Supporting Information

A simple and high-yield route to iridium, rhodium, osmium and ruthenium *nido*-metalladecaborane compounds.

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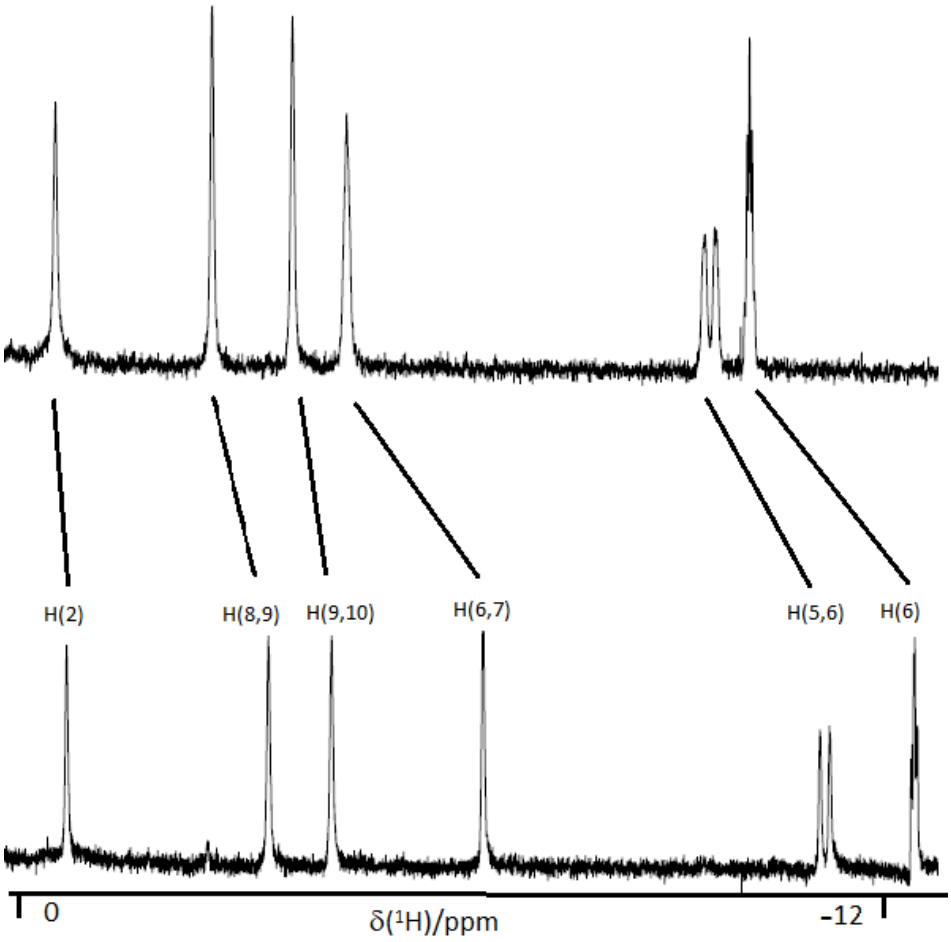
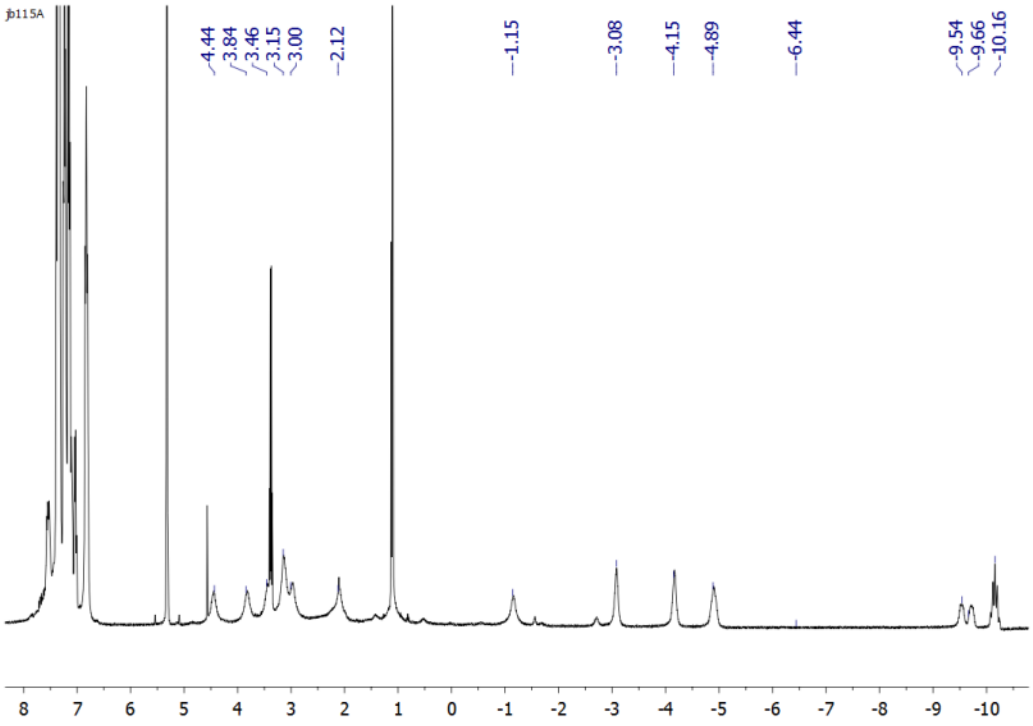

H(2)
H(8,9)
H(9,10)
H(6,7)
H(5,6)
H(6)
0
δ(¹H)/ppm
-12


jb115A
4.44
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3.46
3.15
3.00
2.12
1.15
3.08
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9.54
9.66
10.16
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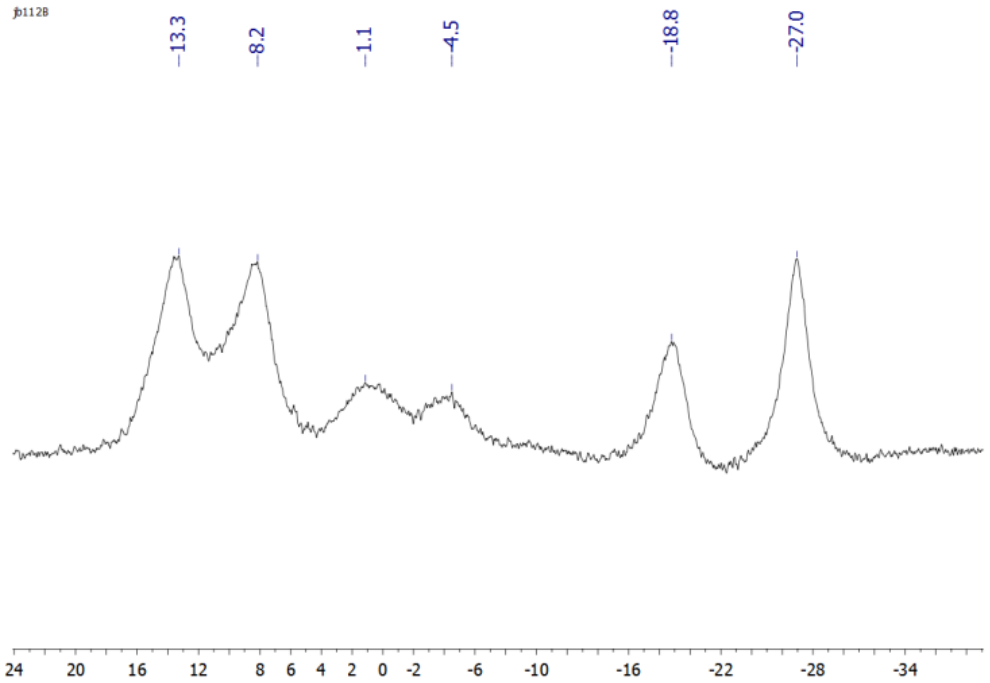

Figure S1. (upper two spectra) ^{1}H-{^{11}B} spectra for [6,6,6-(PPh$_3$)$_2$H-*nido*-6-IrB$_9$H$_{13}$] **1** and [6,6,6-(PPh$_3$)$_2$H-*nido*-6-RhB$_9$H$_{13}$] **2** in the high-field region. (centre) ^{1}H-{^{11}B} NMR spectrum for **2** in CD_2Cl_2 solution at 213 K, 400 MHz. (lower) 128 MHz ^{11}B-{^{1}H} spectrum for **2**. The boron peaks are very broad due to the low temperature. The boron peaks are very broad due to the low temperature.

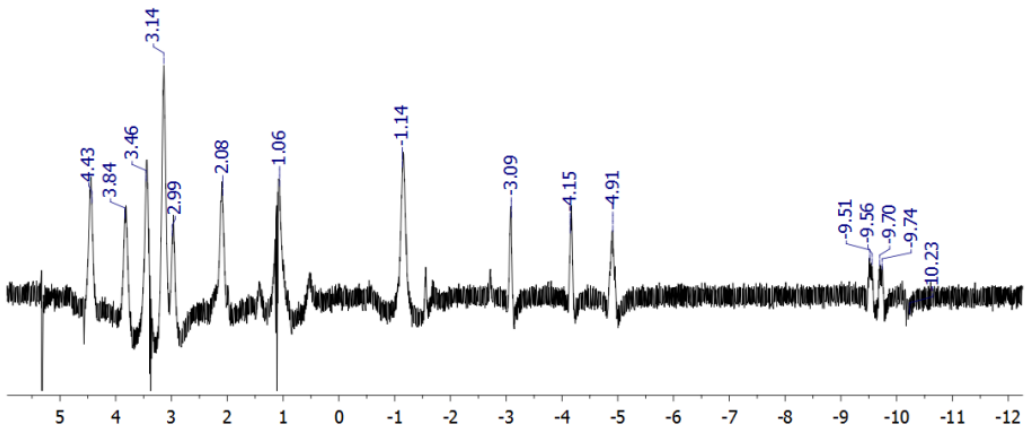

Figure S2. Subtracted ^{1}H-{^{11}B} spectrum of [6,6,6-(PPh$_3$)$_2$H-*nido*-6-RhB$_9$H$_{13}$] **2** obtained by subtracting the "off-resonance" ^{1}H-{^{11}B} spectrum (i.e. with the boron decoupler set at +150 ppm) from the "on-resonance" (i.e. zero ppm) ^{1}H-{^{11}B} spectrum in order to remove non-boron-coupled resonances such as solvent resonances. In CD_2Cl_2 at 213K, 400 MHz.

