4	-B1	-B6	-B2	-108.8(3)
B2	-B1	-B5	-B6	-29.3(2)
B5	-B1	-B2	-N7	-66.1(3)
B3	-B1	-B6	-B5	103.7(3)
B5	-B1	-B2	-B11	-11.6(3)
B4	-B1	-B2	-B11	53.7(3)
B5	-B1	-B6	-B2	-147.4(3)
B4	-B1	-B2	-B6	95.3(3)
B6	-B1	-B2	-B3	-131.2(3)
B5	-B1	-B2	-B3	-101.2(3)
B6	-B2	-B3	-B4	-10.5(3)

B1	-B2	-B3	-N7	135.9(3)
B1	-B2	-B3	-Rh8	106.2(3)
N7	-B2	-B6	-B1	97.3(2)
B6	-B2	-B3	-Rh8	62.5(3)
B1	-B2	-B3	-B4	33.3(2)
B6	-B2	-B3	-N7	92.2(3)
B6	-B2	-B3	-B1	-43.7(2)
B3	-B2	-B11	-B10	71.6(3)
B6	-B2	-B11	-N7	-135.6(3)
N7	-B2	-B3	-Rh8	-29.7(2)
B1	-B2	-B11	-N7	-92.3(3)
B1	-B2	-B6	-B11	-132.0(2)
N7	-B2	-B6	-B5	67.4(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B11	-B2	-B3	-N7	32.1(2)
B1	-B2	-B11	-B6	43.3(2)
N7	-B2	-B3	-B4	-102.6(3)
B3	-B2	-B11	-N7	-32.6(2)
B3	-B2	-B11	-B6	103.0(2)
N7	-B2	-B11	-B10	104.2(3)
B11	-B2	-B3	-Rh8	2.4(3)
B3	-B2	-B6	-B10	-54.1(3)
B11	-B2	-B3	-B1	-103.8(3)
B1	-B2	-B11	-B10	11.9(3)
N7	-B2	-B3	-B1	-135.9(3)
B11	-B2	-B3	-B4	-70.6(3)
B1	-B2	-B6	-B10	-95.9(3)
N7	-B2	-B6	-B10	1.4(3)

N7	-B2	-B6	-B11	-34.7(2)
B6	-B2	-B11	-B10	-31.3(2)
N7	-B2	-B11	-B6	135.6(3)
B11	-B2	-B6	-B1	132.0(2)
B1	-B2	-B6	-B5	-29.9(2)
B11	-B2	-B6	-B10	36.1(3)
B3	-B2	-B6	-B1	41.8(2)
B11	-B2	-B6	-B5	102.1(3)
B3	-B2	-B6	-B5	11.9(3)
B3	-B2	-B6	-B11	-90.2(2)
N7	-B3	-B4	-B1	-94.4(3)
B1	-B3	-B4	-B9	101.3(3)
Rh8	-B3	-B4	-B5	-111.6(2)
B2	-B3	-B4	-B9	68.4(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

N7	-B3	-B4	-Rh8	55.32(19)
Rh8	-B3	-B4	-B9	-48.5(2)
B1	-B3	-B4	-Rh8	149.8(2)
B1	-B3	-B4	-B5	38.1(2)
N7	-B3	-B4	-B5	-56.3(3)
N7	-B3	-B4	-B9	6.9(3)
Rh8	-B3	-B4	-B1	-149.8(2)
B2	-B3	-B4	-B1	-32.9(2)
B2	-B3	-B4	-B5	5.2(3)
B2	-B3	-B4	-Rh8	116.8(2)
B1	-B4	-B5	-B9	142.6(3)
B5	-B4	-B9	-B10	39.2(2)
Rh8	-B4	-B5	-B9	36.0(2)

B3	-B4	-B5	-B9	105.4(3)
B3	-B4	-B5	-B6	1.9(3)
Rh8	-B4	-B9	-B5	-144.6(2)
Rh8	-B4	-B5	-B10	-5.0(3)
Rh8	-B4	-B5	-B1	-106.6(2)
B5	-B4	-B9	-Rh8	144.6(2)
B9	-B4	-B5	-B6	-103.4(3)
Rh8	-B4	-B9	-B10	-105.4(2)
Rh8	-B4	-B5	-B6	-67.4(3)
B1	-B4	-B9	-Rh8	110.4(2)
B1	-B4	-B9	-B5	-34.1(2)
B3	-B4	-B5	-B10	64.3(3)
B9	-B4	-B5	-B1	-142.6(3)
B3	-B4	-B9	-Rh8	48.0(2)
B1	-B4	-B5	-B10	101.5(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B3	-B4	-B5	-B1	-37.2(2)
B3	-B4	-B9	-B10	-57.4(3)
B1	-B4	-B9	-B10	5.1(3)
B1	-B4	-B5	-B6	39.2(2)
B3	-B4	-B9	-B5	-96.6(3)
B9	-B4	-B5	-B10	-41.1(2)
B4	-B5	-B6	-B2	-9.0(3)
B9	-B5	-B6	-B2	-72.2(3)
B9	-B5	-B6	-B10	37.4(3)
B9	-B5	-B6	-B1	-102.1(3)
B4	-B5	-B6	-B1	-38.9(2)
B4	-B5	-B9	-Rh8	-37.3(2)

B1	-B5	-B9	-B4	34.1(2)
B1	-B5	-B10	-B9	103.3(3)
B9	-B5	-B6	-B11	-5.4(4)
B4	-B5	-B6	-B11	57.8(3)
B4	-B5	-B6	-B10	100.5(3)
B1	-B5	-B6	-B11	96.7(3)
B10	-B5	-B6	-B2	-109.5(3)
B10	-B5	-B6	-B11	-42.8(3)
B1	-B5	-B9	-Rh8	-3.2(3)
B4	-B5	-B9	-B10	-135.1(3)
B6	-B5	-B9	-Rh8	61.8(3)
B6	-B5	-B9	-B4	99.1(3)
B1	-B5	-B6	-B10	139.4(3)
B1	-B5	-B9	-B10	-101.0(3)
B1	-B5	-B6	-B2	29.9(2)
B10	-B5	-B9	-B4	135.1(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B1	-B5	-B10	-B6	-36.7(2)
B4	-B5	-B10	-B11	-62.7(3)
B6	-B5	-B10	-B9	140.0(3)
B6	-B5	-B10	-B11	37.6(2)
B10	-B5	-B6	-B1	-139.4(3)
B10	-B5	-B9	-Rh8	97.8(3)
B9	-B5	-B10	-B11	-102.4(3)
B1	-B5	-B10	-B11	0.9(3)
B4	-B5	-B10	-B6	-100.3(3)
B9	-B5	-B10	-B6	-140.0(3)
B6	-B5	-B9	-B10	-36.0(3)

B4	-B5	-B10	-B9	39.7(2)
B5	-B6	-B11	-B10	40.4(3)
B1	-B6	-B11	-B10	102.9(3)
B11	-B6	-B10	-B9	99.9(3)
B2	-B6	-B10	-B9	64.9(3)
B1	-B6	-B11	-N7	-3.0(3)
B5	-B6	-B11	-N7	-65.5(3)
B2	-B6	-B10	-B5	100.3(3)
B1	-B6	-B10	-B11	-99.2(3)
B10	-B6	-B11	-N7	-105.9(3)
B2	-B6	-B11	-B10	144.6(3)
B1	-B6	-B10	-B5	36.0(2)
B2	-B6	-B10	-B11	-35.0(3)
B5	-B6	-B10	-B9	-35.3(2)
B1	-B6	-B11	-B2	-41.7(2)
B10	-B6	-B11	-B2	-144.6(3)
B5	-B6	-B11	-B2	-104.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B1	-B6	-B10	-B9	0.7(3)
B11	-B6	-B10	-B5	135.3(3)
B2	-B6	-B11	-N7	38.6(2)
B5	-B6	-B10	-B11	-135.3(3)
B4	-B9	-B10	-B5	-39.9(2)
Rh8	-B9	-B10	-B6	-74.8(3)
Rh8	-B9	-B10	-B11	-14.6(3)
B4	-B9	-B10	-B11	56.7(3)
Rh8	-B9	-B10	-B5	-111.2(3)
B4	-B9	-B10	-B6	-3.5(3)

B5	-B9	-B10	-B11	96.6(3)
B5	-B9	-B10	-B6	36.4(2)
B9	-B10	-B11	-B2	-69.2(3)
B9	-B10	-B11	-B6	-100.8(3)
B5	-B10	-B11	-B2	-8.0(3)
B6	-B10	-B11	-B2	31.6(2)
B6	-B10	-B11	-N7	95.1(3)
B5	-B10	-B11	-N7	55.6(3)
B9	-B10	-B11	-N7	-5.6(3)
B5	-B10	-B11	-B6	-39.6(2)

Table S8 - Contact Distances(Angstrom)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

Rh8	.H112	3.2400	N7	.H3	2.30(4)
Rh8	.H126	2.9500	N7	.H910	2.48(4)
Rh8	.H216	3.0500	C1S	.Cl2S	2.730(14)
Rh8	.H232	3.5300	C1S	.Cl1S	2.083(13)
Cl1S	.C1S	2.083(13)	C112	.C136	3.232(4)
Cl1S	.C1S_a	2.079(12)	C114	.C124_b	3.562(6)
Cl1S	.Cl1S_a	2.944(11)	C115	.C123_c	3.548(5)
Cl2S	.Cl3S	2.419(15)	C115	.C226	3.574(5)
Cl2S	.Cl2S_a	2.944(16)	C116	.C221	3.399(4)
Cl2S	.C1S	2.730(14)	C116	.C122	3.328(6)
Cl3S	.Cl2S	2.419(15)	C116	.C226	3.379(5)
Cl3S	.C1S_a	2.759(14)	C121	.C222	3.374(5)
Cl3S	.Cl3S_a	2.954(15)	C122	.C116	3.328(6)
P1	.B9	3.181(4)	C122	.C132	3.507(5)
P1	.P2	3.5017(12)	C123	.C115_c	3.548(5)
P1	.B4	3.246(4)	C124	.C114_e	3.562(6)
P2	.P1	3.5017(12)	C126	.C222	3.339(5)

P2	.N7	3.255(2)	C132	.C122	3.507(5)
P1	.H9	3.13(4)	C133	.C133_f	3.555(5)
P2	.H7	2.98(3)	C136	.C112	3.232(4)
N7	.C231	3.227(4)	C111	.H136	2.7500
N7	.C236	3.363(4)	C112	.H232	2.8000
N7	.P2	3.255(2)	C212	.C222	3.543(5)
N7	.B5	3.260(5)	C112	.H136	2.5000
N7	.B9	3.033(5)	C212	.C236	3.341(5)
N7	.B10	2.836(5)	C113	.H232	2.9300
N7	.B1	2.646(4)	C116	.H122	2.9200
N7	.B4	2.824(4)	C121	.H132	2.6800

Table S8 - Contact Distances(Angstrom) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

C221	.C116	3.399(4)	C221	.H212	2.8400
C121	.H116	2.9000	C223	.H213_g	2.9800
C121	.H222	3.0000	C224	.H213_g	3.0900
C222	.C126	3.339(5)	C226	.H232	3.0200
C222	.C212	3.543(5)	C231	.H226	2.7200
C122	.H116	2.6800	C231	.H7	2.63(4)
C222	.C121	3.374(5)	C232	.H3	2.92(4)
C123	.H1_d	2.97(3)	C232	.H226	2.6100
C124	.H114_e	3.0200	C235	.H11_h	3.10(4)
C124	.H1_d	2.97(4)	C236	.H7	2.54(4)
C125	.H222	2.8900	B3	.B5	2.890(6)
C226	.C232	3.301(5)	B3	.B11	2.725(5)
C226	.C115	3.574(5)	B3	.B9	2.966(6)
C126	.H222	2.6200	B3	.B10	3.374(6)
C126	.H132	3.0000	B4	.B10	2.876(5)
C226	.C116	3.379(5)	B4	.P1	3.246(4)

C131	.H4	3.01(4)	B4	.B2	2.984(5)
C131	.H9	3.10(4)	B4	.N7	2.824(4)
C132	.H9	2.75(4)	B4	.B11	3.349(5)
C232	.C226	3.301(5)	B4	.C131	3.457(4)
C134	.H224_c	3.0700	B9	.B11	3.009(5)
C136	.H112	2.9800	B9	.B1	2.909(5)
C136	.H4	3.07(4)	B9	.B3	2.966(6)
C236	.C212	3.341(5)	B9	.C131	3.473(4)
C236	.N7	3.363(4)	B9	.P1	3.181(4)
C211	.H236	2.6200	B9	.N7	3.033(5)
C211	.H222	3.0100	B3	.H7	2.12(4)
C212	.H236	2.7400	B3	.H135_i	2.8800

Table S8 - Contact Distances(Angstrom) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

B3	.H4	2.53(4)	H113	.H133_b	2.4900
B4	.H9	2.69(4)	H113	.H132_b	2.5800
B4	.H3	2.58(4)	H114	.C124_b	3.0200
B4	.H910	2.77(4)	H116	.H122	2.3600
B9	.H4	2.57(4)	H116	.C121	2.9000
B11	.H216	3.0300	H116	.C122	2.6800
H1	.H223_j	2.4400	H122	.C116	2.9200
H1	.C123_j	2.97(3)	H122	.H116	2.3600
H1	.C124_j	2.97(4)	H122	.H122_c	2.5600
H3	.H135_i	2.3700	H126	.Rh8	2.9500
H3	.C232	2.92(4)	H132	.H113_e	2.5800
H4	.C136	3.07(4)	H132	.C121	2.6800
H4	.C131	3.01(4)	H132	.C126	3.0000
H5	.H133_f	2.5900	H132	.H9	2.3800
H6	.H225_k	2.3500	H133	.H5_f	2.5900

H7	.C236	2.54(4)	H133	.H113_e	2.4900
H7	.C231	2.63(4)	H135	.B3_i	2.8800
H9	.C131	3.10(4)	H135	.H3_i	2.3700
H9	.H132	2.3800	H136	.H112	2.3000
H9	.C132	2.75(4)	H136	.C111	2.7500
H10	.H234_e	2.5500	H136	.C112	2.5000
H10	.H214_l	2.4100	H212	.C221	2.8400
H11	.H215_l	2.5900	H213	.C223_g	2.9800
H11	.H235_h	2.4200	H213	.C224_g	3.0900
H11	.C235_h	3.10(4)	H214	.H10_l	2.4100
H112	.H136	2.3000	H215	.H11_l	2.5900
H112	.C136	2.9800	H216	.H910	2.5100
H112	.Rh8	3.2400	H216	.B11	3.0300

Table S8 - Contact Distances(Angstrom) (continued)
for [8,8-(PPh3)2-nido-8,7-RhNB9H11] (1)

H216	.Rh8	3.0500	H232	.Rh8	3.5300
H222	.C125	2.8900	H232	.C112	2.8000
H222	.C126	2.6200	H232	.H226	2.4300
H222	.C211	3.0100	H232	.C113	2.9300
H222	.C121	3.0000	H232	.C226	3.0200
H223	.H1_d	2.4400	H234	.H10_b	2.5500
H224	.C134_c	3.0700	H235	.H11_h	2.4200
H225	.H6_m	2.3500	H236	.C212	2.7400
H226	.C232	2.6100	H236	.C211	2.6200
H226	.C231	2.7200	H910	.H216	2.5100
H226	.H232	2.4300			

Translation of Symmetry Code to Equiv.Pos

a =[2656.00] = 1-x,-y,1-z
b =[1455.00] = -1+x,y,z
c =[2555.00] = -x,-y,-z
d =[1545.00] = x,-1+y,z
e =[1655.00] = 1+x,y,z
f =[2665.00] = 1-x,1-y,-z
g =[2556.00] = -x,-y,1-z
h =[2566.00] = -x,1-y,1-z
i =[2565.00] = -x,1-y,-z
j =[1565.00] = x,1+y,z
k =[1665.00] = 1+x,1+y,z
l =[2666.00] = 1-x,1-y,1-z
m =[1445.00] = -1+x,-1+y,z

Table S1 - Crystal Data and Details of the Structure Determination for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Crystal Data			
Formula			C18 H35 B9 O P2 Pt
Formula Weight			621.78
Crystal System			Monoclinic
Space group		P21/a	(No. 14)
a, b, c [Angstrom]	18.217(2)	13.785(2)	20.778(4)
alpha, beta, gamma [deg]	90	99.890(10)	90
V [Ang**3]			5140.3(14)
Z			8
D(calc) [g/cm**3]			1.607
Mu(MoKa) [/mm]			5.594
F(000)			2432
Crystal Size [mm]		0.15 x 0.40 x 0.60	
Data Collection			
Temperature (K)			200
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.0, 25.0
Dataset		-21: 21 ; 0: 16 ; 0: 24	
Tot., Uniq. Data, R(int)		9459, 9034, 0.000	
Observed data [I > 2.0 sigma(I)]			7155
Refinement			
Nref, Npar			9034, 605