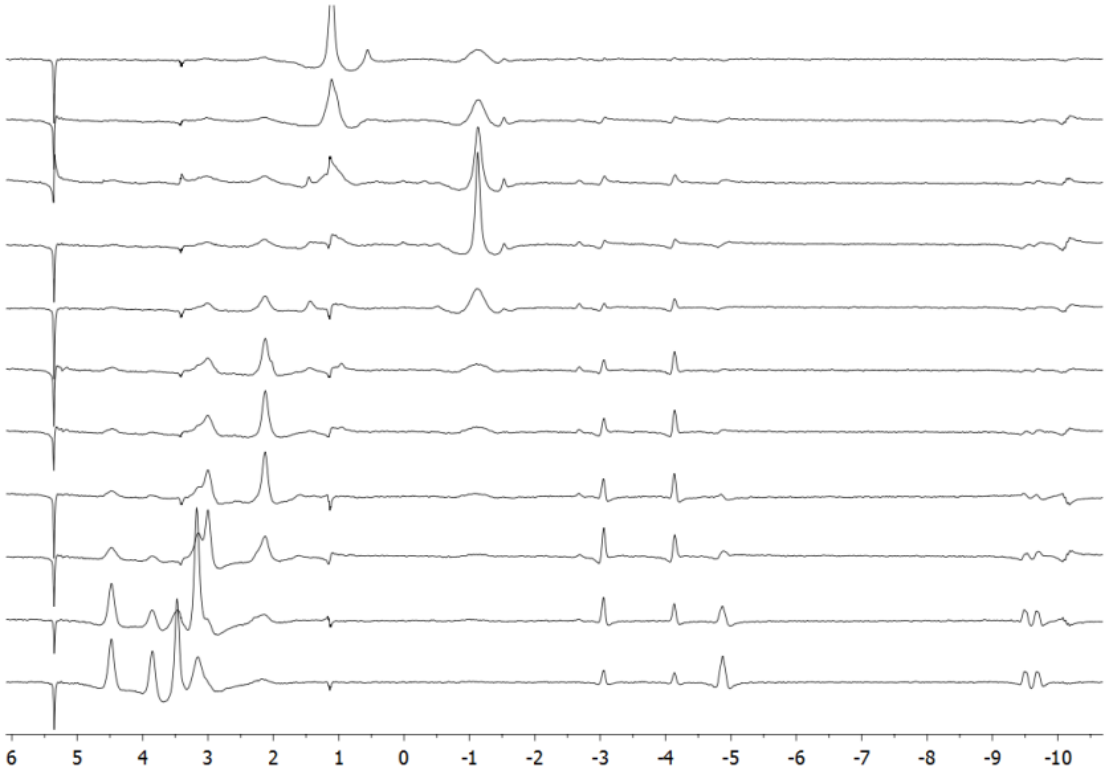

Figure S3. ^{1}H-{$^{11}B_{selective}$} spectra for [6,6,6-$(PPh_3)_2$H-*nido*-6-RhB_9H_{13}] **2**, CD_2Cl_2, 213 K. 400 MHz

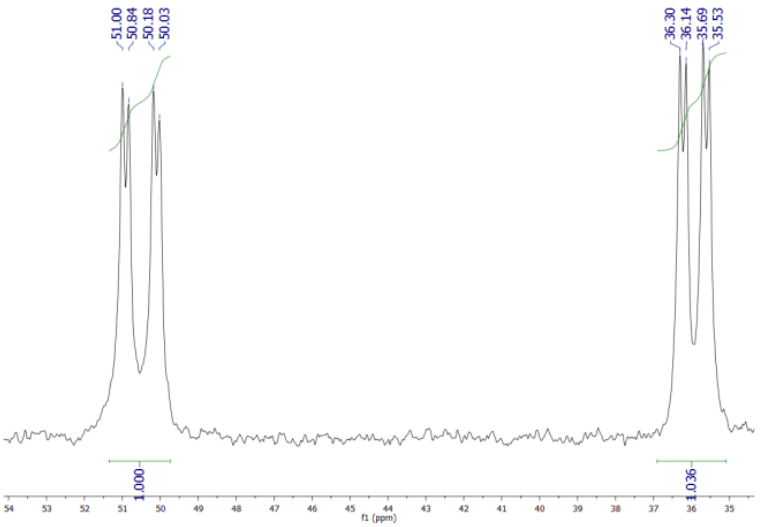

Figure S4. ^{31}P-{^{1}H} NMR spectrum for [6,6,6-$(PPh_3)_2$H-*nido*-6-RhB_9H_{13}] **2** in CD_2Cl_2 at 162 MHz, 213 K.

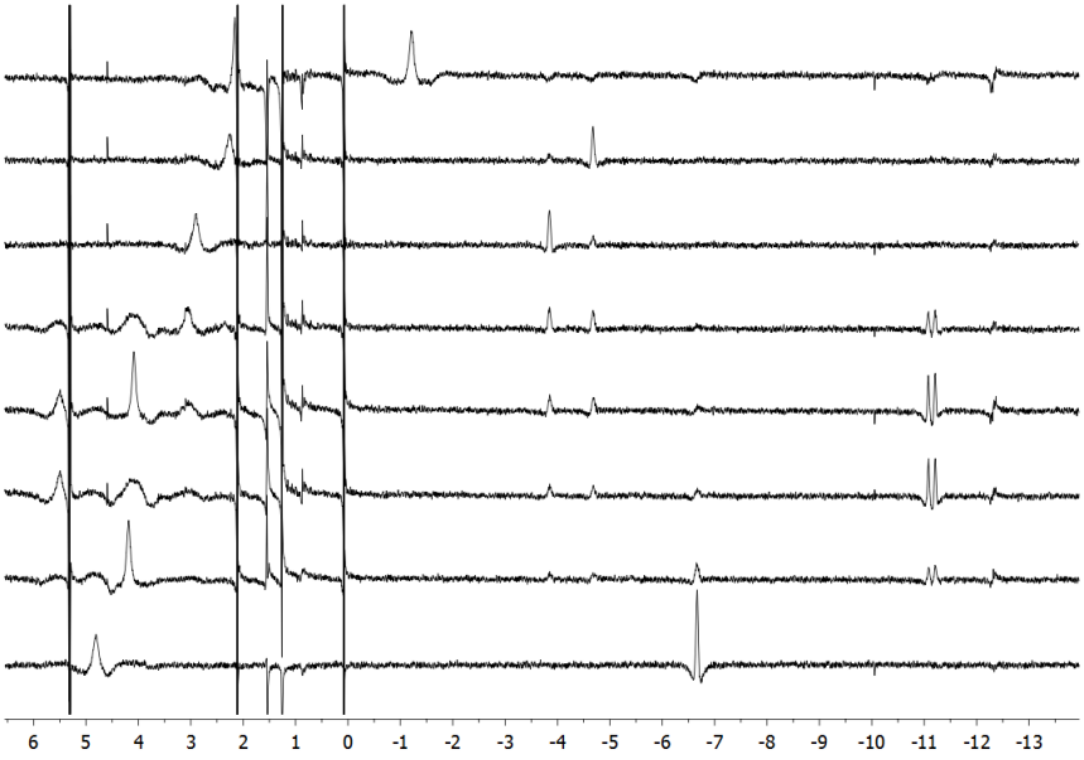

Figure S5 ^{1}H-{^{11}B$_{selective}$} spectra for [6,6,6-(PPh$_3$)$_2$H-*nido*-6-IrB$_9$H$_{13}$] **1**, 500 MHz, CD_2Cl_2, 301K.

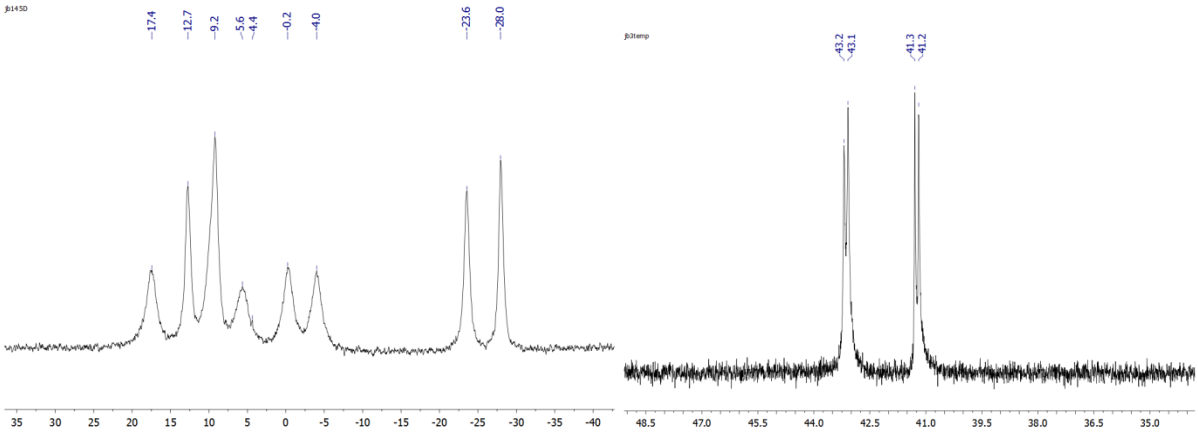

Figure S6. (left) ^{11}B-{^{1}H} NMR spectrum for [6,6,6-(PPh$_3$)$_2$(CO)-*nido*-6-RuB$_9$H$_{13}$] **3**, 192 MHz, and (right) 243 MHz ^{31}P-{^{1}H} NMR spectrum, in CD_2Cl_2, at 292 K.

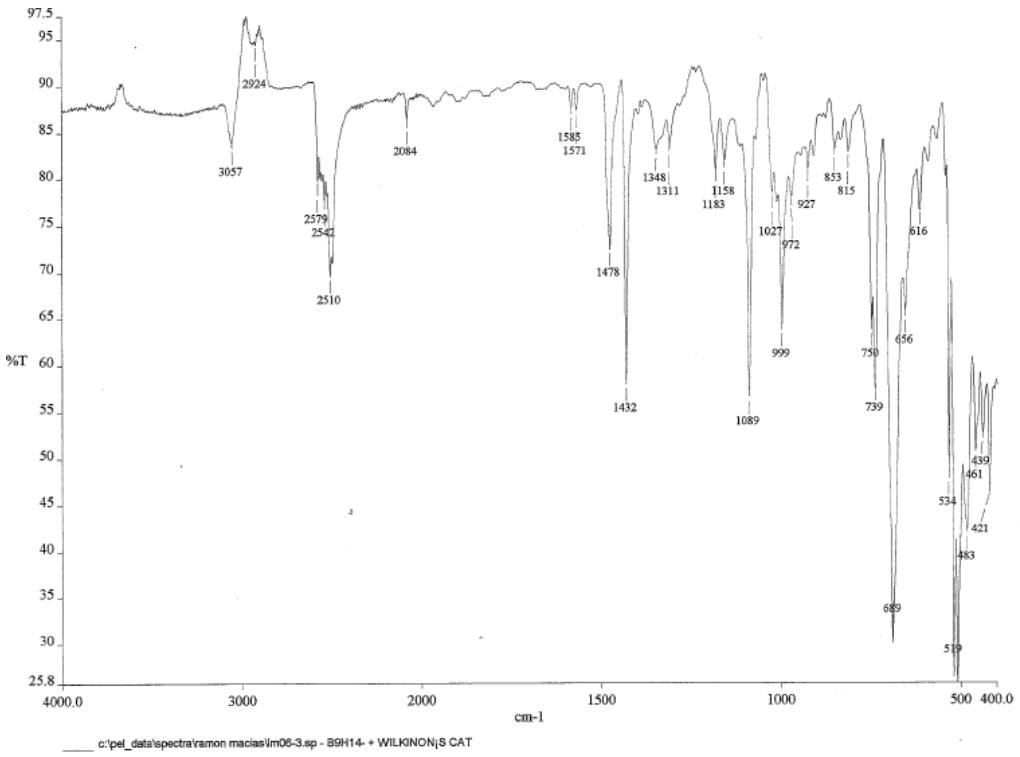

Figure S7. Infrared spectrum (ATR) for [6,6,6-$(PPh_3)_2$H-*nido*-6-RhB_9H_{13}] **2**.