R, wR2, S	0.0202, 0.0505, 0.97
w = 1/[\s^2^(Fo^2^)+(0.0319P)^2^]	where P=(Fo^2^+2Fc^2^)/3
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-1.22, 0.98

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(eq) [Ang^2]
Pt7A	0.25447(1)	0.27923(1)	0.07816(1)	0.0210(1)
P1	0.23977(5)	0.29007(6)	0.18431(4)	0.0234(3)
P2	0.38354(5)	0.30831(7)	0.09729(5)	0.0254(3)
O11A	0.13191(14)	0.42965(17)	0.09651(13)	0.0361(9)
C8A	0.2640(2)	0.2473(3)	-0.0218(2)	0.0354(14)
C11	0.1493(2)	0.2575(3)	0.20322(19)	0.0322(12)
C11A	0.1247(3)	0.5322(3)	0.0854(3)	0.076(2)
C12	0.2569(2)	0.4049(3)	0.22606(18)	0.0311(12)
C21	0.43945(19)	0.1991(3)	0.1121(2)	0.0388(14)
C22	0.4176(2)	0.3645(3)	0.02858(19)	0.0424(14)
C131	0.30125(19)	0.2019(3)	0.23141(18)	0.0288(11)
C132	0.3434(2)	0.2223(3)	0.29184(19)	0.0389(14)
C133	0.3896(2)	0.1518(4)	0.3255(2)	0.0528(18)
C134	0.3928(2)	0.0612(4)	0.2991(3)	0.0549(18)
C135	0.3505(3)	0.0388(3)	0.2392(3)	0.0530(19)
C136	0.3050(2)	0.1097(3)	0.2053(2)	0.0395(14)
C231	0.41878(17)	0.3911(2)	0.16407(17)	0.0226(10)
C232	0.40380(19)	0.4899(2)	0.15434(18)	0.0287(11)
C233	0.4231(2)	0.5555(3)	0.20482(19)	0.0325(11)
C234	0.4558(2)	0.5229(3)	0.26594(19)	0.0333(12)
C235	0.4720(2)	0.4254(3)	0.27577(19)	0.0334(12)
C236	0.45456(18)	0.3596(2)	0.22490(17)	0.0275(11)
B1A	0.1152(2)	0.2086(4)	-0.0449(2)	0.0413(16)
B2A	0.1348(2)	0.2405(3)	0.0392(2)	0.0308(12)
B3A	0.2022(2)	0.1715(3)	-0.0014(2)	0.0347(16)
B4A	0.1947(3)	0.2160(4)	-0.0815(2)	0.0499(19)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(eq) [Ang^2]
B5A	0.1358(3)	0.3159(4)	-0.0892(2)	0.0490(19)
B6A	0.0883(2)	0.3237(4)	-0.0199(2)	0.0413(16)
B9A	0.2318(3)	0.3368(4)	-0.0657(2)	0.0433(19)
B10A	0.1548(3)	0.4130(4)	-0.0340(3)	0.0409(17)
B11A	0.1477(2)	0.3707(3)	0.0473(2)	0.0301(12)
Pt7B	0.23840(1)	0.25565(1)	0.56597(1)	0.0194(1)
P3	0.22288(5)	0.24795(6)	0.67220(4)	0.0223(3)
P4	0.36635(5)	0.22076(6)	0.58481(5)	0.0230(3)
O8B	0.11276(13)	0.11061(16)	0.58168(12)	0.0278(8)
C8B	0.1061(3)	0.0083(3)	0.5713(2)	0.0546(18)
C11B	0.2492(2)	0.2856(3)	0.46559(18)	0.0294(11)
C31	0.13190(19)	0.2801(3)	0.69035(18)	0.0302(12)
C32	0.2403(2)	0.1342(2)	0.71492(18)	0.0303(11)
C41	0.3932(2)	0.1450(3)	0.52122(19)	0.0342(12)
C42	0.42195(19)	0.3297(3)	0.58290(19)	0.0334(11)
C331	0.28363(18)	0.3378(2)	0.71874(17)	0.0252(11)
C332	0.2952(2)	0.4255(2)	0.68845(19)	0.0304(11)
C333	0.3417(2)	0.4951(3)	0.7219(2)	0.0364(14)
C334	0.3764(2)	0.4783(3)	0.7854(2)	0.0382(14)
C335	0.3641(2)	0.3926(3)	0.81515(19)	0.0414(14)
C336	0.3173(2)	0.3229(3)	0.78258(18)	0.0340(12)
C431	0.40757(18)	0.1594(2)	0.65930(18)	0.0272(11)
C432	0.4401(2)	0.2103(3)	0.71463(19)	0.0367(11)
C433	0.4679(2)	0.1616(4)	0.7718(2)	0.0526(16)
C434	0.4642(3)	0.0620(4)	0.7736(3)	0.0631(19)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(eq) [Ang^2]
C435	0.4318(3)	0.0107(3)	0.7196(3)	0.0548(19)
C436	0.4037(2)	0.0590(3)	0.6622(2)	0.0390(14)
B1B	0.1027(2)	0.3364(3)	0.4434(2)	0.0302(12)
B2B	0.1206(2)	0.3007(3)	0.5269(2)	0.0255(12)
B3B	0.0710(2)	0.2224(3)	0.4664(2)	0.0297(12)
B4B	0.1173(3)	0.2300(3)	0.3969(2)	0.0339(14)
B5B	0.1814(2)	0.3252(3)	0.4064(2)	0.0307(12)
B6B	0.1916(2)	0.3657(3)	0.4880(2)	0.0268(12)
B8B	0.1298(2)	0.1703(3)	0.5325(2)	0.0250(11)
B9B	0.1342(2)	0.1296(3)	0.4497(2)	0.0304(12)
B10B	0.2128(3)	0.2016(3)	0.4180(2)	0.0328(12)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(iso) [Ang^2]
H1A	0.07080	0.15400	-0.06260	0.0500
H2A	0.10730	0.20310	0.07650	0.0370
H3A	0.21530	0.09340	0.01020	0.0420
H4A	0.20000	0.16990	-0.12490	0.0600
H5A	0.10790	0.33630	-0.13960	0.0590
H6A	0.02750	0.34090	-0.02490	0.0490
H8A	0.315(2)	0.222(3)	-0.026(2)	0.042(11)
H9A	0.2690(19)	0.377(2)	-0.0952(18)	0.031(10)
H10A	0.143(2)	0.484(3)	-0.054(2)	0.057(13)
H11D	0.07880	0.54550	0.05460	0.1140
H11E	0.12290	0.56530	0.12680	0.1140
H11F	0.16760	0.55590	0.06720	0.1140
H11G	0.13440	0.19400	0.18420	0.0480
H11H	0.15230	0.25470	0.25070	0.0480
H11I	0.11250	0.30630	0.18490	0.0480
H12D	0.30940	0.42280	0.22870	0.0470
H12E	0.24530	0.39930	0.27020	0.0470
H12F	0.22530	0.45500	0.20190	0.0470
H20A	0.49230	0.21570	0.11520	0.0580
H20B	0.42490	0.15340	0.07600	0.0580
H20C	0.43140	0.16920	0.15310	0.0580
H24A	0.47070	0.37950	0.04120	0.0640
H24B	0.38990	0.42440	0.01620	0.0640
H24C	0.41060	0.31970	-0.00860	0.0640
H101	0.203(2)	0.417(3)	0.0092(19)	0.040(11)
H132	0.34070	0.28480	0.31050	0.0470

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(iso) [Ang^2]
H133	0.41890	0.16660	0.36670	0.0630
H134	0.42440	0.01330	0.32220	0.0660
H135	0.35250	-0.02440	0.22130	0.0640
H136	0.27620	0.09480	0.16390	0.0480
H232	0.38010	0.51230	0.11270	0.0340
H233	0.41400	0.62270	0.19750	0.0390
H234	0.46700	0.56740	0.30120	0.0400
H235	0.49530	0.40340	0.31760	0.0400
H236	0.46710	0.29300	0.23170	0.0330
H1B	0.06100	0.39480	0.42680	0.0360
H2B	0.090(2)	0.337(3)	0.5614(19)	0.043(11)
H3B	0.00970	0.20880	0.46170	0.0360
H4B	0.08730	0.21370	0.34640	0.0410
H5B	0.18880	0.37280	0.36430	0.0370
H6B	0.20880	0.44210	0.50130	0.0320
H9B	0.1153(18)	0.060(2)	0.4275(17)	0.028(9)
H10B	0.2438(19)	0.160(3)	0.3885(18)	0.035(10)
H11B	0.2990(18)	0.308(2)	0.4631(16)	0.018(8)
H17A	0.41220	0.37450	0.61710	0.0500
H17B	0.40870	0.36110	0.54020	0.0500
H17C	0.47490	0.31250	0.59040	0.0500
H30A	0.06120	-0.00550	0.53930	0.0820
H30B	0.10250	-0.02400	0.61260	0.0820
H30C	0.15000	-0.01570	0.55490	0.0820
H31A	0.09510	0.23190	0.67100	0.0450

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	x	y	z	U(iso) [Ang^2]
H31B	0.11750	0.34420	0.67210	0.0450
H31C	0.13410	0.28150	0.73780	0.0450
H32A	0.29310	0.11740	0.71880	0.0450
H32B	0.20990	0.08320	0.69060	0.0450
H32C	0.22730	0.14010	0.75860	0.0450
H41A	0.44730	0.13520	0.52990	0.0510
H41B	0.37870	0.17680	0.47880	0.0510
H41C	0.36800	0.08210	0.52070	0.0510
H89	0.181(2)	0.122(2)	0.4906(19)	0.038(11)
H332	0.27120	0.43740	0.64490	0.0370
H333	0.34960	0.55460	0.70110	0.0440
H334	0.40870	0.52580	0.80820	0.0460
H335	0.38810	0.38100	0.85880	0.0500
H336	0.30840	0.26450	0.80430	0.0410
H432	0.44330	0.27910	0.71320	0.0440
H433	0.48950	0.19680	0.80970	0.0630
H434	0.48420	0.02840	0.81260	0.0760
H435	0.42870	-0.05800	0.72160	0.0660
H436	0.38160	0.02330	0.62470	0.0470

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Pt7A	0.0177(1)	0.0274(1)	0.0176(1)	-0.0049(1)	0.0024(1)	0.0006(1)
P1	0.0250(5)	0.0276(5)	0.0184(5)	-0.0013(4)	0.0058(4)	-0.0009(3)
P2	0.0194(4)	0.0350(5)	0.0218(5)	-0.0054(4)	0.0037(4)	-0.0012(3)
O11A	0.0423(16)	0.0330(14)	0.0348(17)	0.0000(11)	0.0120(13)	0.0080(11)
C8A	0.026(2)	0.057(3)	0.024(2)	-0.0193(18)	0.0069(17)	-0.0040(17)
C11	0.031(2)	0.041(2)	0.026(2)	0.0042(16)	0.0087(17)	-0.0015(16)
C11A	0.120(5)	0.037(3)	0.081(4)	0.005(3)	0.043(4)	0.027(3)
C12	0.030(2)	0.039(2)	0.025(2)	-0.0082(16)	0.0067(17)	-0.0008(15)
C21	0.0222(19)	0.040(2)	0.053(3)	-0.0117(19)	0.0031(19)	0.0017(15)
C22	0.037(2)	0.067(3)	0.026(2)	-0.0051(19)	0.0131(19)	-0.0137(19)
C131	0.0271(19)	0.037(2)	0.024(2)	0.0099(15)	0.0094(16)	-0.0013(15)
C132	0.039(2)	0.054(3)	0.024(2)	0.0079(18)	0.0059(19)	-0.0010(18)
C133	0.036(2)	0.086(4)	0.035(3)	0.027(2)	0.002(2)	-0.002(2)
C134	0.036(2)	0.068(3)	0.064(4)	0.039(3)	0.018(3)	0.015(2)
C135	0.050(3)	0.043(3)	0.070(4)	0.014(2)	0.022(3)	0.016(2)
C136	0.037(2)	0.040(2)	0.042(3)	0.0056(19)	0.008(2)	0.0024(17)
C231	0.0168(16)	0.0318(18)	0.0199(19)	-0.0007(14)	0.0049(15)	-0.0023(13)
C232	0.0271(19)	0.0316(19)	0.026(2)	0.0042(15)	0.0008(16)	0.0020(14)
C233	0.031(2)	0.0290(19)	0.037(2)	-0.0030(16)	0.0044(18)	-0.0021(15)
C234	0.029(2)	0.038(2)	0.032(2)	-0.0123(17)	0.0027(18)	-0.0023(15)
C235	0.026(2)	0.052(2)	0.020(2)	-0.0003(17)	-0.0023(17)	0.0037(16)
C236	0.0251(18)	0.0308(19)	0.026(2)	0.0020(15)	0.0027(16)	0.0040(14)
B1A	0.027(2)	0.064(3)	0.031(3)	-0.014(2)	0.000(2)	-0.005(2)
B2A	0.024(2)	0.040(2)	0.028(2)	-0.0073(18)	0.0034(19)	-0.0027(17)
B3A	0.028(2)	0.042(3)	0.033(3)	-0.017(2)	0.002(2)	0.0002(18)
B4A	0.034(3)	0.088(4)	0.027(3)	-0.026(3)	0.003(2)	-0.011(2)

Table S4 - (An)isotropic Displacement Parameters (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
B5A	0.034(3)	0.091(4)	0.020(3)	-0.001(3)	-0.001(2)	-0.005(3)
B6A	0.025(2)	0.062(3)	0.034(3)	0.005(2)	-0.003(2)	0.006(2)
B9A	0.035(3)	0.075(4)	0.021(3)	-0.006(2)	0.008(2)	-0.013(2)
B10A	0.039(3)	0.050(3)	0.032(3)	0.008(2)	0.001(2)	0.002(2)
B11A	0.024(2)	0.037(2)	0.029(2)	0.0022(18)	0.0036(19)	0.0045(16)
Pt7B	0.0190(1)	0.0237(1)	0.0161(1)	-0.0002(1)	0.0047(1)	-0.0021(1)
P3	0.0243(5)	0.0271(5)	0.0168(5)	-0.0004(3)	0.0072(4)	-0.0022(3)
P4	0.0200(4)	0.0275(5)	0.0225(5)	-0.0020(4)	0.0062(4)	-0.0019(3)
O8B	0.0355(14)	0.0249(12)	0.0253(14)	-0.0022(10)	0.0118(12)	-0.0065(10)
C8B	0.095(4)	0.031(2)	0.046(3)	-0.0002(19)	0.035(3)	-0.013(2)
C11B	0.033(2)	0.036(2)	0.0193(19)	0.0090(15)	0.0048(17)	-0.0050(16)
C31	0.029(2)	0.038(2)	0.026(2)	-0.0037(16)	0.0117(17)	0.0016(15)
C32	0.036(2)	0.0283(19)	0.029(2)	0.0049(15)	0.0127(17)	-0.0004(15)
C41	0.034(2)	0.042(2)	0.029(2)	-0.0058(17)	0.0121(18)	0.0025(16)
C42	0.0280(19)	0.038(2)	0.035(2)	-0.0012(17)	0.0081(18)	-0.0096(15)
C331	0.0216(17)	0.0343(19)	0.0204(19)	-0.0036(15)	0.0053(15)	-0.0024(14)
C332	0.032(2)	0.0302(19)	0.030(2)	-0.0029(16)	0.0086(18)	-0.0005(15)
C333	0.036(2)	0.032(2)	0.042(3)	-0.0035(17)	0.009(2)	-0.0065(16)
C334	0.034(2)	0.042(2)	0.040(3)	-0.0169(18)	0.010(2)	-0.0127(17)
C335	0.044(2)	0.061(3)	0.019(2)	-0.0082(19)	0.0053(19)	-0.008(2)
C336	0.039(2)	0.042(2)	0.023(2)	-0.0024(16)	0.0108(18)	-0.0088(17)
C431	0.0194(17)	0.036(2)	0.027(2)	0.0032(15)	0.0061(16)	0.0057(14)
C432	0.0220(19)	0.056(2)	0.032(2)	-0.0006(18)	0.0044(17)	-0.0012(16)
C433	0.032(2)	0.095(4)	0.027(2)	0.004(2)	-0.006(2)	0.005(2)
C434	0.045(3)	0.098(4)	0.045(3)	0.033(3)	0.004(3)	0.030(3)

Table S4 - (An)isotropic Displacement Parameters (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C435	0.049(3)	0.056(3)	0.063(4)	0.027(3)	0.020(3)	0.023(2)
C436	0.036(2)	0.040(2)	0.044(3)	0.0056(18)	0.015(2)	0.0110(17)
B1B	0.030(2)	0.035(2)	0.024(2)	0.0067(17)	0.0003(19)	0.0006(17)
B2B	0.021(2)	0.029(2)	0.027(2)	0.0019(17)	0.0052(18)	-0.0006(15)
B3B	0.028(2)	0.038(2)	0.023(2)	0.0010(18)	0.0042(19)	-0.0054(17)
B4B	0.036(2)	0.048(3)	0.017(2)	0.0009(19)	0.003(2)	-0.0091(19)
B5B	0.029(2)	0.044(2)	0.018(2)	0.0065(18)	0.0009(18)	-0.0070(18)
B6B	0.030(2)	0.031(2)	0.020(2)	0.0019(16)	0.0057(18)	-0.0019(16)
B8B	0.0214(19)	0.030(2)	0.024(2)	-0.0034(16)	0.0050(17)	-0.0038(15)
B9B	0.029(2)	0.037(2)	0.025(2)	-0.0052(18)	0.004(2)	-0.0067(17)
B10B	0.040(2)	0.039(2)	0.022(2)	-0.0007(18)	0.013(2)	-0.0033(19)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Pt7A	-P1	2.2720(9)	C8A	-B3A	1.644(6)
Pt7A	-P2	2.3507(10)	C8A	-B4A	1.668(6)
Pt7A	-C8A	2.159(4)	C8A	-B9A	1.586(7)
Pt7A	-B2A	2.255(4)	C8A	-H8A	1.01(4)
Pt7A	-B3A	2.303(4)	C11	-H11I	0.9800
Pt7A	-B11A	2.314(4)	C11	-H11H	0.9800
Pt7B	-P4	2.3461(10)	C11	-H11G	0.9800
Pt7B	-C11B	2.168(4)	C11A	-H11F	0.9800
Pt7B	-B2B	2.248(4)	C11A	-H11D	0.9800
Pt7B	-B6B	2.276(4)	C11A	-H11E	0.9800
Pt7B	-B8B	2.304(4)	C12	-H12E	0.9800
Pt7B	-P3	2.2754(9)	C12	-H12D	0.9800
P1	-C11	1.815(4)	C12	-H12F	0.9800
P1	-C12	1.806(4)	C21	-H20A	0.9800
P1	-C131	1.820(4)	C21	-H20B	0.9800
P2	-C231	1.826(3)	C21	-H20C	0.9800
P2	-C22	1.824(4)	C22	-H24A	0.9800
P2	-C21	1.814(4)	C22	-H24B	0.9800
P3	-C32	1.803(3)	C22	-H24C	0.9800
P3	-C31	1.817(4)	C131	-C136	1.388(6)
P3	-C331	1.824(3)	C131	-C132	1.384(5)
P4	-C41	1.816(4)	C132	-C133	1.393(6)
P4	-C42	1.816(4)	C133	-C134	1.369(8)
P4	-C431	1.810(4)	C134	-C135	1.382(8)
O11A	-C11A	1.435(5)	C135	-C136	1.392(6)
O11A	-B11A	1.375(5)	C11B	-B5B	1.678(5)
O8B	-C8B	1.429(5)	C11B	-B10B	1.592(6)
O8B	-B8B	1.388(5)	C11B	-B6B	1.645(6)

Table S5 - Bond Distances (Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C231	-C236	1.389(5)	C41	-H41C	0.9800
C231	-C232	1.397(4)	C42	-H17A	0.9800
C232	-C233	1.384(5)	C42	-H17C	0.9800
C132	-H132	0.9500	C42	-H17B	0.9800
C233	-C234	1.382(6)	C331	-C336	1.378(5)
C133	-H133	0.9500	C331	-C332	1.396(4)
C134	-H134	0.9500	C332	-C333	1.385(5)
C234	-C235	1.384(6)	C333	-C334	1.381(6)
C235	-C236	1.388(5)	C334	-C335	1.370(6)
C135	-H135	0.9500	C335	-C336	1.382(6)
C136	-H136	0.9500	C431	-C436	1.388(5)
C8B	-H30B	0.9800	C431	-C432	1.390(5)
C8B	-H30C	0.9800	C432	-C433	1.383(6)
C8B	-H30A	0.9800	C332	-H332	0.9500
C11B	-H11B	0.97(3)	C433	-C434	1.376(8)
C31	-H31B	0.9800	C333	-H333	0.9500
C31	-H31C	0.9800	C334	-H334	0.9500
C31	-H31A	0.9800	C434	-C435	1.371(8)
C32	-H32B	0.9800	C335	-H335	0.9500
C32	-H32C	0.9800	C435	-C436	1.385(7)
C32	-H32A	0.9800	C336	-H336	0.9500
C232	-H232	0.9500	C432	-H432	0.9500
C233	-H233	0.9500	C433	-H433	0.9500
C234	-H234	0.9500	C434	-H434	0.9500
C235	-H235	0.9500	C435	-H435	0.9500
C236	-H236	0.9500	C436	-H436	0.9500
C41	-H41B	0.9800	B1A	-B4A	1.751(7)

C41	-H41A	0.9800	B1A	-B6A	1.765(7)

Table S5 - Bond Distances (Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1A	-B3A	1.760(6)	B1B	-B3B	1.768(6)
B1A	-B2A	1.778(6)	B1B	-B6B	1.769(5)
B1A	-B5A	1.815(7)	B1B	-B4B	1.801(6)
B2A	-B6A	1.784(6)	B1B	-B5B	1.746(5)
B2A	-B11A	1.814(6)	B2B	-B3B	1.781(6)
B2A	-B3A	1.865(6)	B2B	-B6B	1.868(6)
B3A	-B4A	1.757(6)	B2B	-B8B	1.807(6)
B4A	-B9A	1.806(8)	B3B	-B4B	1.796(6)
B4A	-B5A	1.736(8)	B3B	-B9B	1.794(6)
B5A	-B9A	1.757(8)	B3B	-B8B	1.745(6)
B5A	-B10A	1.758(8)	B4B	-B9B	1.760(6)
B5A	-B6A	1.806(6)	B4B	-B10B	1.764(8)
B6A	-B10A	1.786(7)	B4B	-B5B	1.745(6)
B6A	-B11A	1.738(6)	B5B	-B10B	1.800(6)
B9A	-B10A	1.955(8)	B5B	-B6B	1.764(6)
B10A	-B11A	1.813(7)	B8B	-B9B	1.824(6)
B1A	-H1A	1.1200	B9B	-B10B	1.948(6)
B2A	-H2A	1.1200	B1B	-H1B	1.1200
B3A	-H3A	1.1200	B2B	-H2B	1.10(4)
B4A	-H4A	1.1200	B3B	-H3B	1.1200
B5A	-H5A	1.1200	B4B	-H4B	1.1200
B6A	-H6A	1.1200	B5B	-H5B	1.1200
B9A	-H9A	1.13(3)	B6B	-H6B	1.1200
B10A	-H10A	1.07(4)	B8B	-H89	1.53(4)
B10A	-H101	1.14(4)	B9B	-H9B	1.09(3)
B11A	-H101	1.52(4)	B9B	-H89	1.10(4)
B1B	-B2B	1.779(6)	B10B	-H10B	1.07(4)

Table S6 - Bond Angles (Degrees)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

P1	-Pt7A	-P2	96.08(4)	P3	-Pt7B	-P4	96.55(4)
P1	-Pt7A	-C8A	171.76(11)	P3	-Pt7B	-C11B	171.50(11)
P1	-Pt7A	-B2A	95.52(11)	C11	-P1	-C131	102.48(18)
P1	-Pt7A	-B3A	129.50(10)	Pt7A	-P1	-C11	117.17(13)
P1	-Pt7A	-B11A	89.97(10)	Pt7A	-P1	-C12	118.98(13)
P2	-Pt7A	-C8A	87.37(10)	Pt7A	-P1	-C131	108.29(12)
P2	-Pt7A	-B2A	168.00(11)	C11	-P1	-C12	101.61(18)
P2	-Pt7A	-B3A	120.64(10)	C12	-P1	-C131	106.70(18)
P2	-Pt7A	-B11A	136.27(10)	C22	-P2	-C231	101.94(17)
C8A	-Pt7A	-B2A	80.73(14)	Pt7A	-P2	-C21	113.79(13)
C8A	-Pt7A	-B3A	43.09(14)	Pt7A	-P2	-C22	113.88(13)
C8A	-Pt7A	-B11A	92.70(14)	Pt7A	-P2	-C231	116.49(11)
B2A	-Pt7A	-B3A	48.30(14)	C21	-P2	-C22	103.22(18)
B2A	-Pt7A	-B11A	46.76(14)	C21	-P2	-C231	106.02(17)
B3A	-Pt7A	-B11A	85.89(14)	Pt7B	-P3	-C31	117.37(12)
P3	-Pt7B	-B2B	95.35(11)	C31	-P3	-C32	101.52(18)
P3	-Pt7B	-B6B	128.90(10)	Pt7B	-P3	-C32	118.52(12)
P3	-Pt7B	-B8B	91.47(10)	Pt7B	-P3	-C331	108.51(11)
P4	-Pt7B	-C11B	87.01(10)	C31	-P3	-C331	102.50(17)
P4	-Pt7B	-B2B	167.56(11)	C32	-P3	-C331	106.87(16)
P4	-Pt7B	-B6B	119.70(10)	Pt7B	-P4	-C42	111.64(12)
P4	-Pt7B	-B8B	136.27(10)	Pt7B	-P4	-C41	112.37(13)
C11B	-Pt7B	-B2B	80.72(14)	C41	-P4	-C431	103.26(17)
C11B	-Pt7B	-B6B	43.36(14)	Pt7B	-P4	-C431	119.53(12)
C11B	-Pt7B	-B8B	91.26(14)	C41	-P4	-C42	103.82(18)
B2B	-Pt7B	-B6B	48.77(14)	C42	-P4	-C431	104.73(16)
B2B	-Pt7B	-B8B	46.77(15)	C11A	-O11A	-B11A	119.2(3)
B6B	-Pt7B	-B8B	85.89(14)	C8B	-O8B	-B8B	119.9(3)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B3A	-C8A	-B9A	116.2(3)	P2	-C21	-H20B	109.00
B4A	-C8A	-B9A	67.4(3)	P2	-C21	-H20A	109.00
Pt7A	-C8A	-B9A	108.2(3)	H20A	-C21	-H20C	109.00
Pt7A	-C8A	-B3A	73.1(2)	H20B	-C21	-H20C	109.00
Pt7A	-C8A	-B4A	126.4(3)	H20A	-C21	-H20B	109.00
B3A	-C8A	-B4A	64.1(3)	P2	-C21	-H20C	109.00
B3A	-C8A	-H8A	119(2)	P2	-C22	-H24B	110.00
B9A	-C8A	-H8A	118(2)	H24A	-C22	-H24B	109.00
B4A	-C8A	-H8A	116(2)	P2	-C22	-H24C	109.00
Pt7A	-C8A	-H8A	112(2)	H24A	-C22	-H24C	109.00
P1	-C11	-H11G	109.00	H24B	-C22	-H24C	109.00
H11G	-C11	-H11I	109.00	P2	-C22	-H24A	109.00
P1	-C11	-H11H	109.00	C132	-C131	-C136	118.9(4)
H11G	-C11	-H11H	110.00	P1	-C131	-C136	117.9(3)
P1	-C11	-H11I	109.00	P1	-C131	-C132	123.1(3)
H11H	-C11	-H11I	110.00	C131	-C132	-C133	120.5(4)
H11D	-C11A	-H11E	109.00	C132	-C133	-C134	119.9(4)
O11A	-C11A	-H11F	109.00	C133	-C134	-C135	120.6(5)
O11A	-C11A	-H11E	109.00	C134	-C135	-C136	119.4(4)
H11E	-C11A	-H11F	109.00	C131	-C136	-C135	120.7(4)
H11D	-C11A	-H11F	109.00	Pt7B	-C11B	-B5B	126.2(2)
O11A	-C11A	-H11D	110.00	B5B	-C11B	-B6B	64.1(2)
H12D	-C12	-H12F	109.00	Pt7B	-C11B	-B6B	71.8(2)
P1	-C12	-H12D	110.00	Pt7B	-C11B	-B10B	111.2(3)
P1	-C12	-H12F	109.00	B5B	-C11B	-B10B	66.8(3)
H12D	-C12	-H12E	109.00	B6B	-C11B	-B10B	116.5(3)
H12E	-C12	-H12F	109.00	P2	-C231	-C236	123.0(2)
P1	-C12	-H12E	109.00	P2	-C231	-C232	117.7(3)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C232	-C231	-C236	119.1(3)	P3	-C31	-H31A	109.00
C131	-C132	-H132	120.00	H31A	-C31	-H31B	110.00
C231	-C232	-C233	120.6(3)	H31B	-C31	-H31C	109.00
C133	-C132	-H132	120.00	H31A	-C31	-H31C	109.00
C134	-C133	-H133	120.00	H32A	-C32	-H32B	109.00
C132	-C133	-H133	120.00	P3	-C32	-H32B	110.00
C232	-C233	-C234	119.8(4)	H32A	-C32	-H32C	109.00
C135	-C134	-H134	120.00	C233	-C232	-H232	120.00
C133	-C134	-H134	120.00	P3	-C32	-H32C	109.00
C233	-C234	-C235	119.9(4)	C231	-C232	-H232	120.00
C234	-C235	-C236	120.5(3)	P3	-C32	-H32A	109.00
C134	-C135	-H135	120.00	H32B	-C32	-H32C	109.00
C136	-C135	-H135	120.00	C234	-C233	-H233	120.00
C231	-C236	-C235	120.0(3)	C232	-C233	-H233	120.00
C131	-C136	-H136	120.00	C235	-C234	-H234	120.00
C135	-C136	-H136	120.00	C233	-C234	-H234	120.00
H30A	-C8B	-H30C	110.00	C236	-C235	-H235	120.00
O8B	-C8B	-H30B	109.00	C234	-C235	-H235	120.00
H30B	-C8B	-H30C	109.00	C235	-C236	-H236	120.00
H30A	-C8B	-H30B	109.00	C231	-C236	-H236	120.00
O8B	-C8B	-H30C	109.00	H41B	-C41	-H41C	109.00
O8B	-C8B	-H30A	109.00	P4	-C41	-H41B	109.00
Pt7B	-C11B	-H11B	111(2)	H41A	-C41	-H41C	110.00
B5B	-C11B	-H11B	115.8(19)	P4	-C41	-H41C	109.00
B10B	-C11B	-H11B	119.6(18)	H41A	-C41	-H41B	110.00
B6B	-C11B	-H11B	116.8(17)	P4	-C41	-H41A	109.00
P3	-C31	-H31B	109.00	H17B	-C42	-H17C	110.00
P3	-C31	-H31C	109.00	P4	-C42	-H17C	110.00