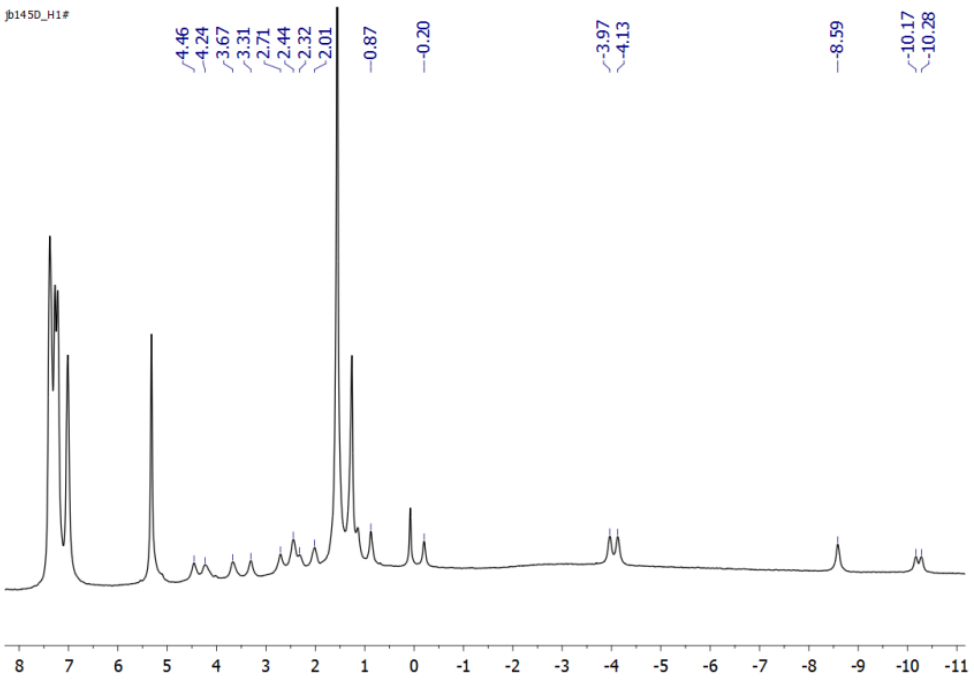

Figure S8 ^{1}H-{^{11}B} NMR spectrum for [6,6,6-$(PPh_3)_2$(CO)-*nido*6-RuB_9H_{13}] **3**, 400 MHz , $CDCl_3$, 292 K.

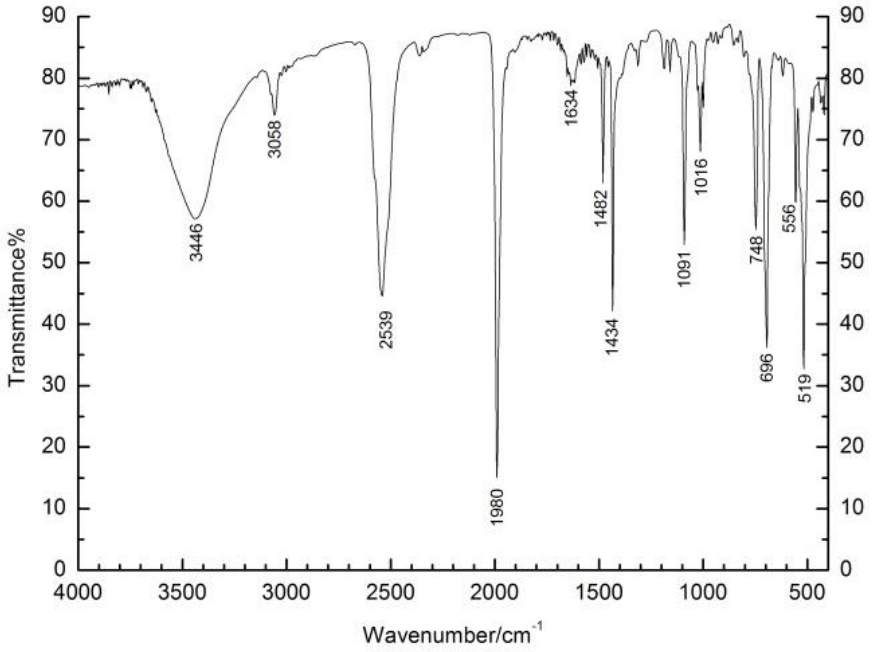

Figure S9 IR spectrum of [6,6,6-$(PPh_3)_2$(CO)-*nido*6-RuB_9H_{13}] **3** (KBr disc).

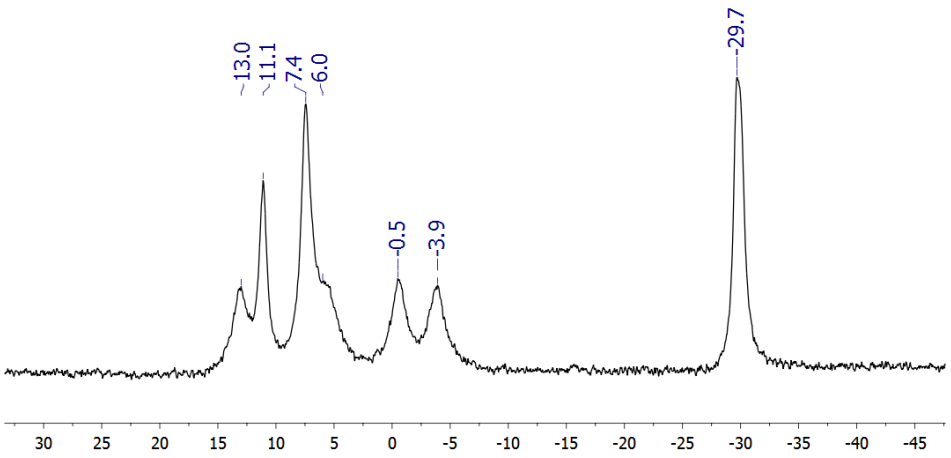

Figure S10. ^{11}B-{^{1}H} NMR spectrum for [6,6,6-$(PPh_3)_2$(CO)-*nido*-6-OsB_9H_{13}] **4** in CD_2Cl_2, 193 MHz, 292 K..

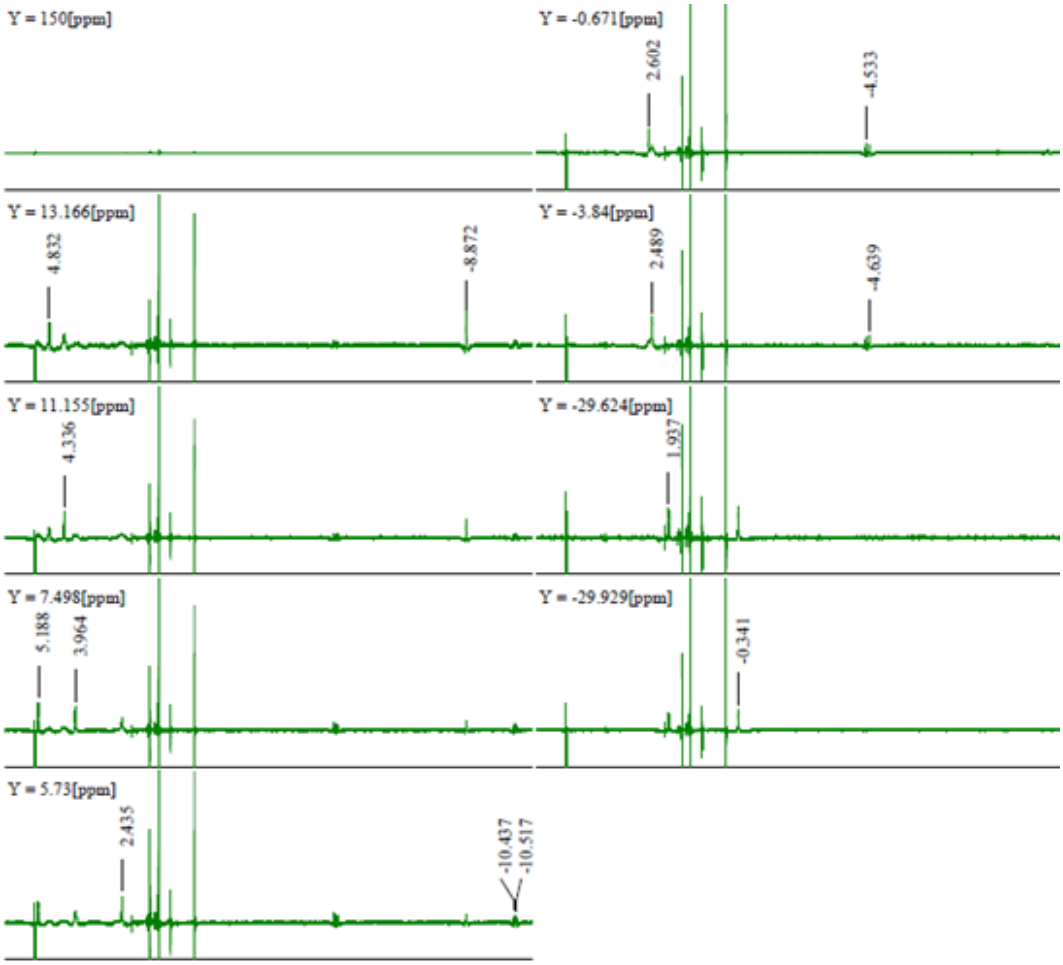

Figure S11. ^{1}H-{$^{11}B_{selective}$} spectra for [6,6,6-$(PPh_3)_2$(CO)-*nido*-6-OsB_9H_{13}] **3**, CD_2Cl_2, 298 K. 600MHz

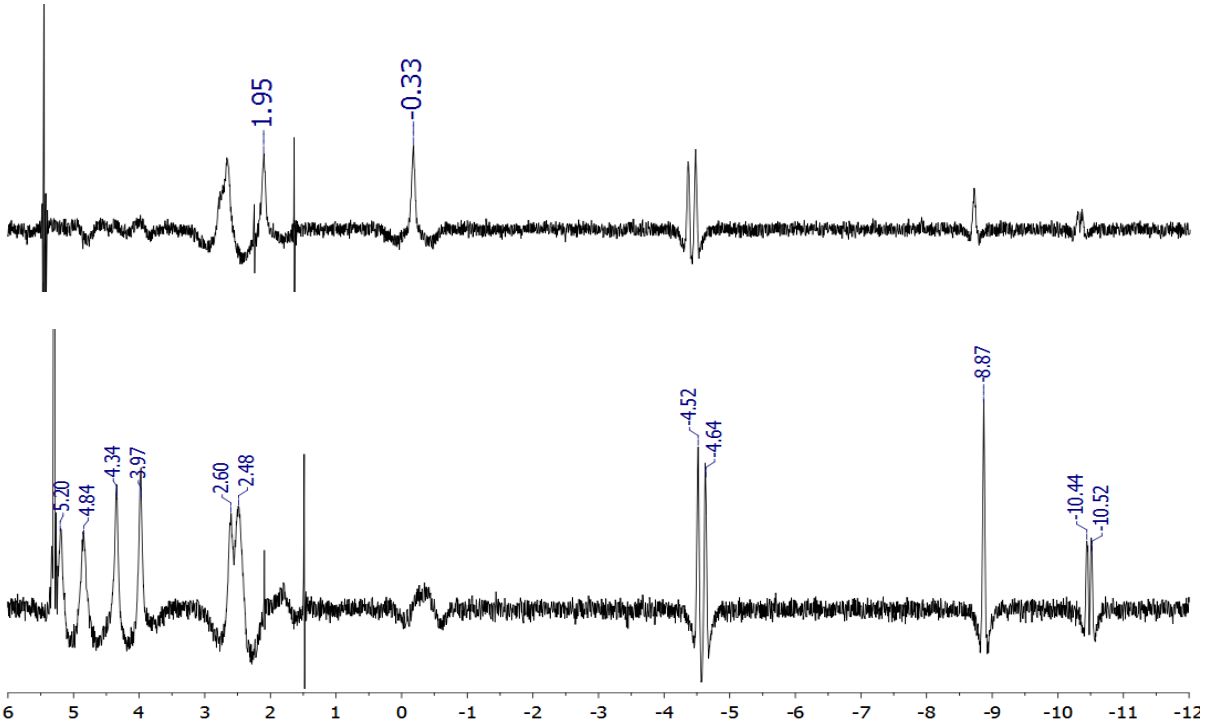

Figure S12. Subtracted $^{1}H-\{^{11}B\}$ spectrum of [6,6,6-$(PPh_3)_2$(CO)-*nido*-6-OsB_9H_{13}] **4** obtained by subtracting the "off-resonance" $^{1}H-\{^{11}B\}$ spectrum (i.e. with the boron decoupler set at +150 ppm) from the "on-resonance" (i.e. zero ppm) $^{1}H-\{^{11}B\}$ spectrum in order to remove non-boron-coupled resonances such as solvent resonances. Broadband decoupling does not efficiently decouple all the resonances simultaneously and therefore the upper spectrum is with the 'on resonance' decoupler set at -30 ppm and the lower is with it set at +9 ppm. In CD_2Cl_2 at 298K, 600 MHz.

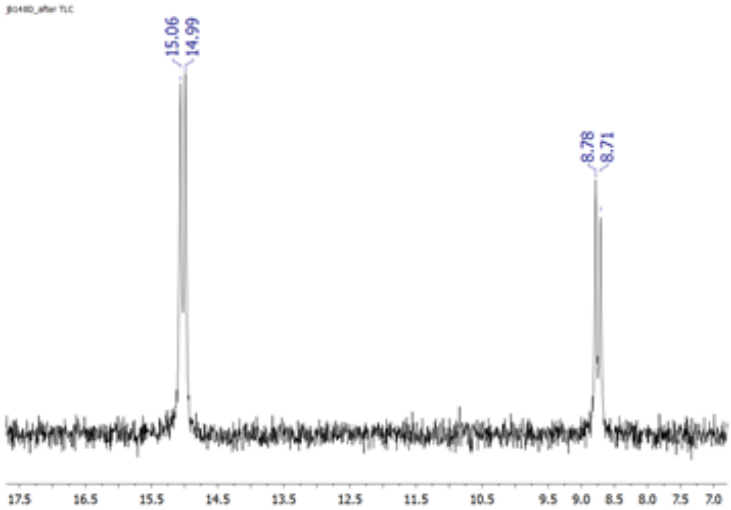

Figure S13. $^{31}P-\{^{1}H\}$ NMR spectrum for [6,6,6-$(PPh_3)_2$(CO)-*nido*-6-OsB_9H_{13}] **4** in CD_2Cl_2, 243 MHz, 292 K.

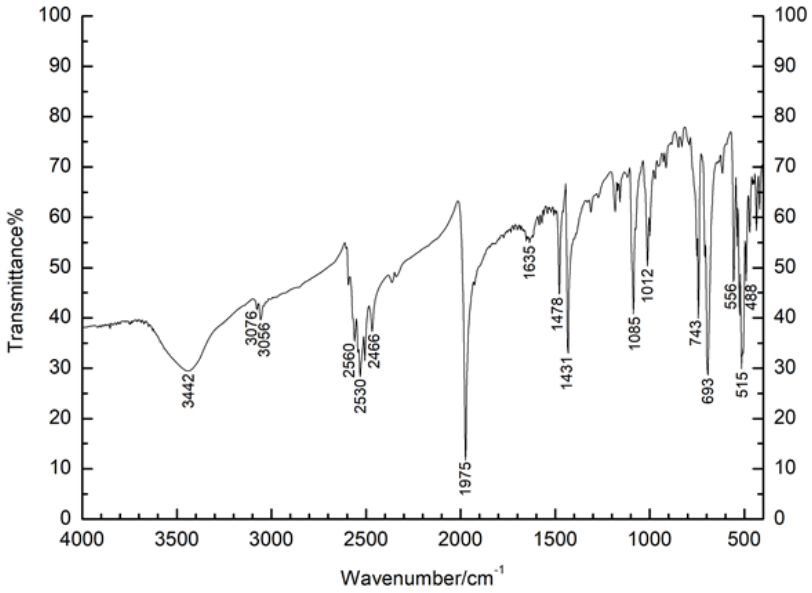

Figure S14. IR spectrum of [6,6,6-$(PPh_3)_2$(CO)-*nido*6-OsB_9H_{13}] **4** (KBr disc).

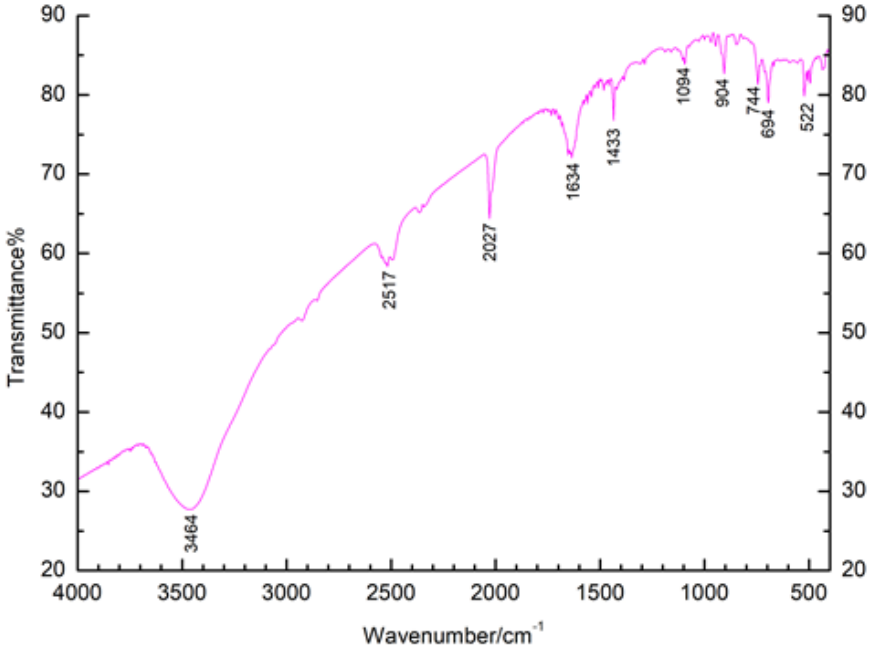

Figure S15. IR spectrum of [1,1,1-(CO)H(PPh_3)-*isocloso*-1-RuB_9H8-μ-(1,2)-{$Pt(PMe_2Ph)_2$}] **5** (KBr disc)

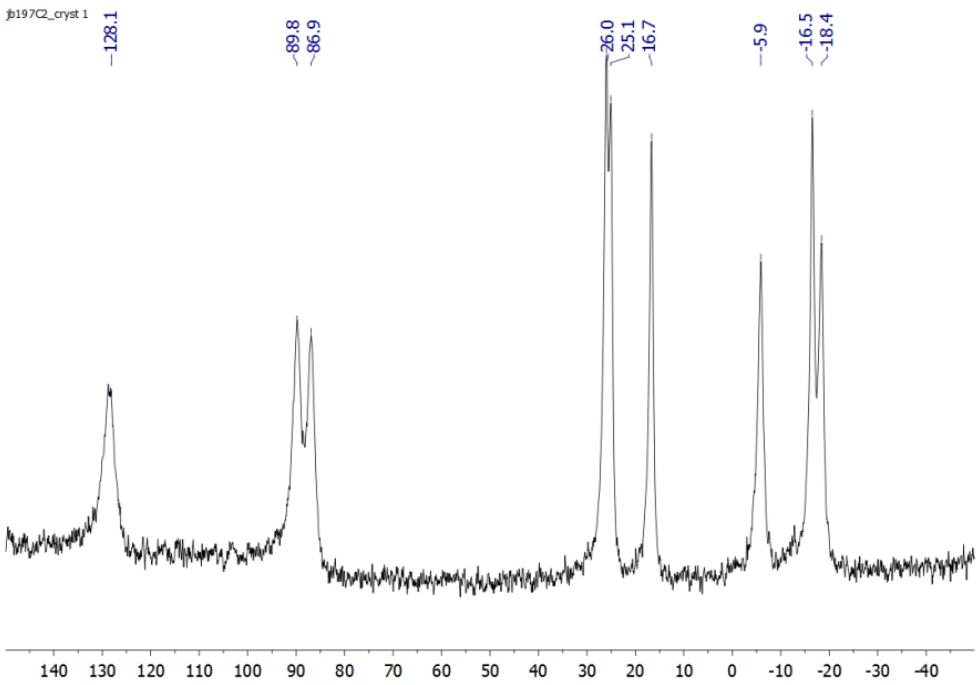

Figure S16. {^{11}B}-^{1}H- NMR spectrum for [1,1,1-(CO)H(PPh$_3$)-*isocloso*-1-RuB$_9$H8-μ-(1,2)-{Pt(PMe$_2$Ph)$_2$}] **5**, 192 MHz , CDCl$_3$, 292 K.