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

H17A	-C42	-H17B	109.00	C335	-C336	-H336	120.00
P4	-C42	-H17A	110.00	C431	-C436	-C435	120.2(4)
H17A	-C42	-H17C	109.00	C431	-C432	-H432	120.00
P4	-C42	-H17B	109.00	C433	-C432	-H432	120.00
P3	-C331	-C332	118.3(3)	C432	-C433	-H433	120.00
C332	-C331	-C336	119.1(3)	C434	-C433	-H433	120.00
P3	-C331	-C336	122.6(3)	C435	-C434	-H434	120.00
C331	-C332	-C333	120.0(4)	C433	-C434	-H434	120.00
C332	-C333	-C334	120.2(4)	C436	-C435	-H435	120.00
C333	-C334	-C335	119.5(4)	C434	-C435	-H435	120.00
C334	-C335	-C336	120.9(4)	C435	-C436	-H436	120.00
C331	-C336	-C335	120.2(4)	C431	-C436	-H436	120.00
C432	-C431	-C436	119.0(3)	B3A	-B1A	-B4A	60.1(2)
P4	-C431	-C432	121.8(2)	B2A	-B1A	-B6A	60.5(2)
P4	-C431	-C436	119.1(3)	B2A	-B1A	-B3A	63.6(2)
C431	-C432	-C433	120.5(4)	B2A	-B1A	-B4A	111.8(3)
C331	-C332	-H332	120.00	B2A	-B1A	-B5A	105.8(3)
C333	-C332	-H332	120.00	B5A	-B1A	-B6A	60.6(3)
C334	-C333	-H333	120.00	B4A	-B1A	-B6A	111.6(4)
C432	-C433	-C434	119.7(4)	B3A	-B1A	-B5A	104.5(3)
C332	-C333	-H333	120.00	B4A	-B1A	-B5A	58.2(3)
C433	-C434	-C435	120.6(5)	B3A	-B1A	-B6A	112.4(3)
C335	-C334	-H334	120.00	B1A	-B2A	-B6A	59.4(3)
C333	-C334	-H334	120.00	B1A	-B2A	-B11A	109.7(3)
C336	-C335	-H335	120.00	Pt7A	-B2A	-B6A	114.2(2)
C334	-C335	-H335	119.00	Pt7A	-B2A	-B11A	68.33(17)
C434	-C435	-C436	120.0(4)	Pt7A	-B2A	-B3A	67.19(17)
C331	-C336	-H336	120.00	B3A	-B2A	-B6A	106.7(3)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1A	-B2A	-B3A	57.7(2)	B1A	-B5A	-B9A	106.0(3)
B3A	-B2A	-B11A	117.5(3)	B4A	-B5A	-B9A	62.3(3)
Pt7A	-B2A	-B1A	115.5(2)	B6A	-B5A	-B10A	60.1(3)
B6A	-B2A	-B11A	57.8(2)	B4A	-B5A	-B6A	110.3(3)
Pt7A	-B3A	-B1A	114.0(3)	B1A	-B5A	-B6A	58.3(3)
B2A	-B3A	-B4A	107.5(3)	B9A	-B5A	-B10A	67.6(3)
Pt7A	-B3A	-B4A	114.2(3)	B2A	-B6A	-B5A	105.9(3)
B1A	-B3A	-B2A	58.6(2)	B1A	-B6A	-B10A	109.9(3)
Pt7A	-B3A	-B2A	64.52(17)	B2A	-B6A	-B10A	107.5(3)
Pt7A	-B3A	-C8A	63.78(19)	B2A	-B6A	-B11A	62.0(2)
C8A	-B3A	-B4A	58.6(3)	B1A	-B6A	-B11A	113.9(3)
C8A	-B3A	-B2A	109.0(3)	B1A	-B6A	-B2A	60.1(3)
B1A	-B3A	-B4A	59.7(3)	B1A	-B6A	-B5A	61.1(3)
C8A	-B3A	-B1A	106.2(3)	B5A	-B6A	-B10A	58.6(3)
B1A	-B4A	-B3A	60.2(2)	B5A	-B6A	-B11A	110.2(3)
C8A	-B4A	-B1A	105.6(3)	B10A	-B6A	-B11A	61.9(3)
B1A	-B4A	-B5A	62.7(3)	C8A	-B9A	-B4A	58.5(3)
B1A	-B4A	-B9A	106.7(4)	B4A	-B9A	-B10A	106.8(4)
C8A	-B4A	-B9A	54.2(3)	B5A	-B9A	-B10A	56.2(3)
B3A	-B4A	-B5A	108.1(3)	C8A	-B9A	-B10A	116.1(3)
C8A	-B4A	-B3A	57.3(2)	B4A	-B9A	-B5A	58.3(3)
C8A	-B4A	-B5A	103.9(3)	C8A	-B9A	-B5A	106.5(4)
B5A	-B4A	-B9A	59.4(3)	B5A	-B10A	-B6A	61.3(3)
B3A	-B4A	-B9A	100.6(3)	B5A	-B10A	-B9A	56.2(3)
B4A	-B5A	-B10A	119.6(4)	B6A	-B10A	-B9A	103.4(3)
B6A	-B5A	-B9A	111.0(3)	B6A	-B10A	-B11A	57.8(3)
B1A	-B5A	-B4A	59.0(3)	B9A	-B10A	-B11A	108.1(3)
B1A	-B5A	-B10A	108.9(3)	B5A	-B10A	-B11A	109.0(4)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

O11A	-B11A	-B2A	127.9(3)	B1A	-B4A	-H4A	121.00
O11A	-B11A	-B6A	129.6(3)	B3A	-B4A	-H4A	124.00
Pt7A	-B11A	-B10A	104.0(2)	B4A	-B5A	-H5A	117.00
Pt7A	-B11A	-B2A	64.91(17)	B1A	-B5A	-H5A	125.00
Pt7A	-B11A	-B6A	113.4(3)	B6A	-B5A	-H5A	122.00
O11A	-B11A	-B10A	124.1(3)	B10A	-B5A	-H5A	115.00
Pt7A	-B11A	-O11A	112.9(2)	B9A	-B5A	-H5A	119.00
B6A	-B11A	-B10A	60.4(3)	B5A	-B6A	-H6A	123.00
B2A	-B11A	-B6A	60.3(3)	B2A	-B6A	-H6A	123.00
B2A	-B11A	-B10A	105.1(3)	B10A	-B6A	-H6A	122.00
B6A	-B1A	-H1A	119.00	B1A	-B6A	-H6A	119.00
B3A	-B1A	-H1A	121.00	B11A	-B6A	-H6A	118.00
B5A	-B1A	-H1A	126.00	B10A	-B9A	-H9A	116.7(15)
B2A	-B1A	-H1A	120.00	C8A	-B9A	-H9A	119.7(17)
B4A	-B1A	-H1A	120.00	B5A	-B9A	-H9A	126.1(19)
B1A	-B2A	-H2A	122.00	B4A	-B9A	-H9A	126.3(16)
Pt7A	-B2A	-H2A	112.00	B6A	-B10A	-H101	111(2)
B3A	-B2A	-H2A	119.00	B9A	-B10A	-H10A	118(2)
B11A	-B2A	-H2A	117.00	B6A	-B10A	-H10A	127(2)
B6A	-B2A	-H2A	124.00	B5A	-B10A	-H10A	116(2)
B1A	-B3A	-H3A	122.00	B5A	-B10A	-H101	126(2)
B4A	-B3A	-H3A	121.00	H10A	-B10A	-H101	110(3)
C8A	-B3A	-H3A	122.00	B11A	-B10A	-H101	56.8(19)
B2A	-B3A	-H3A	122.00	B9A	-B10A	-H101	78.0(19)
Pt7A	-B3A	-H3A	115.00	B11A	-B10A	-H10A	128(2)
B9A	-B4A	-H4A	126.00	B2A	-B11A	-H101	116.9(15)
C8A	-B4A	-H4A	126.00	B6A	-B11A	-H101	96.6(15)
B5A	-B4A	-H4A	121.00	B10A	-B11A	-H101	38.9(15)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

O11A	-B11A	-H101	112.4(15)	B2B	-B3B	-B4B	106.3(3)
Pt7A	-B11A	-H101	76.9(15)	B1B	-B3B	-B4B	60.7(2)
B2B	-B1B	-B3B	60.3(2)	B4B	-B3B	-B8B	110.3(3)
B5B	-B1B	-B6B	60.3(2)	B1B	-B3B	-B2B	60.2(2)
B4B	-B1B	-B6B	105.1(3)	B1B	-B4B	-B10B	106.1(3)
B4B	-B1B	-B5B	58.9(2)	B1B	-B4B	-B3B	58.9(2)
B2B	-B1B	-B4B	106.2(3)	B1B	-B4B	-B5B	59.0(2)
B2B	-B1B	-B5B	112.2(3)	B1B	-B4B	-B9B	109.4(3)
B2B	-B1B	-B6B	63.5(2)	B9B	-B4B	-B10B	67.1(2)
B3B	-B1B	-B4B	60.4(2)	B3B	-B4B	-B10B	111.5(3)
B3B	-B1B	-B5B	111.8(3)	B3B	-B4B	-B5B	110.5(3)
B3B	-B1B	-B6B	111.9(3)	B3B	-B4B	-B9B	60.6(2)
Pt7B	-B2B	-B3B	115.1(2)	B5B	-B4B	-B9B	118.6(3)
Pt7B	-B2B	-B6B	66.40(17)	B5B	-B4B	-B10B	61.7(3)
Pt7B	-B2B	-B8B	68.26(18)	C11B	-B5B	-B6B	57.0(2)
B1B	-B2B	-B3B	59.6(2)	C11B	-B5B	-B4B	103.4(3)
B1B	-B2B	-B6B	58.0(2)	B6B	-B5B	-B10B	101.1(3)
B1B	-B2B	-B8B	109.7(3)	C11B	-B5B	-B10B	54.3(2)
B3B	-B2B	-B6B	106.9(3)	B1B	-B5B	-B4B	62.1(2)
B3B	-B2B	-B8B	58.2(2)	B1B	-B5B	-B6B	60.5(2)
Pt7B	-B2B	-B1B	115.6(2)	B1B	-B5B	-B10B	106.9(3)
B6B	-B2B	-B8B	116.2(3)	B4B	-B5B	-B6B	107.7(3)
B2B	-B3B	-B8B	61.7(2)	B4B	-B5B	-B10B	59.6(3)
B2B	-B3B	-B9B	107.7(3)	C11B	-B5B	-B1B	105.2(3)
B4B	-B3B	-B9B	58.7(2)	C11B	-B6B	-B5B	58.8(2)
B8B	-B3B	-B9B	62.0(2)	B1B	-B6B	-B2B	58.5(2)
B1B	-B3B	-B8B	113.2(3)	B1B	-B6B	-B5B	59.2(2)
B1B	-B3B	-B9B	109.3(3)	B2B	-B6B	-B5B	107.3(3)

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Pt7B	-B6B	-B2B	64.83(17)	B2B	-B1B	-H1B	120.00
Pt7B	-B6B	-B5B	116.0(2)	B3B	-B1B	-H1B	119.00
C11B	-B6B	-B1B	105.6(3)	B4B	-B1B	-H1B	125.00
C11B	-B6B	-B2B	108.9(3)	B5B	-B1B	-H1B	120.00
Pt7B	-B6B	-C11B	64.83(19)	B6B	-B1B	-H1B	121.00
Pt7B	-B6B	-B1B	114.7(2)	Pt7B	-B2B	-H2B	117(2)
O8B	-B8B	-B2B	127.4(3)	B1B	-B2B	-H2B	119(2)
Pt7B	-B8B	-O8B	111.7(2)	B3B	-B2B	-H2B	119(2)
Pt7B	-B8B	-B2B	64.97(17)	B6B	-B2B	-H2B	122(2)
Pt7B	-B8B	-B3B	114.0(2)	B8B	-B2B	-H2B	118(2)
Pt7B	-B8B	-B9B	105.5(2)	B1B	-B3B	-H3B	119.00
O8B	-B8B	-B9B	124.3(3)	B2B	-B3B	-H3B	123.00
B2B	-B8B	-B3B	60.2(2)	B4B	-B3B	-H3B	123.00
O8B	-B8B	-B3B	129.7(3)	B8B	-B3B	-H3B	118.00
B3B	-B8B	-B9B	60.3(2)	B9B	-B3B	-H3B	122.00
B2B	-B8B	-B9B	105.3(3)	B1B	-B4B	-H4B	125.00
B4B	-B9B	-B10B	56.5(3)	B3B	-B4B	-H4B	121.00
B4B	-B9B	-B8B	108.3(3)	B5B	-B4B	-H4B	118.00
B3B	-B9B	-B4B	60.7(2)	B9B	-B4B	-H4B	116.00
B3B	-B9B	-B8B	57.6(2)	B10B	-B4B	-H4B	119.00
B8B	-B9B	-B10B	108.4(3)	C11B	-B5B	-H5B	126.00
B3B	-B9B	-B10B	103.6(3)	B1B	-B5B	-H5B	121.00
C11B	-B10B	-B5B	58.9(2)	B4B	-B5B	-H5B	121.00
C11B	-B10B	-B9B	114.4(3)	B6B	-B5B	-H5B	124.00
C11B	-B10B	-B4B	106.3(3)	B10B	-B5B	-H5B	126.00
B4B	-B10B	-B9B	56.4(2)	Pt7B	-B6B	-H6B	113.00
B5B	-B10B	-B9B	107.0(3)	C11B	-B6B	-H6B	122.00

B4B	-B10B	-B5B	58.6(2)	B1B	-B6B	-H6B	122.00

Table S6 - Bond Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B2B	-B6B	-H6B	122.00	B4B	-B9B	-H89	125.8(16)
B5B	-B6B	-H6B	121.00	B8B	-B9B	-H9B	127.3(18)
Pt7B	-B8B	-H89	79.6(13)	B8B	-B9B	-H89	57.0(19)
O8B	-B8B	-H89	113.3(12)	B10B	-B9B	-H9B	120.0(18)
B2B	-B8B	-H89	117.0(12)	B10B	-B9B	-H89	78.0(18)
B3B	-B8B	-H89	94.8(14)	H9B	-B9B	-H89	113(2)
B9B	-B8B	-H89	37.0(14)	C11B	-B10B	-H10B	123(2)
B3B	-B9B	-H9B	122.7(18)	B4B	-B10B	-H10B	125(2)
B3B	-B9B	-H89	110.9(17)	B5B	-B10B	-H10B	128(2)
B4B	-B9B	-H9B	114.7(18)	B9B	-B10B	-H10B	114(2)

Table S7 - Torsion Angles (Degrees)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

P2	-Pt7A	-P1	-C11	-172.10(15)
B2A	-Pt7A	-P1	-C11	4.80(18)
B3A	-Pt7A	-P1	-C11	-33.3(2)
B11A	-Pt7A	-P1	-C11	51.30(18)
P2	-Pt7A	-P1	-C12	65.03(15)
B2A	-Pt7A	-P1	-C12	-118.08(18)
B3A	-Pt7A	-P1	-C12	-156.22(19)
B11A	-Pt7A	-P1	-C12	-71.57(17)
P2	-Pt7A	-P1	-C131	-56.91(13)
B2A	-Pt7A	-P1	-C131	119.98(17)
B3A	-Pt7A	-P1	-C131	81.85(18)
B11A	-Pt7A	-P1	-C131	166.49(17)
P2	-Pt7A	-C8A	-B9A	-104.6(3)
B2A	-Pt7A	-C8A	-B9A	77.0(3)
B3A	-Pt7A	-C8A	-B9A	112.7(3)
B11A	-Pt7A	-C8A	-B9A	31.6(3)
B3A	-Pt7A	-B2A	-B11A	-134.9(3)
C8A	-Pt7A	-B11A	-B10A	-25.8(3)
P1	-Pt7A	-P2	-C21	90.22(15)
C8A	-Pt7A	-P2	-C21	-82.26(18)
B3A	-Pt7A	-P2	-C21	-53.53(19)
B11A	-Pt7A	-P2	-C21	-173.4(2)
P1	-Pt7A	-P2	-C22	-151.85(15)
C8A	-Pt7A	-P2	-C22	35.67(18)
B3A	-Pt7A	-P2	-C22	64.40(19)
B11A	-Pt7A	-P2	-C22	-55.5(2)
P1	-Pt7A	-P2	-C231	-33.59(12)
C8A	-Pt7A	-P2	-C231	153.92(16)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B3A	-Pt7A	-P2	-C231	-177.34(16)
B11A	-Pt7A	-P2	-C231	62.76(19)
B11A	-Pt7A	-B3A	-C8A	98.4(2)
P1	-Pt7A	-B3A	-B1A	88.0(3)
P1	-Pt7A	-B11A	-O11A	24.9(2)
P2	-Pt7A	-B11A	-O11A	-73.9(3)
P1	-Pt7A	-B2A	-B1A	-173.0(3)
C8A	-Pt7A	-B2A	-B1A	-0.4(3)
P2	-Pt7A	-C8A	-B3A	142.74(19)
B2A	-Pt7A	-C8A	-B3A	-35.7(2)
B11A	-Pt7A	-C8A	-B3A	-81.1(2)
P2	-Pt7A	-C8A	-B4A	-179.5(4)
B2A	-Pt7A	-C8A	-B4A	2.1(3)
B3A	-Pt7A	-C8A	-B4A	37.8(3)
B11A	-Pt7A	-C8A	-B4A	-43.3(4)
P2	-Pt7A	-B11A	-B6A	126.7(2)
C8A	-Pt7A	-B11A	-B6A	37.7(3)
B2A	-Pt7A	-B11A	-B6A	-36.9(2)
B3A	-Pt7A	-B11A	-B6A	-4.9(3)
P1	-Pt7A	-B11A	-B10A	162.0(2)
P2	-Pt7A	-B11A	-B10A	63.3(3)
B2A	-Pt7A	-B11A	-B10A	-100.4(3)
B3A	-Pt7A	-B11A	-B10A	-68.3(3)
C8A	-Pt7A	-B11A	-O11A	-162.9(3)
B2A	-Pt7A	-B11A	-O11A	122.5(3)
B3A	-Pt7A	-B11A	-O11A	154.5(3)
P1	-Pt7A	-B11A	-B2A	-97.61(17)

P2	-Pt7A	-B11A	-B2A	163.61(15)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C8A	-Pt7A	-B11A	-B2A	74.6(2)
B3A	-Pt7A	-B11A	-B2A	32.01(19)
P1	-Pt7A	-B11A	-B6A	-134.5(2)
P1	-Pt7A	-B3A	-C8A	-175.03(16)
P2	-Pt7A	-B3A	-C8A	-44.7(2)
B2A	-Pt7A	-B3A	-C8A	129.6(3)
B3A	-Pt7A	-B2A	-B6A	-98.8(3)
B11A	-Pt7A	-B2A	-B6A	36.1(2)
P1	-Pt7A	-B2A	-B11A	84.75(17)
P2	-Pt7A	-B3A	-B1A	-141.7(2)
P1	-Pt7A	-B2A	-B3A	-140.34(16)
B11A	-Pt7A	-B2A	-B3A	134.9(3)
C8A	-Pt7A	-B3A	-B1A	-97.0(3)
B2A	-Pt7A	-B3A	-B1A	32.6(2)
B11A	-Pt7A	-B3A	-B1A	1.4(3)
B3A	-Pt7A	-B2A	-B1A	-32.7(3)
B11A	-Pt7A	-B2A	-B1A	102.3(3)
C8A	-Pt7A	-B2A	-B11A	-102.7(2)
P1	-Pt7A	-B3A	-B2A	55.4(2)
P1	-Pt7A	-B2A	-B6A	120.8(2)
C8A	-Pt7A	-B2A	-B6A	-66.6(3)
P2	-Pt7A	-B3A	-B4A	-75.6(3)
C8A	-Pt7A	-B3A	-B4A	-30.9(3)
B2A	-Pt7A	-B3A	-B4A	98.7(3)
B11A	-Pt7A	-B3A	-B2A	-31.15(19)
B11A	-Pt7A	-B3A	-B4A	67.5(3)
C8A	-Pt7A	-B2A	-B3A	32.26(19)