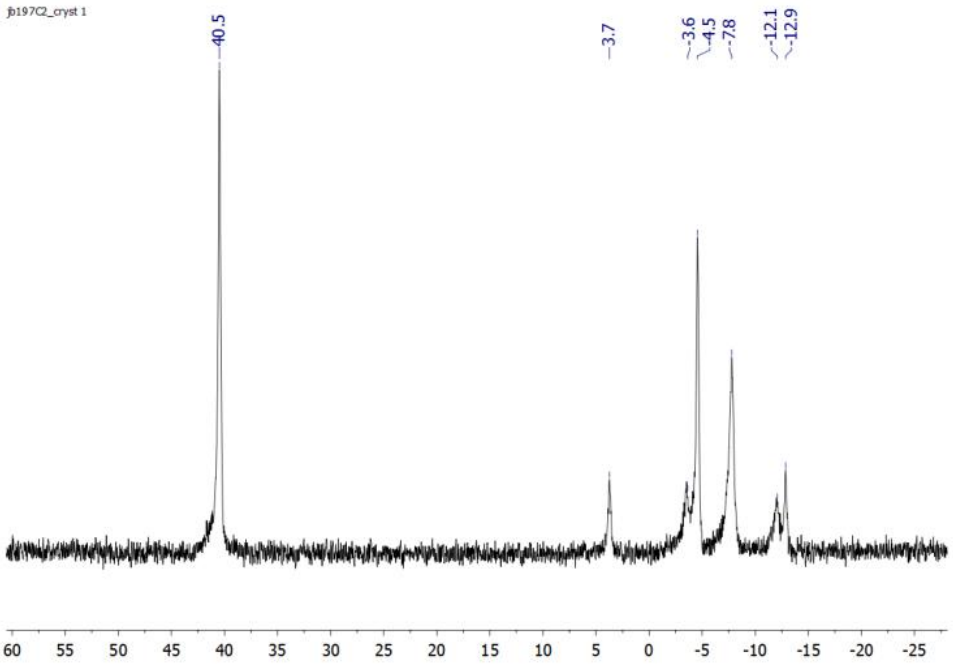

Figure S17. ^{31}P-{^{1}H} NMR spectrum for [1,1,1-(CO)H(PPh$_3$)-*isocloso*-1-RuB$_9$H$_8$-μ-(1,2)-{Pt(PMe$_2$Ph)$_2$}] **5**, 243 MHz , CDCl$_3$, 203 K.

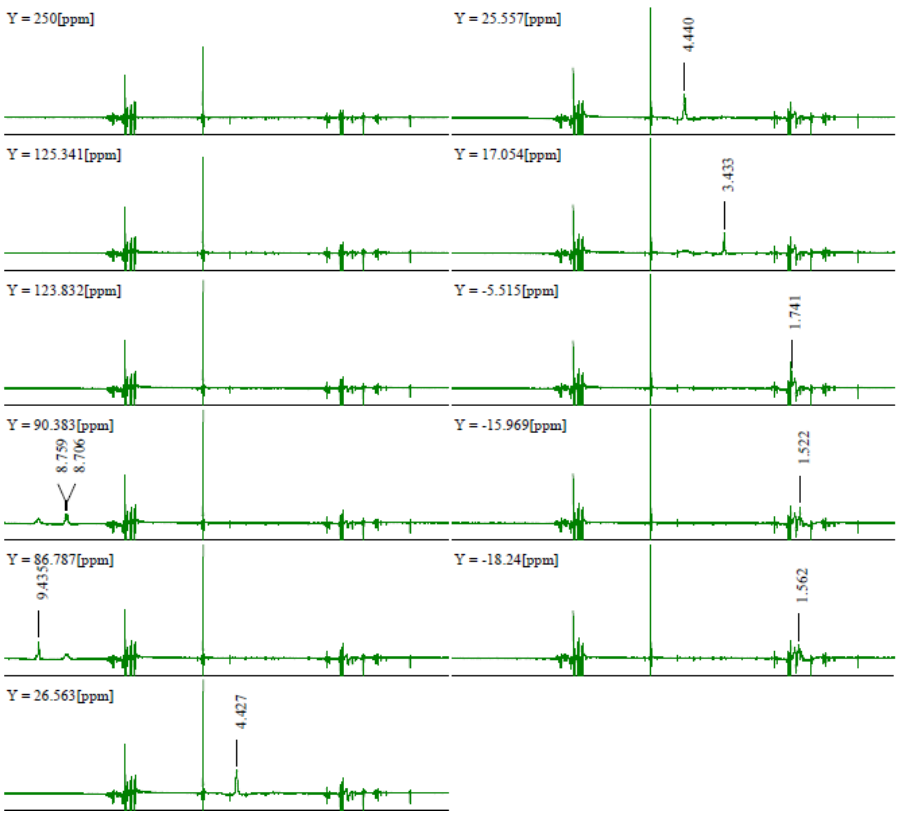

Figure S18. ^{1}H-{$^{11}B_{selective}$} spectra for [1,1,1-(CO)H(PPh_3)-*isocloso*-1-RuB_9H_8-μ-(1,2)-{$Pt(PMe_2Ph)_2$}] **5**, CD_2Cl_2, 298 K. 600MHz.

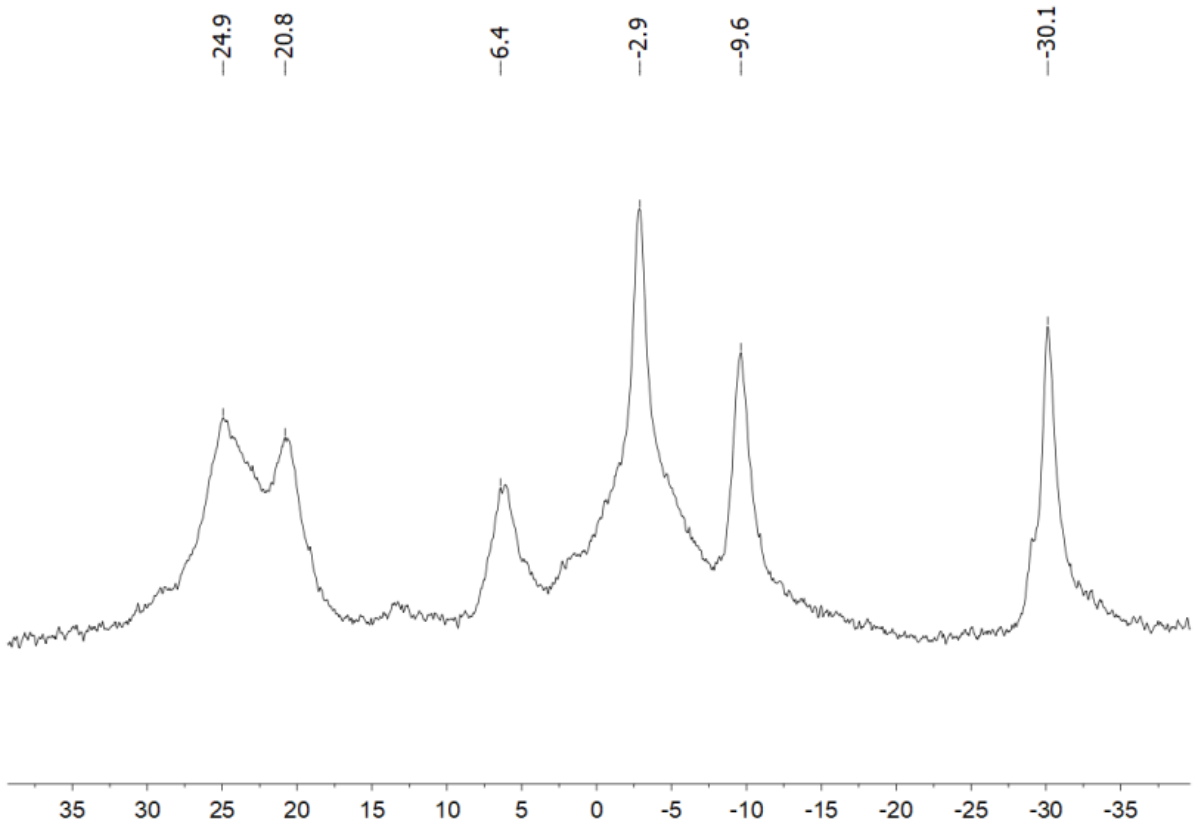

Figure S19. $^{11}B-\{^{1}H\}$ NMR spectrum for [7,7-$(PMe_2Ph)_2$-9,9,9-$(CO)(PPh_3)_2$-*nido*-7,9-$PtOsB_9H_{11}$].CH_2Cl_2 **6**

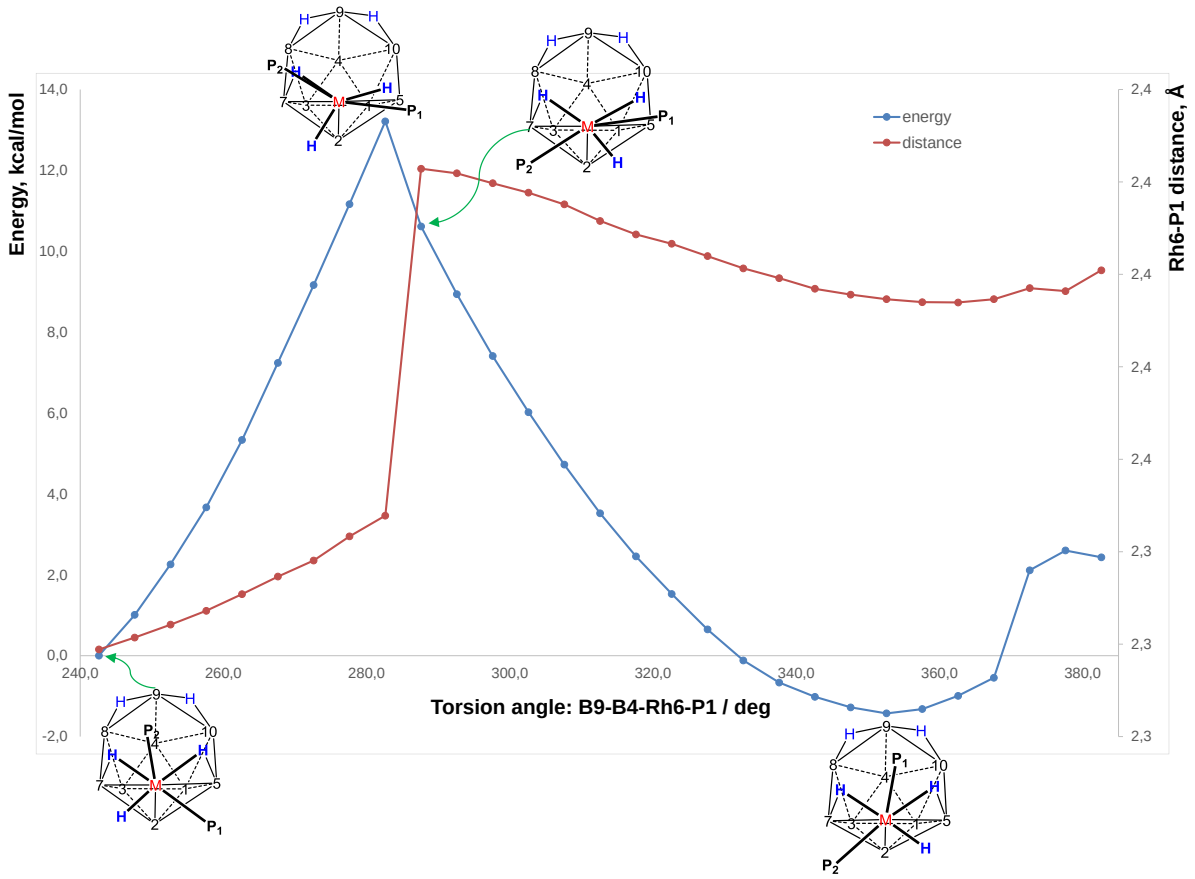

Figure S20. Variation of energy and the PH_3–Rh6 distances in the PES scan upon the rotation of the {Rh(H)(PH_3)$_2$} ligand sphere in [6,6,6-(H)(PH_3)$_2$-*nido*-RhB_9H_{13}], using as a reference the dihedral angle defined by B9−B4−Rh6−P1. (n.b. to reduce the computational load, H atoms were used instead of phenyl rings on the PPh_3 ligand)

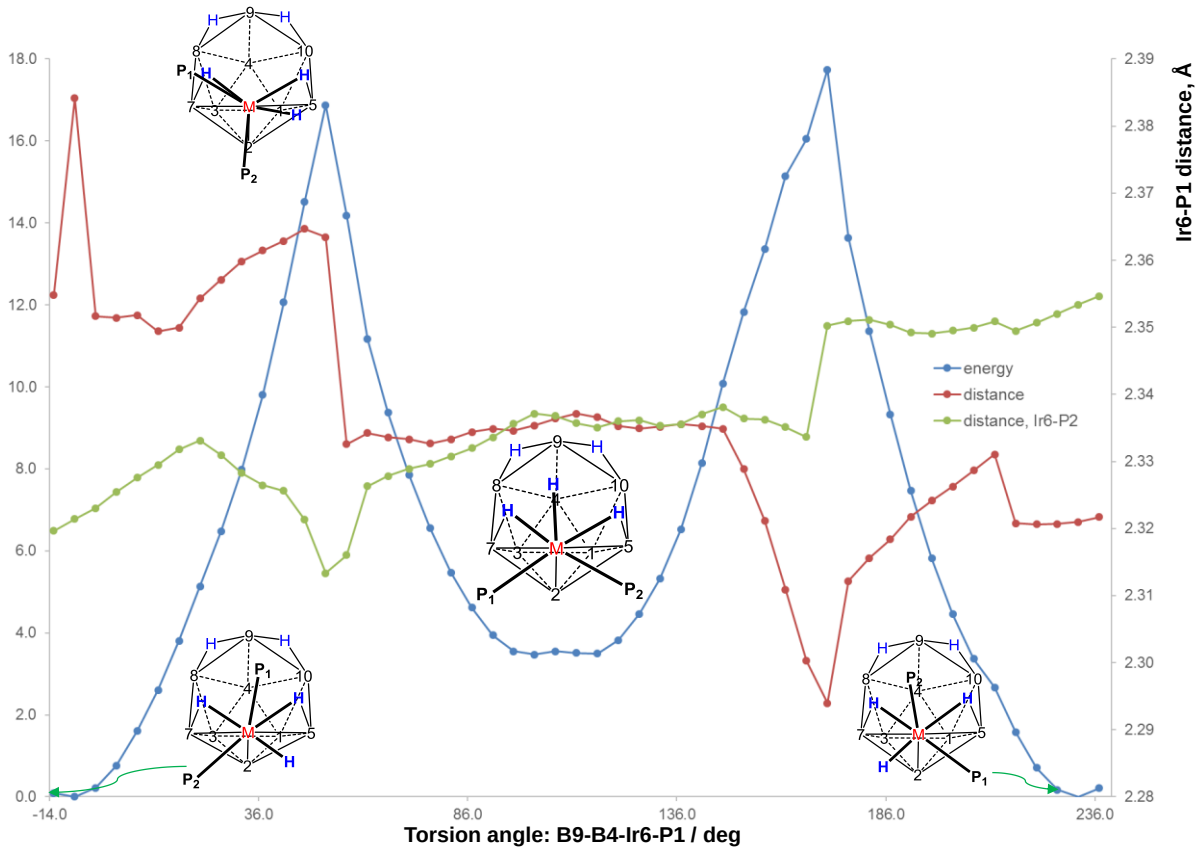

Figure S21. Variation of energy and the PMe_3–Ir6 distances in the relaxed PES scan upon the rotation of the {Ir(H)(PMe_3)$_2$} ligand sphere in [6,6,6-(H)(PMe_3)$_2$-*nido*-IrB_9H_{13}], using as a reference the dihedral angle defined by B9−B4−Ir6−P1.

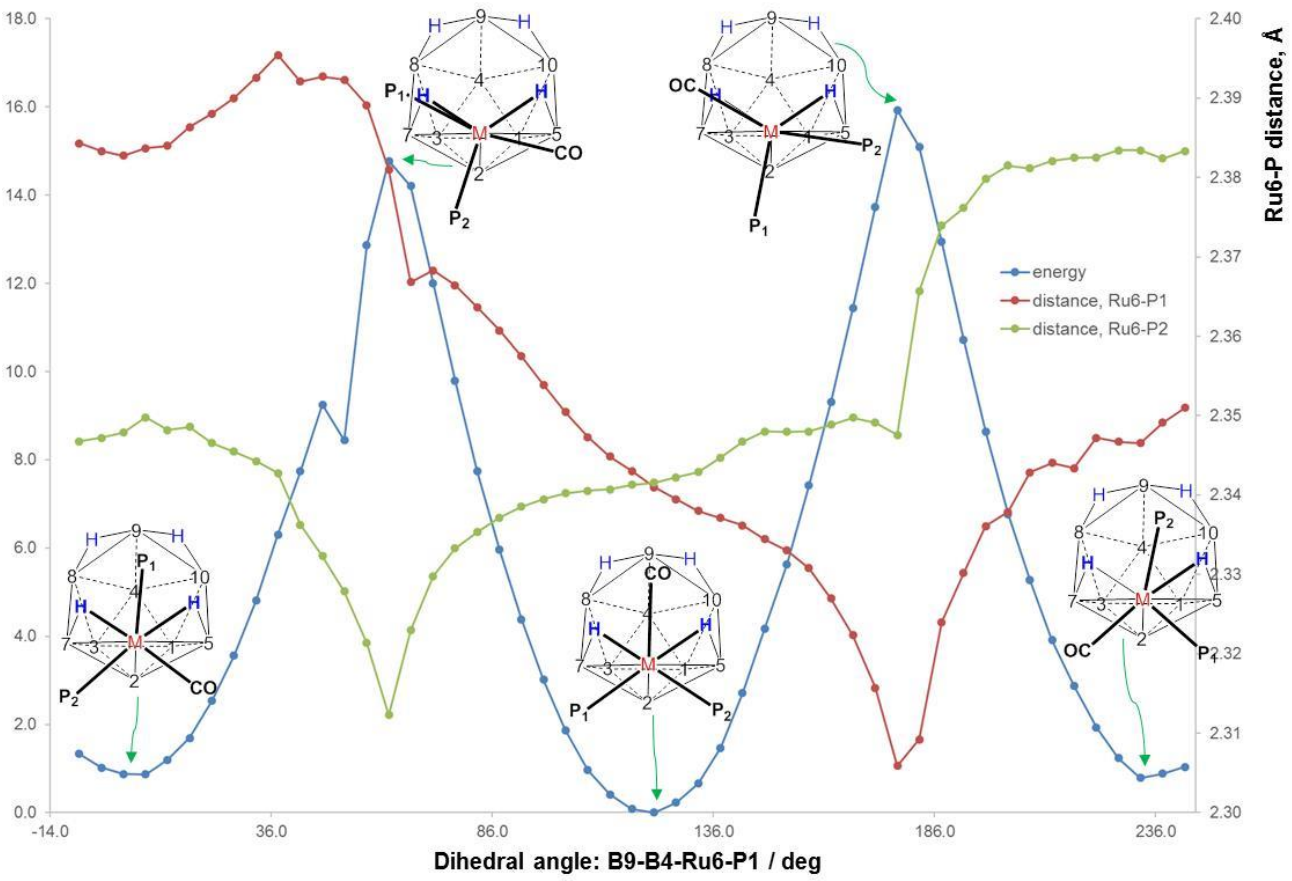

Figure S22. Variation of energy and the PH_3–Ru6 distances in the PES scan upon the rotation of the {Ru(CO)$(PH_3)_2$} ligand sphere, in the PH_3-ligated ruthenadecaborane model, [6,6,6-(CO)$(PH_3)_2$-*nido*-RuB_9H_{13}], using as a reference the dihedral angle defined by B9−B4−Ru6−P1. (n.b. to reduce the computational load, H atoms were used instead of phenyl rings on the PPh_3 ligand)

CRYSTALLOGRAPHIC DATA: DISTANCES AND ANGLES

Twin analysis, resolution and refinement of the X-ray structure determination of compound 3

Twin analysis. The collected reflections were analysed with Cell Now[i] and were assigned to three different domains, 8.2% of the reflections remaining unassigned.

The following twin matrixes (real space) relate the encountered domains:

Domains 1 and 2 [1.000 –0.019 0.000 0.001 1.000 –0.003 0.002 –0.025 –1.000]

Domains 1 and 3 [0.448 –0.552 0.248 –1.446 –0.448 –0.247 –0.001 –0.002 –1.000]

Only contributions from domains 1 and 2 are significant:

18202 data (7549 unique) involve domain 1 only, mean I/sigma 9.4

22114 data (9024 unique) involve domain 2 only, mean I/sigma 6.3

42162 data (14645 unique) involve domain 3 only, mean I/sigma 0.5

35160 data (15710 unique) involve 2 domains, mean I/sigma 11.8

12070 data (6155 unique) involve 3 domains, mean I/sigma 12.9

3 data (3 unique) involve 4 domains, mean I/sigma 9.6

Both single and composite contributions from domains 1 and 2 were used.