P1	-Pt7A	-B3A	-B4A	154.1(2)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C8A	-Pt7A	-B3A	-B2A	-129.6(3)
P2	-Pt7A	-B3A	-B2A	-174.22(15)
B6B	-Pt7B	-P4	-C42	41.20(19)
B8B	-Pt7B	-P4	-C42	159.7(2)
P3	-Pt7B	-P4	-C431	21.35(12)
C11B	-Pt7B	-P4	-C431	-166.40(16)
B6B	-Pt7B	-P4	-C431	163.82(16)
P3	-Pt7B	-B6B	-C11B	175.21(15)
B8B	-Pt7B	-P4	-C431	-77.70(19)
P3	-Pt7B	-P4	-C42	-101.27(14)
C11B	-Pt7B	-P4	-C42	70.98(18)
P4	-Pt7B	-B8B	-B3B	-127.0(2)
C11B	-Pt7B	-B8B	-B3B	-40.0(3)
B2B	-Pt7B	-B8B	-B3B	36.0(2)
B6B	-Pt7B	-B2B	-B1B	31.7(2)
P3	-Pt7B	-B2B	-B6B	139.15(16)
B6B	-Pt7B	-P4	-C41	-74.97(19)
P3	-Pt7B	-B2B	-B3B	-122.5(2)
B8B	-Pt7B	-P4	-C41	43.5(2)
P3	-Pt7B	-B8B	-B3B	132.0(2)
B6B	-Pt7B	-B8B	-B2B	-32.9(2)
B8B	-Pt7B	-B2B	-B3B	-35.5(2)
C11B	-Pt7B	-B2B	-B1B	-1.6(3)
P4	-Pt7B	-B6B	-C11B	46.3(2)
B8B	-Pt7B	-B2B	-B1B	-102.2(3)
P3	-Pt7B	-B8B	-B2B	95.96(17)

P4	-Pt7B	-P3	-C32	-62.68(14)
C11B	-Pt7B	-B2B	-B3B	65.1(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B6B	-Pt7B	-B2B	-B3B	98.3(3)
C11B	-Pt7B	-B8B	-B2B	-76.0(2)
B6B	-Pt7B	-C11B	-B5B	-36.0(3)
B6B	-Pt7B	-B8B	-B3B	3.1(3)
B2B	-Pt7B	-B6B	-C11B	-128.0(3)
B2B	-Pt7B	-B8B	-B9B	99.9(3)
B6B	-Pt7B	-B8B	-B9B	67.0(2)
B6B	-Pt7B	-B2B	-B8B	133.9(3)
B8B	-Pt7B	-C11B	-B10B	-29.5(3)
P3	-Pt7B	-B2B	-B1B	170.8(2)
B8B	-Pt7B	-P3	-C31	-48.24(18)
C11B	-Pt7B	-P4	-C41	-45.19(18)
B2B	-Pt7B	-P3	-C31	-1.54(18)
B6B	-Pt7B	-B8B	-O8B	-155.3(3)
P4	-Pt7B	-B8B	-B2B	-162.98(15)
P3	-Pt7B	-P4	-C41	142.56(15)
B2B	-Pt7B	-C11B	-B5B	0.9(3)
B2B	-Pt7B	-B6B	-B1B	-31.6(2)
B8B	-Pt7B	-C11B	-B5B	46.7(3)
P3	-Pt7B	-B8B	-B9B	-164.1(2)
P4	-Pt7B	-B8B	-B9B	-63.0(3)
C11B	-Pt7B	-B8B	-B9B	24.0(2)
B8B	-Pt7B	-B2B	-B6B	-133.9(3)
P3	-Pt7B	-B2B	-B8B	-86.98(17)
B2B	-Pt7B	-C11B	-B10B	-75.2(3)
B6B	-Pt7B	-P3	-C31	37.7(2)

P4	-Pt7B	-P3	-C31	174.83(15)
B2B	-Pt7B	-B8B	-O8B	-122.4(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

P4	-Pt7B	-B6B	-B1B	142.7(2)
C11B	-Pt7B	-B6B	-B1B	96.4(3)
P4	-Pt7B	-C11B	-B5B	-177.1(3)
B6B	-Pt7B	-P3	-C331	-77.83(17)
B6B	-Pt7B	-C11B	-B10B	-112.1(3)
B8B	-Pt7B	-B6B	-B1B	0.2(3)
P3	-Pt7B	-B6B	-B2B	-56.8(2)
P4	-Pt7B	-C11B	-B6B	-141.07(18)
C11B	-Pt7B	-B2B	-B6B	-33.25(19)
P4	-Pt7B	-B6B	-B2B	174.25(15)
B2B	-Pt7B	-C11B	-B6B	36.9(2)
B8B	-Pt7B	-P3	-C331	-163.73(15)
P3	-Pt7B	-B6B	-B5B	-154.66(18)
B8B	-Pt7B	-B6B	-C11B	-96.2(2)
P3	-Pt7B	-B6B	-B1B	-88.4(3)
P3	-Pt7B	-B8B	-O8B	-26.4(2)
P4	-Pt7B	-B8B	-O8B	74.7(3)
C11B	-Pt7B	-B8B	-O8B	161.7(3)
P4	-Pt7B	-P3	-C331	59.34(11)
B8B	-Pt7B	-C11B	-B6B	82.7(2)
C11B	-Pt7B	-B2B	-B8B	100.6(2)
P4	-Pt7B	-B6B	-B5B	76.4(2)
C11B	-Pt7B	-B6B	-B5B	30.1(2)
B2B	-Pt7B	-B6B	-B5B	-97.9(3)
B8B	-Pt7B	-B6B	-B5B	-66.1(2)

B6B	-Pt7B	-P3	-C32	160.16(18)
B2B	-Pt7B	-P3	-C331	-117.03(15)
B2B	-Pt7B	-P3	-C32	120.96(17)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B8B	-Pt7B	-P3	-C32	74.26(17)
P4	-Pt7B	-C11B	-B10B	106.8(3)
B8B	-Pt7B	-B6B	-B2B	31.78(19)
C11B	-Pt7B	-B6B	-B2B	128.0(3)
C11	-P1	-C131	-C132	-98.4(3)
C11	-P1	-C131	-C136	81.0(3)
Pt7A	-P1	-C131	-C132	137.2(3)
C12	-P1	-C131	-C136	-172.7(3)
C12	-P1	-C131	-C132	8.0(4)
Pt7A	-P1	-C131	-C136	-43.5(3)
C22	-P2	-C231	-C232	51.5(3)
C21	-P2	-C231	-C236	-25.6(3)
Pt7A	-P2	-C231	-C236	102.1(3)
C22	-P2	-C231	-C236	-133.3(3)
Pt7A	-P2	-C231	-C232	-73.1(3)
C21	-P2	-C231	-C232	159.2(3)
C32	-P3	-C331	-C336	-16.9(3)
Pt7B	-P3	-C331	-C336	-145.8(3)
C32	-P3	-C331	-C332	164.1(3)
Pt7B	-P3	-C331	-C332	35.2(3)
C31	-P3	-C331	-C332	-89.6(3)
C31	-P3	-C331	-C336	89.4(3)
C42	-P4	-C431	-C432	32.5(3)
Pt7B	-P4	-C431	-C436	83.6(3)
C41	-P4	-C431	-C432	140.9(3)

C41	-P4	-C431	-C436	-42.0(3)
C42	-P4	-C431	-C436	-150.4(3)
Pt7B	-P4	-C431	-C432	-93.5(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C11A	-O11A	-B11A	-B2A	-161.5(4)
C11A	-O11A	-B11A	-B6A	-81.5(5)
C11A	-O11A	-B11A	-Pt7A	123.3(3)
C11A	-O11A	-B11A	-B10A	-3.9(5)
C8B	-O8B	-B8B	-Pt7B	-120.7(3)
C8B	-O8B	-B8B	-B3B	85.2(5)
C8B	-O8B	-B8B	-B2B	164.9(4)
C8B	-O8B	-B8B	-B9B	7.5(5)
B4A	-C8A	-B3A	-Pt7A	-146.7(3)
Pt7A	-C8A	-B9A	-B4A	-122.6(3)
Pt7A	-C8A	-B9A	-B5A	-88.2(3)
B4A	-C8A	-B3A	-B1A	-37.6(3)
B9A	-C8A	-B3A	-Pt7A	-102.4(3)
B9A	-C8A	-B3A	-B2A	-55.0(4)
Pt7A	-C8A	-B3A	-B4A	146.7(3)
B3A	-C8A	-B4A	-B1A	37.7(3)
B9A	-C8A	-B4A	-B5A	-34.4(3)
Pt7A	-C8A	-B4A	-B1A	-3.0(5)
Pt7A	-C8A	-B4A	-B3A	-40.7(3)
Pt7A	-C8A	-B4A	-B5A	62.1(4)
Pt7A	-C8A	-B4A	-B9A	96.5(4)
B4A	-C8A	-B3A	-B2A	-99.3(3)
Pt7A	-C8A	-B3A	-B1A	109.2(3)
B3A	-C8A	-B9A	-B4A	-42.9(3)

B3A	-C8A	-B9A	-B5A	-8.5(5)
B9A	-C8A	-B3A	-B4A	44.4(4)
B9A	-C8A	-B3A	-B1A	6.8(4)
B3A	-C8A	-B4A	-B9A	137.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B3A	-C8A	-B9A	-B10A	51.5(5)
B4A	-C8A	-B9A	-B5A	34.4(3)
Pt7A	-C8A	-B3A	-B2A	47.4(2)
B9A	-C8A	-B4A	-B3A	-137.2(3)
B3A	-C8A	-B4A	-B5A	102.8(3)
B4A	-C8A	-B9A	-B10A	94.4(4)
Pt7A	-C8A	-B9A	-B10A	-28.2(4)
B9A	-C8A	-B4A	-B1A	-99.5(4)
B5B	-C11B	-B6B	-B1B	37.8(3)
B5B	-C11B	-B10B	-B9B	-95.8(3)
Pt7B	-C11B	-B5B	-B10B	-100.0(4)
Pt7B	-C11B	-B10B	-B9B	25.7(4)
Pt7B	-C11B	-B6B	-B1B	-110.4(2)
B10B	-C11B	-B6B	-B1B	-5.2(4)
B10B	-C11B	-B6B	-B2B	56.3(4)
B5B	-C11B	-B6B	-B2B	99.3(3)
Pt7B	-C11B	-B6B	-B2B	-48.9(2)
Pt7B	-C11B	-B6B	-B5B	-148.2(2)
Pt7B	-C11B	-B5B	-B1B	0.1(4)
Pt7B	-C11B	-B5B	-B4B	-64.3(4)
Pt7B	-C11B	-B10B	-B5B	121.5(3)
B5B	-C11B	-B10B	-B4B	-35.9(3)
B6B	-C11B	-B5B	-B10B	-138.4(3)
B6B	-C11B	-B10B	-B4B	6.0(4)
B6B	-C11B	-B5B	-B1B	-38.3(3)
Pt7B	-C11B	-B5B	-B6B	38.4(3)
B10B	-C11B	-B5B	-B6B	138.4(3)
B10B	-C11B	-B6B	-Pt7B	105.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B10B	-C11B	-B5B	-B4B	35.8(3)
B6B	-C11B	-B5B	-B4B	-102.6(3)
B6B	-C11B	-B10B	-B9B	-54.0(4)
B10B	-C11B	-B6B	-B5B	-43.0(3)
Pt7B	-C11B	-B10B	-B4B	85.6(3)
B5B	-C11B	-B6B	-Pt7B	148.2(2)
B6B	-C11B	-B10B	-B5B	41.9(3)
B10B	-C11B	-B5B	-B1B	100.1(3)
P1	-C131	-C136	-H136	0.00
P2	-C231	-C236	-C235	-172.3(3)
C132	-C131	-C136	-H136	180.00
C136	-C131	-C132	-H132	-179.00
P2	-C231	-C232	-C233	174.3(3)
P1	-C131	-C132	-H132	0.00
C232	-C231	-C236	-C235	2.8(5)
C236	-C231	-C232	-C233	-1.1(5)
H132	-C132	-C133	-H133	-1.00
H132	-C132	-C133	-C134	179.00
C231	-C232	-C233	-C234	-1.7(5)
C131	-C132	-C133	-H133	179.00
C232	-C233	-C234	-C235	2.7(6)
H133	-C133	-C134	-H134	0.00
C132	-C133	-C134	-H134	180.00
H133	-C133	-C134	-C135	-180.00
H134	-C134	-C135	-H135	1.00
C133	-C134	-C135	-H135	-179.00
H134	-C134	-C135	-C136	-179.00
C233	-C234	-C235	-C236	-1.0(6)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

H135	-C135	-C136	-C131	179.00
C134	-C135	-C136	-H136	179.00
C234	-C235	-C236	-C231	-1.7(5)
H135	-C135	-C136	-H136	-1.00
C336	-C331	-C332	-H332	-178.00
C332	-C331	-C336	-H336	178.00
P4	-C431	-C436	-C435	-177.1(3)
C436	-C431	-C432	-C433	-0.3(5)
P3	-C331	-C332	-H332	1.00
P3	-C331	-C336	-H336	-1.00
C432	-C431	-C436	-C435	0.2(6)
P4	-C431	-C432	-C433	176.8(3)
C431	-C432	-C433	-C434	0.9(6)
H332	-C332	-C333	-C334	180.00
H332	-C332	-C333	-H333	0.00
C331	-C332	-C333	-H333	180.00
H333	-C333	-C334	-C335	179.00
C332	-C333	-C334	-H334	179.00
H333	-C333	-C334	-H334	-1.00
C432	-C433	-C434	-C435	-1.4(7)
C333	-C334	-C335	-H335	180.00
H334	-C334	-C335	-H335	0.00
H334	-C334	-C335	-C336	-180.00
C433	-C434	-C435	-C436	1.2(8)
H335	-C335	-C336	-C331	-178.00
C334	-C335	-C336	-H336	-178.00
C434	-C435	-C436	-C431	-0.6(7)
H335	-C335	-C336	-H336	2.00