Diffraction data have been corrected for absorption corrections with TWINABS.[ii]

Resolution and refinement details. The asymmetric unit contains two chemically equivalent molecules. B-H hydrogen atoms of molecule 1 were encountered in the Fourier difference map and were refined freely.

Molecule 2 presented static disorder. The disordered P(3) atom, the phenyl groups (C(39)>C(44), C(45)>C(50), C(51)>C(56), C(69)>C(74)) and the B9-cluster were included in the model using two sets of atomic coordinates with complementary occupancy factors (aprox. 0.50/0.50). AFIX, EADP and SADI restraints were used. Anisotropic refinement was applied to P(3), while disordered carbon and boron atoms were refined isotropically. C-H hydrogen atoms were included at calculated positions and refined according to the riding model. B-H hydrogen atoms were found in the difference Fourier map and refined using SADI restraints and fixed isotropic displacement parameter (1.2 times the equivalent Ueq for the C/B atom attached).

Table S1. Bond lengths [Å] and angles [°] for [6,6,6-(CO)(PPh_3)$_2$-*nido*-6-RuB_9H_{13}] **3** with s.u.s. in parentheses

Molecule 1					
B(1)-B(10)	1.750(4)	B(4)-B(8)	1.782(4)	B(9)-H(90B)	1.28(3)
B(1)-B(2)	1.768(4)	B(4)-B(9)	1.721(4)	B(9)-H(9B)	1.06(3)
B(1)-B(3)	1.787(4)	B(4)-H(4B)	1.09(3)	B(10)-H(10B)	1.06(3)
B(1)-B(4)	1.789(4)	B(5)-B(10)	2.003(4)	B(10)-H(90B)	1.20(3)
B(1)-B(5)	1.735(4)	B(5)-H(5B)	1.11(3)	C(1)-O(1)	1.146(3)
B(1)-H(1B)	1.07(3)	B(5)-H(65B)	1.22(3)	C(1)-Ru(6)	1.873(3)
B(2)-B(3)	1.777(4)	B(5)-Ru(6)	2.305(3)	C(2)-P(1)	1.839(2)
B(2)-B(5)	1.810(4)	B(7)-B(8)	2.031(4)	C(8)-P(1)	1.848(2)
B(2)-B(7)	1.826(4)	B(7)-H(76B)	1.28(3)	C(14)-P(1)	1.828(2)
B(2)-H(2B)	1.05(3)	B(7)-H(7B)	1.05(3)	C(20)-P(2)	1.836(2)
B(2)-Ru(6)	2.298(3)	B(7)-Ru(6)	2.325(3)	C(26)-P(2)	1.835(2)
B(3)-B(4)	1.794(4)	B(8)-B(9)	1.782(4)	C(32)-P(2)	1.826(2)
B(3)-B(7)	1.753(4)	B(8)-H(89B)	1.23(3)	P(1)-Ru(6)	2.3731(8)
B(3)-B(8)	1.745(4)	B(8)-H(8B)	1.06(3)	P(2)-Ru(6)	2.3806(8)
B(3)-H(3B)	1.11(3)	B(9)-B(10)	1.792(4)	Ru(6)-H(65B)	1.61(3)
B(4)-B(10)	1.789(4)	B(9)-H(89B)	1.27(3)	Ru(6)-H(76B)	1.76(3)
Molecule 2					
B(11A)-B(12A)	1.782(9)	B(14A)-B(19A)	1.712(8)	B(19A)-H(19X)	1.07(4)
B(11A)-B(13A)	1.783(8)	B(14A)-B(20A)	1.768(7)	B(19A)-H(89X)	1.28(5)
B(11A)-B(14A)	1.797(8)	B(14A)-H(14X)	1.09(4)	B(19A)-H(90X)	1.32(4)
B(11A)-B(15A)	1.749(9)	B(14B)-B(18B)	1.769(8)	B(19B)-B(20B)	1.789(8)
B(11A)-B(20A)	1.732(8)	B(14B)-B(19B)	1.708(8)	B(19B)-H(19Y)	1.07(4)
B(11A)-H(11X)	1.10(4)	B(14B)-B(20B)	1.781(7)	B(19B)-H(89Y)	1.28(5)
B(11B)-B(12B)	1.778(9)	B(14B)-H(14Y)	1.09(4)	B(19B)-H(90Y)	1.32(4)
B(11B)-B(13B)	1.793(8)	B(15A)-B(20A)	2.045(8)	B(20A)-H(20X)	1.11(4)
B(11B)-B(14B)	1.790(8)	B(15A)-H(15X)	1.10(3)	B(20A)-H(90X)	1.22(5)
B(11B)-B(15B)	1.759(10)	B(15A)-H(56X)	1.26(3)	B(20B)-H(20Y)	1.11(4)
B(11B)-B(20B)	1.734(9)	B(15A)-Ru(16)	2.419(7)	B(20B)-H(90Y)	1.22(5)
B(11B)-H(11Y)	1.10(4)	B(15B)-B(20B)	2.044(8)	C(38)-O(2)	1.144(3)
B(12A)-B(13A)	1.773(9)	B(15B)-H(15Y)	1.10(3)	C(38)-Ru(16)	1.869(3)
B(12A)-B(15A)	1.818(13)	B(15B)-H(56Y)	1.26(3)	C(57)-P(4)	1.831(2)
B(12A)-B(17A)	1.808(11)	B(15B)-Ru(16)	2.203(8)	C(63)-P(4)	1.838(3)
B(12A)-H(12X)	1.09(3)	B(17A)-B(18A)	2.022(8)	C(69A)-P(4)	1.855(3)
B(12A)-Ru(16)	2.341(10)	B(17A)-H(17X)	1.08(3)	C(69B)-P(4)	1.831(3)
B(12B)-B(13B)	1.779(9)	B(17A)-H(76X)	1.37(3)	P(3A)-C(39A)	1.849(7)
B(12B)-B(15B)	1.811(14)	B(17A)-Ru(16)	2.365(7)	P(3A)-C(45A)	1.858(6)
B(12B)-B(17B)	1.808(13)	B(17B)-B(18B)	2.009(8)	P(3A)-C(51A)	1.852(7)
B(12B)-H(12Y)	1.09(3)	B(17B)-H(17Y)	1.08(3)	P(3A)-Ru(16)	2.382(8)
B(12B)-Ru(16)	2.248(11)	B(17B)-H(76Y)	1.37(3)	P(3B)-C(39B)	1.866(8)
B(13A)-B(14A)	1.793(7)	B(17B)-Ru(16)	2.250(7)	P(3B)-C(45B)	1.851(7)
B(13A)-B(17A)	1.715(9)	B(18A)-B(19A)	1.781(7)	P(3B)-C(51B)	1.849(8)
B(13A)-B(18A)	1.755(9)	B(18A)-H(18X)	1.14(4)	P(3B)-Ru(16)	2.353(9)
B(13A)-H(13X)	1.12(3)	B(18A)-H(89X)	1.23(4)	P(4)-Ru(16)	2.3871(8)
B(13B)-B(14B)	1.789(7)	B(18B)-B(19B)	1.792(7)	Ru(16)-H(56X)	1.77(3)
B(13B)-B(17B)	1.728(10)	B(18B)-H(18Y)	1.13(4)	Ru(16)-H(56Y)	1.77(3)
B(13B)-B(18B)	1.731(9)	B(18B)-H(89Y)	1.23(4)	Ru(16)-H(76X)	1.67(3)
B(13B)-H(13Y)	1.12(3)	B(19A)-B(20A)	1.786(7)	Ru(16)-H(76Y)	1.68(3)
B(14A)-B(18A)	1.763(8)				

Molecule 1					
B(2)-Ru(6)-B(5)	46.32(9)	B(5)-Ru(6)-P(1)	115.99(7)	C(1)-Ru(6)-H(65B)	92.3(12)
B(2)-Ru(6)-B(7)	46.51(9)	B(5)-Ru(6)-P(2)	142.43(6)	C(1)-Ru(6)-H(76B)	173.2(9)
B(2)-Ru(6)-H(65B)	71.9(12)	B(7)-Ru(6)-H(65B)	87.6(12)	C(1)-Ru(6)-P(1)	93.37(7)
B(2)-Ru(6)-H(76B)	76.7(9)	B(7)-Ru(6)-H(76B)	33.0(9)	C(1)-Ru(6)-P(2)	89.65(7)
B(2)-Ru(6)-P(1)	157.33(6)	B(7)-Ru(6)-P(1)	125.66(7)	P(1)-Ru(6)-H(65B)	87.5(12)
B(2)-Ru(6)-P(2)	99.61(7)	B(7)-Ru(6)-P(2)	85.62(7)	P(1)-Ru(6)-H(76B)	92.6(9)
B(5)-Ru(6)-B(7)	79.40(9)	C(1)-Ru(6)-B(2)	96.58(10)	P(1)-Ru(6)-P(2)	100.77(3)
B(5)-Ru(6)-H(65B)	30.3(12)	C(1)-Ru(6)-B(5)	81.11(10)	P(2)-Ru(6)-H(65B)	171.4(12)
B(5)-Ru(6)-H(76B)	93.4(9)	C(1)-Ru(6)-B(7)	140.89(10)	P(2)-Ru(6)-H(76B)	92.3(9)
Molecule 2					

B(12A)-Ru(16)-B(15A)	44.9(3)	C(38)-Ru(16)-B(12A)	97.3(2)	C(38)-Ru(16)-P(3A)	96.54(16)
B(12A)-Ru(16)-B(17A)	45.2(3)	C(38)-Ru(16)-B(12B)	96.9(3)	C(38)-Ru(16)-P(3B)	90.48(17)
B(12A)-Ru(16)-H(56X)	73.9(13)	C(38)-Ru(16)-B(15A)	139.82(19)	C(38)-Ru(16)-P(4)	90.19(8)
B(12A)-Ru(16)-H(76X)	75.0(14)	C(38)-Ru(16)-B(15B)	142.8(2)	H(56X)-Ru(16)-H(76X)	86(3)
B(12A)-Ru(16)-P(3A)	153.6(3)	C(38)-Ru(16)-B(17A)	84.49(18)	H(56Y)-Ru(16)-H(76Y)	84(3)
B(12A)-Ru(16)-P(4)	99.7(2)	C(38)-Ru(16)-B(17B)	77.8(2)	H(65B)-Ru(6)-H(76B)	84.8(15)
B(12B)-Ru(16)-B(17B)	47.4(3)	C(38)-Ru(16)-H(56X)	169.5(13)	P(3A)-Ru(16)-B(15A)	123.4(2)
B(12B)-Ru(16)-H(56Y)	78.5(14)	C(38)-Ru(16)-H(56Y)	173(2)	P(3A)-Ru(16)-H(56X)	93.8(12)
B(12B)-Ru(16)-H(76Y)	79.6(16)	C(38)-Ru(16)-H(76X)	97(2)	P(3A)-Ru(16)-H(76X)	81.0(12)
B(12B)-Ru(16)-P(3B)	157.4(3)	C(38)-Ru(16)-H(76Y)	90(3)	P(3A)-Ru(16)-P(4)	102.55(16)
B(12B)-Ru(16)-P(4)	102.2(3)	B(17A)-Ru(16)-B(15A)	76.0(2)	P(3B)-Ru(16)-H(56Y)	92.0(12)
B(15A)-Ru(16)-H(56X)	30.2(11)	B(17A)-Ru(16)-H(56X)	93.0(18)	P(3B)-Ru(16)-H(76Y)	79.1(14)
B(15A)-Ru(16)-H(76X)	86(2)	B(17A)-Ru(16)-H(76X)	34.7(11)	P(3B)-Ru(16)-P(4)	99.16(18)
B(15B)-Ru(16)-B(12B)	48.0(3)	B(17A)-Ru(16)-P(3A)	114.5(2)	P(4)-Ru(16)-B(15A)	85.15(16)
B(15B)-Ru(16)-B(17B)	83.2(3)	B(17A)-Ru(16)-P(4)	142.95(15)	P(4)-Ru(16)-H(56X)	85.7(19)
B(15B)-Ru(16)-H(56Y)	34.8(11)	B(17B)-Ru(16)-H(56Y)	95(2)	P(4)-Ru(16)-H(56Y)	96(2)
B(15B)-Ru(16)-H(76Y)	94(3)	B(17B)-Ru(16)-H(76Y)	37.5(11)	P(4)-Ru(16)-H(76X)	171(2)
B(15B)-Ru(16)-P(3B)	126.6(3)	B(17B)-Ru(16)-P(3B)	114.5(3)	P(4)-Ru(16)-H(76Y)	178.2(15)
B(15B)-Ru(16)-P(4)	86.80(19)	B(17B)-Ru(16)-P(4)	144.10(18)		