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B5A	-B1A	-B4A	-B9A	41.3(3)
B3A	-B1A	-B4A	-C8A	-36.3(3)
B3A	-B1A	-B4A	-B5A	-134.2(3)
B5A	-B1A	-B4A	-B3A	134.2(3)
B2A	-B1A	-B4A	-B5A	-95.6(4)
B3A	-B1A	-B6A	-B11A	-6.2(4)
B2A	-B1A	-B4A	-B9A	-54.3(4)
B3A	-B1A	-B4A	-B9A	-92.9(3)
B5A	-B1A	-B4A	-C8A	97.9(4)
B3A	-B1A	-B6A	-B5A	94.5(3)
B6A	-B1A	-B3A	-B2A	37.0(3)
B6A	-B1A	-B3A	-C8A	-65.7(4)
B6A	-B1A	-B3A	-B4A	-102.8(4)
B2A	-B1A	-B4A	-C8A	2.2(5)
B3A	-B1A	-B6A	-B10A	61.0(4)
B4A	-B1A	-B6A	-B2A	-103.6(3)
B2A	-B1A	-B4A	-B3A	38.6(3)
B6A	-B1A	-B5A	-B4A	147.7(3)
B5A	-B1A	-B6A	-B11A	-100.8(3)
B6A	-B1A	-B4A	-C8A	67.9(4)
B6A	-B1A	-B4A	-B3A	104.2(3)
B3A	-B1A	-B6A	-B2A	-38.3(3)
B2A	-B1A	-B6A	-B5A	132.8(3)
B4A	-B1A	-B6A	-B5A	29.2(3)
B3A	-B1A	-B5A	-B10A	-73.9(4)
B5A	-B1A	-B6A	-B2A	-132.8(3)
B5A	-B1A	-B6A	-B10A	-33.6(3)
B2A	-B1A	-B6A	-B10A	99.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B2A	-B1A	-B6A	-B11A	32.0(3)
B3A	-B1A	-B5A	-B4A	39.9(3)
B3A	-B1A	-B5A	-B9A	-2.6(4)
B6A	-B1A	-B3A	-Pt7A	2.3(4)
B4A	-B1A	-B2A	-B11A	73.7(4)
B4A	-B1A	-B5A	-B10A	-113.8(4)
B4A	-B1A	-B3A	-B2A	139.8(3)
B3A	-B1A	-B2A	-Pt7A	36.0(3)
B4A	-B1A	-B6A	-B10A	-4.3(4)
B3A	-B1A	-B5A	-B6A	-107.8(3)
B2A	-B1A	-B5A	-B10A	-7.7(4)
B4A	-B1A	-B6A	-B11A	-71.5(4)
B4A	-B1A	-B2A	-B6A	103.2(4)
B2A	-B1A	-B3A	-B4A	-139.8(3)
B5A	-B1A	-B3A	-Pt7A	66.0(3)
B5A	-B1A	-B3A	-C8A	-2.0(4)
B5A	-B1A	-B3A	-B2A	100.7(3)
B5A	-B1A	-B3A	-B4A	-39.0(3)
B6A	-B1A	-B5A	-B10A	33.9(3)
B4A	-B1A	-B5A	-B9A	-42.6(3)
B6A	-B1A	-B2A	-B11A	-29.6(3)
B4A	-B1A	-B3A	-Pt7A	105.1(3)
B5A	-B1A	-B2A	-Pt7A	-62.6(3)
B5A	-B1A	-B2A	-B3A	-98.7(3)
B6A	-B1A	-B4A	-B5A	-30.0(3)
B6A	-B1A	-B4A	-B9A	11.3(4)
B4A	-B1A	-B2A	-B3A	-37.1(3)
B4A	-B1A	-B5A	-B6A	-147.7(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B6A	-B1A	-B2A	-B3A	-140.3(3)
B4A	-B1A	-B3A	-C8A	37.1(3)
B2A	-B1A	-B5A	-B4A	106.2(3)
B2A	-B1A	-B5A	-B6A	-41.6(3)
B2A	-B1A	-B5A	-B9A	63.6(4)
B3A	-B1A	-B2A	-B6A	140.3(3)
B4A	-B1A	-B2A	-Pt7A	-1.0(5)
B5A	-B1A	-B2A	-B6A	41.6(3)
B2A	-B1A	-B3A	-Pt7A	-34.7(2)
B2A	-B1A	-B3A	-C8A	-102.7(3)
B6A	-B1A	-B2A	-Pt7A	-104.3(3)
B3A	-B1A	-B2A	-B11A	110.7(3)
B6A	-B1A	-B5A	-B9A	105.2(3)
B5A	-B1A	-B2A	-B11A	12.1(4)
B6A	-B2A	-B11A	-O11A	119.0(4)
B6A	-B2A	-B11A	-B10A	-41.9(3)
B11A	-B2A	-B3A	-B1A	-96.9(3)
B1A	-B2A	-B11A	-O11A	149.2(3)
B3A	-B2A	-B6A	-B11A	-112.3(3)
B11A	-B2A	-B3A	-Pt7A	47.9(2)
B6A	-B2A	-B3A	-B4A	0.7(4)
B3A	-B2A	-B11A	-B10A	51.3(4)
B3A	-B2A	-B6A	-B5A	-7.6(4)
B11A	-B2A	-B3A	-C8A	0.9(4)
Pt7A	-B2A	-B6A	-B10A	3.0(4)
B6A	-B2A	-B11A	-Pt7A	-140.6(2)
B1A	-B2A	-B11A	-B6A	30.1(3)
B6A	-B2A	-B3A	-B1A	-35.1(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B3A	-B2A	-B11A	-B6A	93.2(3)
B3A	-B2A	-B11A	-O11A	-147.8(3)
B1A	-B2A	-B6A	-B11A	-146.7(3)
B3A	-B2A	-B11A	-Pt7A	-47.4(2)
B1A	-B2A	-B11A	-Pt7A	-110.4(2)
B3A	-B2A	-B6A	-B10A	-69.0(4)
B6A	-B2A	-B3A	-C8A	62.8(4)
B6A	-B2A	-B3A	-Pt7A	109.8(3)
B1A	-B2A	-B3A	-B4A	35.8(3)
B3A	-B2A	-B6A	-B1A	34.3(3)
Pt7A	-B2A	-B6A	-B5A	64.4(4)
Pt7A	-B2A	-B11A	-B6A	140.6(2)
Pt7A	-B2A	-B11A	-B10A	98.7(3)
Pt7A	-B2A	-B3A	-C8A	-47.0(2)
Pt7A	-B2A	-B3A	-B1A	-144.8(3)
B11A	-B2A	-B3A	-B4A	-61.2(4)
Pt7A	-B2A	-B6A	-B1A	106.4(3)
B1A	-B2A	-B3A	-C8A	97.8(3)
Pt7A	-B2A	-B11A	-O11A	-100.4(4)
B11A	-B2A	-B6A	-B5A	104.8(3)
B1A	-B2A	-B3A	-Pt7A	144.8(3)
B11A	-B2A	-B6A	-B10A	43.3(3)
Pt7A	-B2A	-B3A	-B4A	-109.0(3)
B11A	-B2A	-B6A	-B1A	146.7(3)
Pt7A	-B2A	-B6A	-B11A	-40.3(2)
B1A	-B2A	-B6A	-B10A	-103.4(3)
B1A	-B2A	-B11A	-B10A	-11.8(4)
B1A	-B2A	-B6A	-B5A	-41.9(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1A	-B3A	-B4A	-C8A	137.3(4)
Pt7A	-B3A	-B4A	-B1A	-104.7(3)
Pt7A	-B3A	-B4A	-C8A	32.7(3)
C8A	-B3A	-B4A	-B9A	-34.1(3)
B1A	-B3A	-B4A	-B9A	103.2(4)
C8A	-B3A	-B4A	-B5A	-95.2(4)
B2A	-B3A	-B4A	-B5A	6.8(4)
C8A	-B3A	-B4A	-B1A	-137.3(4)
B2A	-B3A	-B4A	-B1A	-35.3(3)
B1A	-B3A	-B4A	-B5A	42.1(3)
B2A	-B3A	-B4A	-C8A	102.0(3)
Pt7A	-B3A	-B4A	-B5A	-62.5(4)
Pt7A	-B3A	-B4A	-B9A	-1.4(4)
B2A	-B3A	-B4A	-B9A	67.9(4)
C8A	-B4A	-B5A	-B10A	-5.3(5)
B3A	-B4A	-B9A	-C8A	35.6(3)
B1A	-B4A	-B5A	-B10A	95.4(4)
B1A	-B4A	-B5A	-B6A	29.0(3)
B1A	-B4A	-B9A	-B5A	-43.0(3)
B1A	-B4A	-B9A	-B10A	-13.3(4)
B3A	-B4A	-B5A	-B10A	54.5(5)
C8A	-B4A	-B5A	-B9A	32.1(3)
C8A	-B4A	-B5A	-B1A	-100.6(3)
B9A	-B4A	-B5A	-B1A	-132.7(3)
C8A	-B4A	-B9A	-B10A	-110.8(3)
B1A	-B4A	-B5A	-B9A	132.7(3)
B3A	-B4A	-B5A	-B1A	-40.9(3)
B3A	-B4A	-B5A	-B9A	91.8(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C8A	-B4A	-B5A	-B6A	-71.7(4)
B1A	-B4A	-B9A	-C8A	97.5(3)
B5A	-B4A	-B9A	-B10A	29.7(3)
C8A	-B4A	-B9A	-B5A	-140.5(3)
B3A	-B4A	-B9A	-B5A	-104.9(3)
B3A	-B4A	-B9A	-B10A	-75.2(4)
B3A	-B4A	-B5A	-B6A	-11.9(5)
B5A	-B4A	-B9A	-C8A	140.5(3)
B9A	-B4A	-B5A	-B10A	-37.4(4)
B9A	-B4A	-B5A	-B6A	-103.8(3)
B10A	-B5A	-B6A	-B11A	-35.6(4)
B10A	-B5A	-B6A	-B1A	-142.5(3)
B9A	-B5A	-B6A	-B11A	10.6(5)
B10A	-B5A	-B6A	-B2A	-101.1(3)
B1A	-B5A	-B10A	-B9A	100.0(4)
B10A	-B5A	-B9A	-C8A	110.7(4)
B4A	-B5A	-B10A	-B6A	-97.7(4)
B9A	-B5A	-B6A	-B2A	-54.9(5)
B4A	-B5A	-B6A	-B2A	12.2(4)
B9A	-B5A	-B6A	-B10A	46.2(4)
B6A	-B5A	-B9A	-C8A	68.1(5)
B4A	-B5A	-B6A	-B11A	77.7(5)
B1A	-B5A	-B9A	-B10A	-104.3(3)
B1A	-B5A	-B10A	-B11A	0.5(5)
B6A	-B5A	-B9A	-B4A	102.6(4)
B10A	-B5A	-B9A	-B4A	145.2(3)
B1A	-B5A	-B10A	-B6A	-33.2(3)
B1A	-B5A	-B9A	-C8A	6.4(4)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1A	-B5A	-B9A	-B4A	40.9(3)
B4A	-B5A	-B6A	-B10A	113.3(4)
B6A	-B5A	-B10A	-B9A	133.2(3)
B9A	-B5A	-B6A	-B1A	-96.3(4)
B1A	-B5A	-B6A	-B11A	106.9(4)
B4A	-B5A	-B6A	-B1A	-29.2(3)
B6A	-B5A	-B9A	-B10A	-42.6(4)
B4A	-B5A	-B10A	-B9A	35.5(4)
B4A	-B5A	-B10A	-B11A	-64.0(5)
B4A	-B5A	-B9A	-B10A	-145.2(3)
B6A	-B5A	-B10A	-B11A	33.7(3)
B4A	-B5A	-B9A	-C8A	-34.5(3)
B1A	-B5A	-B6A	-B2A	41.4(3)
B1A	-B5A	-B6A	-B10A	142.5(3)
B9A	-B5A	-B10A	-B6A	-133.2(3)
B9A	-B5A	-B10A	-B11A	-99.5(4)
B10A	-B6A	-B11A	-B2A	-132.1(3)
B11A	-B6A	-B10A	-B9A	103.2(3)
B5A	-B6A	-B11A	-B10A	34.3(3)
B11A	-B6A	-B10A	-B5A	141.7(4)
B5A	-B6A	-B11A	-B2A	-97.8(4)
B5A	-B6A	-B10A	-B9A	-38.5(3)
B2A	-B6A	-B10A	-B9A	59.8(4)
B5A	-B6A	-B11A	-Pt7A	-59.0(4)
B5A	-B6A	-B10A	-B11A	-141.7(4)
B1A	-B6A	-B11A	-B2A	-31.4(3)
B10A	-B6A	-B11A	-O11A	111.5(5)
B2A	-B6A	-B10A	-B11A	-43.4(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B2A	-B6A	-B10A	-B5A	98.3(4)
B1A	-B6A	-B10A	-B11A	-107.2(3)
B1A	-B6A	-B11A	-Pt7A	7.4(4)
B1A	-B6A	-B11A	-O11A	-147.8(4)
B5A	-B6A	-B11A	-O11A	145.8(4)
B2A	-B6A	-B11A	-B10A	132.1(3)
B2A	-B6A	-B11A	-O11A	-116.4(4)
B10A	-B6A	-B11A	-Pt7A	-93.3(3)
B1A	-B6A	-B11A	-B10A	100.7(3)
B1A	-B6A	-B10A	-B9A	-4.0(4)
B1A	-B6A	-B10A	-B5A	34.5(3)
B2A	-B6A	-B11A	-Pt7A	38.8(2)
B4A	-B9A	-B10A	-B11A	70.6(4)
B4A	-B9A	-B10A	-B6A	10.6(4)
B4A	-B9A	-B10A	-B5A	-30.5(3)
C8A	-B9A	-B10A	-B11A	8.1(5)
B5A	-B9A	-B10A	-B6A	41.1(3)
C8A	-B9A	-B10A	-B5A	-93.1(4)
C8A	-B9A	-B10A	-B6A	-52.0(5)
B5A	-B9A	-B10A	-B11A	101.1(4)
B9A	-B10A	-B11A	-B2A	-52.8(4)
B6A	-B10A	-B11A	-B2A	41.9(3)
B9A	-B10A	-B11A	-B6A	-94.6(4)
B5A	-B10A	-B11A	-Pt7A	74.1(4)
B9A	-B10A	-B11A	-O11A	145.4(4)
B5A	-B10A	-B11A	-B6A	-35.1(3)
B9A	-B10A	-B11A	-Pt7A	14.6(4)
B6A	-B10A	-B11A	-O11A	-120.0(4)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B6A	-B10A	-B11A	-Pt7A	109.2(3)
B5A	-B10A	-B11A	-B2A	6.8(4)
B5A	-B10A	-B11A	-O11A	-155.1(4)
B5B	-B1B	-B2B	-B3B	-103.2(3)
B6B	-B1B	-B2B	-Pt7B	-34.6(2)
B4B	-B1B	-B2B	-B3B	-40.8(3)
B4B	-B1B	-B2B	-B6B	99.1(3)
B6B	-B1B	-B2B	-B3B	-139.9(3)
B6B	-B1B	-B2B	-B8B	-109.2(3)
B5B	-B1B	-B2B	-B8B	-72.6(3)
B4B	-B1B	-B3B	-B8B	101.1(3)
B4B	-B1B	-B3B	-B9B	34.1(3)
B5B	-B1B	-B3B	-B2B	103.9(3)
B5B	-B1B	-B3B	-B4B	-30.0(3)
B4B	-B1B	-B2B	-B8B	-10.1(4)
B5B	-B1B	-B2B	-B6B	36.7(3)
B3B	-B1B	-B2B	-Pt7B	105.3(3)
B6B	-B1B	-B5B	-C11B	36.7(3)
B5B	-B1B	-B3B	-B9B	4.1(4)
B6B	-B1B	-B3B	-B2B	38.5(3)
B6B	-B1B	-B3B	-B4B	-95.4(3)
B5B	-B1B	-B3B	-B8B	71.2(4)
B4B	-B1B	-B5B	-B6B	-134.0(3)
B4B	-B1B	-B5B	-B10B	-40.7(3)
B3B	-B1B	-B6B	-B2B	-37.1(3)
B3B	-B1B	-B6B	-B5B	103.4(3)
B3B	-B1B	-B2B	-B6B	139.9(3)
B3B	-B1B	-B2B	-B8B	30.7(2)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B4B	-B1B	-B2B	-Pt7B	64.6(3)
B4B	-B1B	-B6B	-B5B	39.6(3)
B5B	-B1B	-B6B	-Pt7B	-106.7(3)
B5B	-B1B	-B6B	-C11B	-37.6(3)
B5B	-B1B	-B6B	-B2B	-140.5(3)
B5B	-B1B	-B2B	-Pt7B	2.1(4)
B6B	-B1B	-B4B	-B5B	-40.3(3)
B6B	-B1B	-B4B	-B9B	72.1(4)
B6B	-B1B	-B4B	-B10B	1.2(4)
B2B	-B1B	-B3B	-B4B	-133.9(3)
B2B	-B1B	-B3B	-B8B	-32.8(3)
B2B	-B1B	-B3B	-B9B	-99.8(3)
B4B	-B1B	-B3B	-B2B	133.9(3)
B3B	-B1B	-B5B	-C11B	-66.9(4)
B3B	-B1B	-B5B	-B4B	30.5(3)
B3B	-B1B	-B5B	-B6B	-103.6(3)
B3B	-B1B	-B5B	-B10B	-10.2(4)
B4B	-B1B	-B5B	-C11B	-97.4(3)
B5B	-B1B	-B4B	-B3B	147.2(3)
B5B	-B1B	-B4B	-B9B	112.4(4)
B5B	-B1B	-B4B	-B10B	41.5(3)
B6B	-B1B	-B5B	-B4B	134.0(3)
B6B	-B1B	-B5B	-B10B	93.4(3)
B2B	-B1B	-B6B	-Pt7B	33.8(2)
B2B	-B1B	-B6B	-C11B	102.8(3)
B2B	-B1B	-B6B	-B5B	140.5(3)
B3B	-B1B	-B6B	-Pt7B	-3.3(4)
B6B	-B1B	-B3B	-B8B	5.7(4)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B6B	-B1B	-B3B	-B9B	-61.4(4)
B4B	-B1B	-B6B	-Pt7B	-67.1(3)
B4B	-B1B	-B6B	-C11B	2.0(4)
B4B	-B1B	-B6B	-B2B	-100.8(3)
B3B	-B1B	-B4B	-B10B	-105.7(3)
B2B	-B1B	-B4B	-B9B	5.8(4)
B2B	-B1B	-B4B	-B10B	-65.1(3)
B3B	-B1B	-B4B	-B5B	-147.2(3)
B6B	-B1B	-B4B	-B3B	107.0(3)
B2B	-B1B	-B5B	-B6B	-38.0(3)
B2B	-B1B	-B5B	-B10B	55.4(4)
B2B	-B1B	-B4B	-B3B	40.7(3)
B2B	-B1B	-B4B	-B5B	-106.6(3)
B3B	-B1B	-B4B	-B9B	-34.9(3)
B2B	-B1B	-B5B	-C11B	-1.3(4)
B2B	-B1B	-B5B	-B4B	96.0(3)
B3B	-B1B	-B6B	-C11B	65.7(4)
B3B	-B2B	-B6B	-Pt7B	-110.6(2)
B1B	-B2B	-B6B	-C11B	-97.2(3)
B1B	-B2B	-B6B	-B5B	-35.0(3)
B1B	-B2B	-B6B	-Pt7B	-146.1(2)
Pt7B	-B2B	-B3B	-B4B	-65.3(3)
Pt7B	-B2B	-B3B	-B8B	39.4(2)
Pt7B	-B2B	-B3B	-B1B	-106.2(3)
B1B	-B2B	-B8B	-Pt7B	110.6(2)
Pt7B	-B2B	-B3B	-B9B	-3.6(3)
B1B	-B2B	-B3B	-B4B	40.9(3)

B1B -B2B -B3B -B8B 145.6(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1B	-B2B	-B3B	-B9B	102.6(3)
B6B	-B2B	-B3B	-B1B	-34.8(2)
Pt7B	-B2B	-B6B	-B5B	111.1(2)
B6B	-B2B	-B8B	-B9B	-52.8(3)
B6B	-B2B	-B8B	-B3B	-94.3(3)
B8B	-B2B	-B6B	-C11B	0.6(4)
B8B	-B2B	-B6B	-B1B	97.8(3)
B8B	-B2B	-B6B	-B5B	62.8(4)
Pt7B	-B2B	-B8B	-O8B	99.0(3)
Pt7B	-B2B	-B8B	-B3B	-141.8(2)
Pt7B	-B2B	-B8B	-B9B	-100.3(2)
Pt7B	-B2B	-B6B	-B1B	146.1(2)
Pt7B	-B2B	-B6B	-C11B	48.9(2)
B1B	-B2B	-B8B	-O8B	-150.4(3)
B1B	-B2B	-B8B	-B3B	-31.2(3)
B1B	-B2B	-B8B	-B9B	10.3(3)
B3B	-B2B	-B8B	-Pt7B	141.8(2)
B3B	-B2B	-B8B	-O8B	-119.2(4)
B3B	-B2B	-B6B	-C11B	-61.7(3)
B3B	-B2B	-B6B	-B1B	35.5(3)
B3B	-B2B	-B6B	-B5B	0.5(4)
B8B	-B2B	-B6B	-Pt7B	-48.3(2)
B6B	-B2B	-B8B	-O8B	146.4(3)
B6B	-B2B	-B3B	-B9B	67.8(3)
B8B	-B2B	-B3B	-B1B	-145.6(3)
B8B	-B2B	-B3B	-B4B	-104.7(3)
B8B	-B2B	-B3B	-B9B	-43.0(3)

B6B -B2B -B3B -B4B 6.1(4)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B6B	-B2B	-B3B	-B8B	110.8(3)
B6B	-B2B	-B8B	-Pt7B	47.4(2)
B3B	-B2B	-B8B	-B9B	41.5(2)
B1B	-B3B	-B8B	-Pt7B	-5.7(4)
B1B	-B3B	-B8B	-O8B	147.9(4)
B9B	-B3B	-B4B	-B10B	-45.4(3)
B8B	-B3B	-B4B	-B10B	-9.5(4)
B9B	-B3B	-B4B	-B1B	-141.8(3)
B2B	-B3B	-B8B	-B9B	-132.6(3)
B1B	-B3B	-B4B	-B10B	96.4(3)
B4B	-B3B	-B8B	-Pt7B	60.2(3)
B4B	-B3B	-B8B	-O8B	-146.3(4)
B4B	-B3B	-B8B	-B2B	98.1(3)
B4B	-B3B	-B8B	-B9B	-34.6(3)
B9B	-B3B	-B8B	-Pt7B	94.8(2)
B9B	-B3B	-B4B	-B5B	-112.1(4)
B8B	-B3B	-B4B	-B9B	35.9(3)
B8B	-B3B	-B9B	-B4B	-141.5(3)
B9B	-B3B	-B8B	-O8B	-111.7(4)
B9B	-B3B	-B8B	-B2B	132.6(3)
B1B	-B3B	-B9B	-B4B	-34.9(3)
B1B	-B3B	-B8B	-B2B	32.2(3)
B8B	-B3B	-B4B	-B5B	-76.2(4)
B1B	-B3B	-B4B	-B9B	141.8(3)
B2B	-B3B	-B8B	-O8B	115.7(4)
B2B	-B3B	-B9B	-B4B	-98.7(3)
B2B	-B3B	-B4B	-B1B	-40.7(3)
B2B	-B3B	-B4B	-B5B	-11.0(4)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B2B	-B3B	-B4B	-B9B	101.1(3)
B2B	-B3B	-B4B	-B10B	55.7(4)
B8B	-B3B	-B4B	-B1B	-105.9(3)
B8B	-B3B	-B9B	-B10B	-103.4(3)
B1B	-B3B	-B4B	-B5B	29.7(3)
B1B	-B3B	-B9B	-B10B	3.2(3)
B1B	-B3B	-B8B	-B9B	-100.4(3)
B2B	-B3B	-B8B	-Pt7B	-37.9(2)
B1B	-B3B	-B9B	-B8B	106.6(3)
B2B	-B3B	-B9B	-B8B	42.8(3)
B2B	-B3B	-B9B	-B10B	-60.6(3)
B4B	-B3B	-B9B	-B10B	38.1(3)
B4B	-B3B	-B9B	-B8B	141.5(3)
B3B	-B4B	-B5B	-B1B	-29.7(3)
B3B	-B4B	-B5B	-B6B	11.4(4)
B3B	-B4B	-B5B	-C11B	70.7(4)
B10B	-B4B	-B5B	-C11B	-33.4(3)
B10B	-B4B	-B5B	-B1B	-133.7(3)
B1B	-B4B	-B5B	-B10B	133.7(3)
B3B	-B4B	-B9B	-B8B	-33.6(3)
B1B	-B4B	-B5B	-B6B	41.1(3)
B3B	-B4B	-B9B	-B10B	-134.0(3)
B5B	-B4B	-B9B	-B3B	98.7(3)
B5B	-B4B	-B9B	-B8B	65.0(4)
B5B	-B4B	-B9B	-B10B	-35.3(3)
B10B	-B4B	-B9B	-B3B	134.0(3)
B10B	-B4B	-B9B	-B8B	100.4(3)
B9B	-B4B	-B5B	-B10B	37.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B9B	-B4B	-B5B	-C11B	3.8(4)
B9B	-B4B	-B5B	-B1B	-96.5(4)
B10B	-B4B	-B5B	-B6B	-92.7(3)
B1B	-B4B	-B9B	-B3B	34.2(3)
B1B	-B4B	-B9B	-B8B	0.5(4)
B1B	-B4B	-B9B	-B10B	-99.8(3)
B9B	-B4B	-B10B	-B5B	-144.8(3)
B9B	-B4B	-B10B	-C11B	-108.8(3)
B1B	-B4B	-B5B	-C11B	100.3(3)
B3B	-B4B	-B10B	-C11B	-66.4(4)
B9B	-B4B	-B5B	-B6B	-55.4(4)
B3B	-B4B	-B10B	-B5B	-102.5(3)
B3B	-B4B	-B10B	-B9B	42.3(3)
B5B	-B4B	-B10B	-C11B	36.0(3)
B3B	-B4B	-B5B	-B10B	104.1(3)
B1B	-B4B	-B10B	-B9B	104.7(3)
B1B	-B4B	-B10B	-C11B	-4.1(4)
B1B	-B4B	-B10B	-B5B	-40.1(3)
B5B	-B4B	-B10B	-B9B	144.8(3)
B4B	-B5B	-B6B	-Pt7B	62.7(3)
B4B	-B5B	-B6B	-C11B	94.8(3)
B1B	-B5B	-B6B	-B2B	34.7(3)
C11B	-B5B	-B6B	-B1B	-136.6(3)
B1B	-B5B	-B6B	-Pt7B	104.6(3)
B1B	-B5B	-B6B	-C11B	136.6(3)
B1B	-B5B	-B10B	-B4B	41.9(3)
B1B	-B5B	-B10B	-B9B	11.8(4)
B4B	-B5B	-B10B	-C11B	-138.8(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B4B	-B5B	-B10B	-B9B	-30.1(3)
B6B	-B5B	-B10B	-C11B	-34.6(3)
C11B	-B5B	-B6B	-B2B	-102.0(3)
C11B	-B5B	-B6B	-Pt7B	-32.1(2)
B10B	-B5B	-B6B	-Pt7B	1.3(3)
B10B	-B5B	-B6B	-B1B	-103.3(3)
B10B	-B5B	-B6B	-B2B	-68.6(3)
C11B	-B5B	-B10B	-B4B	138.8(3)
C11B	-B5B	-B10B	-B9B	108.6(3)
B1B	-B5B	-B10B	-C11B	-96.9(3)
B4B	-B5B	-B6B	-B1B	-41.8(3)
B4B	-B5B	-B6B	-B2B	-7.2(4)
B6B	-B5B	-B10B	-B9B	74.1(3)
B10B	-B5B	-B6B	-C11B	33.3(3)
B6B	-B5B	-B10B	-B4B	104.2(3)
O8B	-B8B	-B9B	-B4B	155.0(3)
O8B	-B8B	-B9B	-B10B	-145.2(3)
O8B	-B8B	-B9B	-B3B	120.1(4)
B3B	-B8B	-B9B	-B10B	94.8(3)
Pt7B	-B8B	-B9B	-B4B	-74.3(3)
Pt7B	-B8B	-B9B	-B3B	-109.1(2)
Pt7B	-B8B	-B9B	-B10B	-14.4(3)
B3B	-B8B	-B9B	-B4B	34.9(3)
B2B	-B8B	-B9B	-B3B	-41.4(2)
B2B	-B8B	-B9B	-B10B	53.3(3)
B2B	-B8B	-B9B	-B4B	-6.6(4)
B4B	-B9B	-B10B	-B5B	31.0(3)

B3B -B9B -B10B -B5B -9.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B4B	-B9B	-B10B	-C11B	94.0(4)
B3B	-B9B	-B10B	-B4B	-40.2(3)
B8B	-B9B	-B10B	-C11B	-6.3(4)
B3B	-B9B	-B10B	-C11B	53.8(4)
B8B	-B9B	-B10B	-B5B	-69.2(3)
B8B	-B9B	-B10B	-B4B	-100.2(3)

Table S8 - Contact Distances(Angstrom)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

Pt7A	.H136	3.0900	C8A	.B1A	2.723(5)
Pt7B	.H332	3.0000	C8A	.C22	3.245(5)
P1	.O11A	3.108(3)	C8A	.P2	3.118(4)
P1	.C231	3.636(3)	C8A	.B10A	3.011(7)
P1	.B2A	3.352(4)	C8A	.B2A	2.860(5)
P1	.B11A	3.242(4)	C8A	.B6A	3.376(5)
P1	.P2	3.4378(15)	C8A	.B11A	3.239(6)
P2	.P1	3.4378(15)	C11	.O11A	3.226(5)
P2	.C131	3.688(4)	C11B	.B9B	2.981(6)
P2	.C8A	3.118(4)	C11B	.B8B	3.198(5)
P3	.O8B	3.139(3)	C11B	.P4	3.110(4)
P3	.P4	3.4495(15)	C11B	.B3B	3.364(5)
P3	.B8B	3.280(4)	C11B	.B1B	2.721(5)
P3	.C431	3.632(3)	C11B	.B2B	2.860(5)
P3	.B2B	3.344(4)	C11B	.C41	3.306(6)
P4	.C11B	3.110(4)	C12	.C32_a	3.388(5)
P4	.P3	3.4495(15)	C12	.C232	3.482(5)
P2	.H8A	2.91(4)	C12	.C231	3.420(5)
P4	.H11B	2.88(3)	C12	.O11A	3.231(5)
O8B	.C31	3.226(5)	C21	.C136	3.591(5)
O8B	.C32	3.310(4)	C31	.O8B	3.226(5)
O11A	.C11	3.226(5)	C32	.C431	3.457(5)
O11A	.C12	3.231(5)	C32	.O8B	3.310(4)
O8B	.H32B	2.6500	C32	.C12_n	3.388(5)
O8B	.H17C_m	2.7600	C32	.C436	3.501(5)
O8B	.H31A	2.5600	C8A	.H24C	2.8200
O11A	.H12F	2.5600	C8A	.H101	2.71(4)
O11A	.H11I	2.5700	C8A	.H3A	2.4400

Table S8 - Contact Distances(Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C8B	.H17B_b	3.0600	C132	.H236	2.9300
C8B	.H32B	3.0300	C232	.C12	3.482(5)
C11	.H2A	2.7200	C134	.H31B_b	3.0600
C11A	.H12F	2.9700	C234	.C334_e	3.406(5)
C11A	.H10A	3.05(4)	C135	.H20C	3.0800
C11B	.H41B	2.7700	C235	.C333_e	3.559(5)
C11B	.H6B	2.4400	C235	.C334_e	3.494(5)
C11B	.H89	2.67(3)	C236	.C132	3.254(5)
C12	.H32B_a	3.0100	C136	.H20C	2.8300
C12	.H132	2.6900	C236	.C131	3.560(5)
C21	.H236	2.7700	C231	.H12D	2.6200
C22	.H232	2.8400	C331	.C432	3.362(5)
C22	.H8A	2.81(4)	C232	.H1A_d	3.0400
C31	.H2B	2.77(4)	C232	.H24B	2.9800
C131	.C236	3.560(5)	C232	.H12D	2.6700
C32	.H336	2.7200	C333	.C235_o	3.559(5)
C132	.C236	3.254(5)	C233	.H4A_d	3.0000
C32	.H12F_n	3.0200	C233	.H12D	2.8700
C134	.C435_c	3.431(7)	C334	.C235_o	3.494(5)
C136	.C21	3.591(5)	C334	.C234_o	3.406(5)
C41	.H436	2.7600	C234	.H12D	2.9800
C41	.H11B	2.96(3)	C234	.H30B_a	2.9700
C42	.H11B	3.06(3)	C235	.H12D	2.9600
C42	.H432	2.7600	C235	.H30B_a	2.9600
C231	.C12	3.420(5)	C235	.H334_e	3.0900
C132	.H12D	3.0800	C235	.H4B_f	3.0300
C132	.H12E	3.0100	C336	.C433	3.568(6)
C132	.H10B	3.05(4)	C236	.H20C	3.0100

Table S8 - Contact Distances(Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C236	.H12D	2.8000	B2A	.P1	3.352(4)
C336	.C432	3.239(5)	B2A	.C11	3.381(6)
C431	.C32	3.457(5)	B2A	.B4A	2.921(6)
C331	.H432	3.0400	B2A	.B9A	3.310(6)
C432	.C336	3.239(5)	B2A	.B10A	2.879(7)
C332	.H17A	2.8800	B2B	.P3	3.344(4)
C432	.C331	3.362(5)	B2B	.O8B	2.870(5)
C433	.C336	3.568(6)	B2B	.B10B	3.334(6)
C334	.H11G_p	3.0500	B2B	.C11B	2.860(5)
C335	.H9A_q	2.76(4)	B2B	.C31	3.379(6)
C435	.C134_s	3.431(7)	B2B	.B5B	2.926(6)
C336	.H432	2.9700	B2B	.B9B	2.887(6)
C436	.C32	3.501(5)	B3A	.B6A	2.929(6)
C336	.H32C	3.0000	B3A	.B11A	3.146(6)
C336	.H9A_q	2.92(4)	B3A	.B9A	2.741(7)
C431	.H32A	2.6600	B6B	.B10B	2.752(6)
C432	.H32A	2.9800	B6B	.B3B	2.931(6)
C432	.H17A	3.0200	B6B	.B8B	3.120(6)
C433	.H5A_r	2.8800	B8B	.P3	3.280(4)
C434	.H11E_n	2.8200	B8B	.B1B	2.933(6)
C435	.H134_s	2.9200	B8B	.C11B	3.198(5)
C435	.H32A	2.9200	B8B	.B10B	3.061(6)
C436	.H32A	2.6300	B8B	.B6B	3.120(6)
C436	.H41C	2.9200	B11A	.B3A	3.146(6)
C436	.H1B_b	3.0600	B11A	.P1	3.242(4)
C436	.H5B_b	3.0700	B11A	.B9A	3.052(6)
B2A	.O11A	2.871(5)	B11A	.B1A	2.937(6)
B2A	.C8A	2.860(5)	B11A	.C8A	3.239(6)

Table S8 - Contact Distances(Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

B1B	.H436_a	2.9800	H4B	.H11H	2.5500
B2A	.H101	2.85(4)	H5A	.C433_i	2.8800
B2A	.H3A	2.6300	H5A	.H433_i	2.2800
B2B	.H6B	2.6400	H5B	.H436_a	2.4700
B2B	.H89	2.85(3)	H5B	.C436_a	3.0700
B3A	.H8A	2.31(4)	H5B	.H12E	2.3900
B3A	.H2A	2.6000	H6A	.H11D_j	2.4800
B5B	.H436_a	2.9900	H6B	.H41C_a	2.3800
B6B	.H11B	2.25(3)	H8A	.H11F_g	2.4800
B6B	.H2B	2.62(4)	H8A	.H24C	2.1800
B8B	.H2B	2.51(4)	H8A	.C22	2.81(4)
B9B	.H30C	2.9400	H9A	.C335_h	2.76(4)
B10A	.H11F	2.8600	H9A	.C336_h	2.92(4)
B11A	.H2A	2.5300	H9A	.H335_h	2.5200
H1A	.C232_g	3.0400	H10A	.C11A	3.05(4)
H1A	.H232_g	2.4500	H10B	.C132	3.05(4)
H1B	.C436_a	3.0600	H11B	.C41	2.96(3)
H1B	.H436_a	2.4000	H11B	.C42	3.06(3)
H2A	.H11G	2.2100	H11B	.H41B	2.3100
H2A	.C11	2.7200	H11B	.H17B	2.4500
H2B	.C31	2.77(4)	H11D	.H6A_j	2.4800
H2B	.H31B	2.2700	H11E	.H434_a	2.5500
H2B	.H41A_m	2.6000	H11E	.C434_a	2.8200
H4A	.H32C_h	2.5900	H11F	.B10A	2.8600
H4A	.C233_g	3.0000	H11F	.H101	2.4100
H4A	.H233_g	2.4400	H11F	.H8A_d	2.4800
H4B	.H235_k	2.3300	H11G	.C334_b	3.0500
H4B	.C235_k	3.0300	H11G	.H334_b	2.4600

Table S8 - Contact Distances(Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

H11G	.H2A	2.2100	H20C	.C136	2.8300
H11H	.H4B	2.5500	H20C	.H236	2.3700
H11I	.O11A	2.5700	H20C	.C236	3.0100
H11I	.H20A_k	2.4300	H24B	.C232	2.9800
H12D	.C235	2.9600	H24B	.H232	2.3800
H12D	.C233	2.8700	H24C	.C8A	2.8200
H12D	.C234	2.9800	H24C	.H8A	2.1800
H12D	.C132	3.0800	H30A	.H17B_b	2.5900
H12D	.C231	2.6200	H30A	.H30A_t	2.5300
H12D	.C232	2.6700	H30B	.C235_n	2.9600
H12D	.C236	2.8000	H30B	.C234_n	2.9700
H12D	.H132	2.5500	H30C	.H89	2.4400
H12E	.H5B	2.3900	H30C	.B9B	2.9400
H12E	.C132	3.0100	H31A	.H17C_m	2.5900
H12E	.H132	2.3900	H31A	.O8B	2.5600
H12F	.O11A	2.5600	H31B	.H134_p	2.4600
H12F	.C11A	2.9700	H31B	.H2B	2.2700
H12F	.C32_a	3.0200	H31B	.C134_p	3.0600
H17A	.C332	2.8800	H31C	.H32C	2.5700
H17A	.H432	2.3800	H32A	.C432	2.9800
H17A	.C432	3.0200	H32A	.C431	2.6600
H17B	.H11B	2.4500	H32A	.C435	2.9200
H17B	.C8B_a	3.0600	H32A	.C436	2.6300
H17B	.H30A_a	2.5900	H32B	.C8B	3.0300
H17C	.O8B_f	2.7600	H32B	.O8B	2.6500
H17C	.H31A_f	2.5900	H32B	.C12_n	3.0100
H20A	.H11I_l	2.4300	H32C	.H4A_q	2.5900
H20C	.C135	3.0800	H32C	.C336	3.0000

Table S8 - Contact Distances(Angstrom) (continued)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

H32C	.H31C	2.5700	H235	.H4B_f	2.3300
H32C	.H336	2.3500	H236	.C132	2.9300
H41A	.H2B_f	2.6000	H236	.H20C	2.3700
H41B	.H133	2.5600	H236	.C21	2.7700
H41B	.C11B	2.7700	H332	.Pt7B	3.0000
H41B	.H11B	2.3100	H334	.H11G_p	2.4600
H41C	.C436	2.9200	H334	.C235_o	3.0900
H41C	.H436	2.2800	H335	.H9A_q	2.5200
H41C	.H6B_b	2.3800	H336	.C32	2.7200
H89	.H30C	2.4400	H336	.H32C	2.3500
H101	.H11F	2.4100	H432	.C42	2.7600
H132	.H12E	2.3900	H432	.C331	3.0400
H132	.C12	2.6900	H432	.C336	2.9700
H132	.H12D	2.5500	H432	.H17A	2.3800
H133	.H41B	2.5600	H433	.H5A_r	2.2800
H134	.H31B_b	2.4600	H434	.H11E_n	2.5500
H134	.C435_c	2.9200	H436	.C41	2.7600
H136	.Pt7A	3.0900	H436	.H41C	2.2800
H232	.C22	2.8400	H436	.B1B_b	2.9800
H232	.H1A_d	2.4500	H436	.B5B_b	2.9900
H232	.H24B	2.3800	H436	.H1B_b	2.4000
H233	.H4A_d	2.4400	H436	.H5B_b	2.4700

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for [9-(OMe)-8,8-(PMe2Ph)2-NIDO-8,7-PtCB9H11] (2)

C11	--	H11G	..	H2A	0.9800	2.2100	2.7200	111.00	.
C11	--	H11I	..	O11A	0.9800	2.5700	3.226(5)	124.00	.
C12	--	H12F	..	O11A	0.9800	2.5600	3.231(5)	126.00	.
C31	--	H31A	..	O8B	0.9800	2.5600	3.226(5)	125.00	.
C31	--	H31B	..	H2B	0.9800	2.2700	2.77(4)	111.00	.
C433	--	H433	..	H5A	0.9500	2.2800	2.8800	120.00	4_556

Translation of Symmetry Code to Equiv.Pos

a =[2556.00] = 1/2-x,1/2+y,1-z
b =[2546.00] = 1/2-x,-1/2+y,1-z
c =[3656.00] = 1-x,-y,1-z
d =[2555.00] = 1/2-x,1/2+y,-z
e =[3666.00] = 1-x,1-y,1-z
f =[4555.00] = 1/2+x,1/2-y,z
g =[2545.00] = 1/2-x,-1/2+y,-z
h =[1554.00] = x,y,-1+z
i =[4454.00] = -1/2+x,1/2-y,-1+z
j =[3565.00] = -x,1-y,-z
k =[4455.00] = -1/2+x,1/2-y,z
l =[4555.00] = 1/2+x,1/2-y,z
m =[4455.00] = -1/2+x,1/2-y,z
n =[2546.00] = 1/2-x,-1/2+y,1-z
o =[3666.00] = 1-x,1-y,1-z
p =[2556.00] = 1/2-x,1/2+y,1-z
q =[1556.00] = x,y,1+z
r =[4556.00] = 1/2+x,1/2-y,1+z
s =[3656.00] = 1-x,-y,1-z
t =[3556.00] = -x,-y,1-z

Table 18 Selected interatomic distances (Å) for [8,8-(PPh_3)-*nido*-8,7-$RhSB_9H_{10}$] (**4**), with estimated standard uncertainties (s.u) in parentheses; and the corresponding calculated for the model compound [8,8-(PH_3)-*nido*-8,7-$RhSB_9H_{10}$] (**4a**)

(a) From the metal atom

	Compound **4**	Compound **4a**
P(1)-Rh(8)	2.2906(5)	2.291
P(2)-Rh(8)	2.4197(5)	2.403
B(3)-Rh(8)	2.242(4)	2.294
B(4)-Rh(8)	2.236(3)	2.244
B(9)-Rh(8)	2.146(3)	2.226
S(7)-Rh(8)	2.3769(6)	2.430

(b) Heteroatom-boron

	Compound **4**	Compound **4a**
S(7)-B(2)	1.986(4)	2.004
S (7)-B(3)	2.035(4)	2.071
S (7)-B(11)	1.908(4)	1.936

(c) Boron-boron

	Compound **4**	Compound **4a**
B(2)-B(3)(longest)	1.887(5)	1.874
B(6)-B(11)(shortest)	1.713(6)	1.719
B(9)-B(10)	1.863(7)	1.828

Table S19 Calculated coordinates (DFT; B3LYP / 6-31G*, LANL2DZ) for [isonido-$(PH_3)_2HRhSB_9H_9$] (compound **4b**).

Rh	-0.600953	0.006326	0.253231
B	1.564117	1.302350	-1.026824
B	1.216561	1.409606	0.821672
B	0.546023	0.286545	2.039341
S	0.580530	-0.099088	-1.874579
P	-2.186431	-1.758533	-0.062135
P	-2.011345	1.863365	-0.152477
B	1.096106	-1.245248	1.241448
B	1.198075	-1.483008	-0.583621
B	2.205092	0.095249	1.651201
B	2.512418	-0.289781	-1.251153
B	2.746801	0.788416	0.102358
H	-3.159644	-1.768303	-1.093354
H	1.649196	2.296367	-1.671497
H	-3.064551	-2.039947	1.007951
H	-1.695207	-3.067536	-0.258925
H	1.075309	2.557782	1.124562
H	-2.045624	2.852862	0.852614
H	-1.717469	2.706094	-1.248896
H	-0.964815	0.085112	1.829980
H	0.314815	0.558215	3.177725
H	-3.408516	1.760780	-0.364073
B	2.610883	-1.015473	0.320924
H	3.224979	-0.513180	-2.171311
H	3.728285	1.459231	0.178977
H	0.986271	-2.565639	-1.025600
H	2.933834	0.203007	2.586018
H	0.873397	-2.262734	1.823672
H	3.510394	-1.777122	0.492459

Table S20 - Calculated coordinates (DFT; B3LYP / 6-31G*, LANL2DZ) for [nido-$(PH_3)_2HRhSB_9H_9$] (compound **4a**).

Rh	0.781332	-0.009079	-0.192080
B	-2.361683	-1.323040	0.710801
B	-1.964487	0.117768	1.860122
B	-0.464816	1.023003	1.336088
S	-0.980592	-1.629778	-0.610115
P	2.347328	-1.703281	0.480944
P	2.233964	1.762148	-0.136120
B	-0.771896	1.600787	-0.369018
B	-1.082874	0.234130	-1.506236
B	-2.054313	1.597592	0.854421

B	-2.667126	-0.607265	-0.964423
B	-3.126376	0.206386	0.534611
H	3.306787	-2.234234	-0.417500
H	-2.857348	-2.330840	1.096091
H	3.240586	-1.450977	1.548904
H	1.842876	-2.938049	0.948596
H	-2.316406	0.095161	2.996991
H	2.497449	2.363087	-1.386651
H	1.905132	2.911394	0.607706
H	-0.749803	-0.249579	1.819258
H	0.225149	1.546167	2.155840
H	3.574698	1.606579	0.296826
B	-2.417750	1.130370	-0.835867
H	-3.372736	-1.151259	-1.747117
H	-4.267321	0.264210	0.871001
H	-0.754689	0.173076	-2.647895
H	-2.477238	2.618038	1.298740
H	-0.359553	2.652057	-0.765264
H	-3.070810	1.828509	-1.544925

Table S21 -Calculated coordinates (DFT; B3LYP / 6-31G*, LANL2DZ) for $[(PH_3)_2HRhSB_9H_9]$ (compound **4** transition state).

Rh	0.599210	-0.000385	0.255319
B	-1.362597	-1.414941	-0.813839
B	-1.161988	-1.347189	1.036963
B	-0.551134	-0.003498	2.065751
S	-0.559020	0.002526	-1.878299
P	2.089838	-1.809755	-0.099711
P	2.089206	1.810359	-0.096675
B	-1.161741	1.343793	1.041726
B	-1.361754	1.417223	-0.809018
B	-2.212516	-0.002556	1.642235
B	-2.512036	0.002268	-1.282331
B	-2.679816	-0.913648	0.186086
H	3.495185	1.639230	-0.101149
H	-1.281848	-2.469957	-1.354628
H	2.027348	2.860373	0.843733
H	1.992896	2.593408	-1.271254
H	-0.989434	-2.441943	1.482963
H	2.028293	-2.861358	0.838891
H	1.994291	-2.590901	-1.275640
H	0.962914	-0.002577	1.835550
H	-0.330205	-0.005870	3.238223
H	3.495688	-1.637741	-0.103570
B	-2.679507	0.913474	0.189098
H	-3.226439	0.004086	-2.227769
H	-3.623857	-1.632026	0.294184
H	-1.280096	2.473876	-1.346469
H	-2.942526	-0.004156	2.582273
H	-0.989144	2.437078	1.491285
H	-3.623410	1.631719	0.299262

Table S22 - Calculated coordinates (DFT; B3LYP / 6-31G*, LANL2DZ) for $[(PH_3)_2HRhNB_9H_{10}]$ (compound **1a** ground state).

Rh,0,-0.7029041093,-0.0877582892,-0.1278077119
B,0,1.1427603348,-0.0558248966,-1.4932965783
B,0,0.8534322887,1.5045249661,-0.5621045064
B,0,0.5675606393,1.2452138558,1.1805677761
N,0,1.1752559394,-1.2858546645,-0.4828270356
H,0,0.9430980432,-2.2003726464,-0.8582514432
P,0,-2.2152455187,-1.9301475836,0.1463929983
P,0,-2.2830308077,1.5020078021,0.0188806517
B,0,1.9725976753,0.2853857551,1.7890133425
B,0,2.1596137177,-1.2799234366,0.7115254423
B,0,2.1787910421,1.6307645665,0.6279128887
B,0,2.705719127,-0.7827170975,-0.9352563495
B,0,2.4947037912,0.9540989,-0.9945003423
H,0,-3.3695612705,-2.0859828524,-0.6610004813
H,0,0.7706017607,-0.2868057551,-2.6000535788
H,0,-2.8616733316,-2.1137782792,1.3924173446
H,0,-1.744649473,-3.2606751302,0.011651483
H,0,0.4363216304,2.4729485921,-1.1221263847
H,0,-1.9152907622,2.8276752348,-0.2869183674
H,0,-2.9303257502,1.7344514571,1.2563397492
H,0,0.7332937973,-0.0011386647,1.7927632629
H,0,-0.0783391159,1.9099745331,1.9323892734
H,0,-3.4415419776,1.3975679291,-0.7899017751
B,0,3.1566965373,0.1261335258,0.4883937023
H,0,3.3248049023,-1.513581476,-1.6332045144
H,0,3.1364754455,1.5832405335,-1.7749524875
H,0,2.4151610476,-2.3331573347,1.2002198879
H,0,2.671552517,2.6663160841,0.9483016696
H,0,2.341872242,0.2945275043,2.9206481048
H,0,4.2868627645,0.1427119628,0.8624329142

Table S23 - Calculated coordinates (DFT; B3LYP / 6-31G*, LANL2DZ) for $[(PH_3)_2HRhNB_9H_{10}]$ (compound **1a** transition state).

Rh,0,-0.7029041093,-0.0877582892,-0.1278077119
B,0,1.1427603348,-0.0558248966,-1.4932965783
B,0,0.8534322887,1.5045249661,-0.5621045064
B,0,0.5675606393,1.2452138558,1.1805677761
N,0,1.1752559394,-1.2858546645,-0.4828270356
H,0,0.9430980432,-2.2003726464,-0.8582514432
P,0,-2.2152455187,-1.9301475836,0.1463929983
P,0,-2.2830308077,1.5020078021,0.0188806517
B,0,1.9725976753,0.2853857551,1.7890133425
B,0,2.1596137177,-1.2799234366,0.7115254423
B,0,2.1787910421,1.6307645665,0.6279128887
B,0,2.705719127,-0.7827170975,-0.9352563495

B,0,2.4947037912,0.9540989,-0.9945003423
H,0,-3.3695612705,-2.0859828524,-0.6610004813
H,0,0.7706017607,-0.2868057551,-2.6000535788
H,0,-2.8616733316,-2.1137782792,1.3924173446
H,0,-1.744649473,-3.2606751302,0.011651483
H,0,0.4363216304,2.4729485921,-1.1221263847
H,0,-1.9152907622,2.8276752348,-0.2869183674
H,0,-2.9303257502,1.7344514571,1.2563397492
H,0,0.7332937973,-0.0011386647,1.7927632629
H,0,-0.0783391159,1.9099745331,1.9323892734
H,0,-3.4415419776,1.3975679291,-0.7899017751
B,0,3.1566965373,0.1261335258,0.4883937023
H,0,3.3248049023,-1.513581476,-1.6332045144
H,0,3.1364754455,1.5832405335,-1.7749524875
H,0,2.4151610476,-2.3331573347,1.2002198879
H,0,2.671552517,2.6663160841,0.9483016696
H,0,2.341872242,0.2945275043,2.9206481048
H,0,4.2868627645,0.1427119628,0.8624329142