Table S2 Bond lengths [Å] and angles [°] for [1,1,1-(CO)H(PPh_3)-*isocloso*-1-RuB_9H_8-μ-(1,2)-{$Pt(PMe_2Ph)_2$}] (**5**) with s.u.s. in parentheses

Pt1–Ru1	2.9152(3)	Pt1–H1	1.65(6)
Pt1–B2	2.032(4)	Pt1–P1	2.3397(9)
Pt1–P2	2.2426(10)	Ru1–H1	1.93(6)
Ru1–B2	2.091(4)	Ru1–B3	2.183(5)
Ru1–B4	2.191(4)	Ru1–B5	2.412(5)
Ru1–B6	2.424(4)	Ru1–B7	2.438(4)
Ru1–C1	1.950(4)	Ru1–P3	2.4169(10)
B2–B5	1.757(6)	B2–B7	1.745(6)
B2–B8	1.733(6)	B3–H3	1.21(5)
B3–B5	1.734(6)	B3–B6	1.729(7)
B3–B9	1.742(7)	B4–H4	1.12(5)
B4–B6	1.729(7)	B4–B7	1.733(6)
B4–B10	1.747(7)	B5–H5	1.05(5)
B5–B8	1.804(7)	B5–B9	1.790(6)
B6–H6	1.10(5)	B6–B9	1.816(7)
B6–B10	1.817(7)	B7–H7	1.06(5)
B7–B8	1.806(6)	B7–B10	1.782(6)
B8–H8	1.10(5)	B8–B9	1.806(6)
B8–B10	1.798(6)	B9–H9	1.12(5)
B9–B10	1.801(7)	B10–H10	1.06(5)
C1–O1	1.135(6)	P1–C11	1.821(4)
P1–C17	1.823(4)	P1–C18	1.822(4)
C11–C12	1.398(6)	C11–C16	1.399(6)
C12–H12	0.950	C12–C13	1.380(7)
C13–H13	0.950	C13–C14	1.388(7)
C14–H14	0.950	C14–C15	1.374(8)
C15–H15	0.950	C15–C16	1.388(7)
C16–H16	0.950	C17–H17A	0.980
C17–H17B	0.980	C17–H17C	0.980
C18–H18A	0.980	C18–H18B	0.980
C18–H18C	0.980	P2–C21	1.823(4)
P2–C27	1.822(5)	P2–C28	1.806(5)
C21–C22	1.392(6)	C21–C26	1.400(6)
C22–H22	0.950	C22–C23	1.389(7)
C23–H23	0.950	C23–C24	1.381(8)
C24–H24	0.950	C24–C25	1.382(8)
C25–H25	0.950	C25–C26	1.388(7)
C26–H26	0.950	C27–H27A	0.980
C27–H27B	0.980	C27–H27C	0.980
C28–H28A	0.980	C28–H28B	0.980
C28–H28C	0.980	P3–C311	1.829(4)
P3–C321	1.824(4)	P3–C331	1.838(4)
C311–C312	1.381(6)	C311–C316	1.400(6)
C312–H312	0.950	C312–C313	1.394(6)
C313–H313	0.950	C313–C314	1.375(7)
C314–H314	0.950	C314–C315	1.386(7)
C315–H315	0.950	C315–C316	1.379(6)
C316–H316	0.950	C321–C322	1.392(6)
C321–C326	1.398(6)	C322–H322	0.950
C322–C323	1.382(7)	C323–H323	0.950
C323–C324	1.387(8)	C324–H324	0.950
C324–C325	1.374(7)	C325–H325	0.950

C325–C326	1.383(6)	C326–H326	0.950
C331–C332	1.387(6)	C331–C336	1.387(6)
C332–H332	0.950	C332–C333	1.392(6)
C333–H333	0.950	C333–C334	1.380(7)
C334–H334	0.950	C334–C335	1.385(7)
C335–H335	0.950	C335–C336	1.388(6)
C336–H336	0.950		

Ru1–Pt1–H1	39(2)	Ru1–Pt1–B2	45.83(12)
Ru1–Pt1–P1	120.94(3)	Ru1–Pt1–P2	133.14(3)
H1–Pt1–B2	85(2)	H1–Pt1–P1	83(2)
H1–Pt1–P2	172(2)	B2–Pt1–P1	165.80(12)
B2–Pt1–P2	87.36(12)	P1–Pt1–P2	105.36(3)
Pt1–Ru1–H1	32.5(19)	Pt1–Ru1–B2	44.18(11)
Pt1–Ru1–B3	116.71(12)	Pt1–Ru1–B4	119.65(12)
Pt1–Ru1–B5	75.19(10)	Pt1–Ru1–B6	138.48(11)
Pt1–Ru1–B7	77.84(10)	Pt1–Ru1–C1	98.57(12)
Pt1–Ru1–P3	106.43(2)	H1–Ru1–B2	76.6(19)
H1–Ru1–B3	134.8(18)	H1–Ru1–B4	133.7(18)
H1–Ru1–B5	102.9(19)	H1–Ru1–B6	170.9(19)
H1–Ru1–B7	102.5(18)	H1–Ru1–C1	78.5(18)
H1–Ru1–P3	80.4(19)	B2–Ru1–B3	87.65(18)
B2–Ru1–B4	86.71(17)	B2–Ru1–B5	45.24(16)
B2–Ru1–B6	94.41(17)	B2–Ru1–B7	44.50(15)
B2–Ru1–C1	126.32(17)	B2–Ru1–P3	132.24(12)
B3–Ru1–B4	86.07(17)	B3–Ru1–B5	43.98(16)
B3–Ru1–B6	43.69(17)	B3–Ru1–B7	94.30(17)
B3–Ru1–C1	77.69(18)	B3–Ru1–P3	136.00(13)
B4–Ru1–B5	94.31(16)	B4–Ru1–B6	43.64(17)
B4–Ru1–B7	43.57(15)	B4–Ru1–C1	141.73(17)
B4–Ru1–P3	79.83(12)	B5–Ru1–B6	70.25(16)
B5–Ru1–B7	71.46(16)	B5–Ru1–C1	97.36(17)
B5–Ru1–P3	173.98(12)	B6–Ru1–B7	69.96(16)
B6–Ru1–C1	107.89(17)	B6–Ru1–P3	105.83(12)
B7–Ru1–C1	168.77(16)	B7–Ru1–P3	103.04(11)
C1–Ru1–P3	88.17(13)	Pt1–B2–Ru1	89.98(17)
Pt1–B2–B5	119.4(3)	Pt1–B2–B7	127.1(3)
Pt1–B2–B8	162.6(3)	Ru1–B2–B5	77.1(2)
Ru1–B2–B7	78.3(2)	Ru1–B2–B8	106.9(2)
B5–B2–B7	107.9(3)	B5–B2–B8	62.3(3)
B7–B2–B8	62.6(3)	Ru1–B3–H3	125(3)
Ru1–B3–B5	75.0(2)	Ru1–B3–B6	75.6(2)
Ru1–B3–B9	104.0(3)	H3–B3–B5	128(2)
H3–B3–B6	124(2)	H3–B3–B9	131(3)
B5–B3–B6	106.9(4)	B5–B3–B9	62.0(3)
B6–B3–B9	63.1(3)	Ru1–B4–H4	130(2)
Ru1–B4–B6	75.4(2)	Ru1–B4–B7	75.8(2)
Ru1–B4–B10	103.7(3)	H4–B4–B6	126(3)
H4–B4–B7	124(3)	H4–B4–B10	126(2)
B6–B4–B7	107.2(3)	B6–B4–B10	63.0(3)
B7–B4–B10	61.6(3)	Ru1–B5–B2	57.69(19)
Ru1–B5–B3	61.0(2)	Ru1–B5–H5	130(3)
Ru1–B5–B8	92.7(2)	Ru1–B5–B9	94.1(2)
B2–B5–B3	116.0(3)	B2–B5–H5	117(3)
B2–B5–B8	58.2(3)	B2–B5–B9	108.8(3)

B3–B5–H5	115(3)	B3–B5–B8	110.2(3)
B3–B5–B9	59.2(3)	H5–B5–B8	129(3)
H5–B5–B9	128(3)	B8–B5–B9	60.3(2)
Ru1–B6–B3	60.7(2)	Ru1–B6–B4	60.99(19)
Ru1–B6–H6	133(3)	Ru1–B6–B9	93.0(2)
Ru1–B6–B10	93.1(2)	B3–B6–B4	119.4(3)
B3–B6–H6	116(3)	B3–B6–B9	58.8(3)
B3–B6–B10	109.7(3)	B4–B6–H6	115(3)
B4–B6–B9	109.9(3)	B4–B6–B10	59.0(3)
H6–B6–B9	127(3)	H6–B6–B10	127(3)
B9–B6–B10	59.4(3)	Ru1–B7–B2	57.16(18)
Ru1–B7–B4	60.6(2)	Ru1–B7–H7	131(3)
Ru1–B7–B8	91.8(2)	Ru1–B7–B10	93.6(2)
B2–B7–B4	115.5(3)	B2–B7–H7	115(2)
B2–B7–B8	58.4(2)	B2–B7–B10	108.8(3)
B4–B7–H7	117(2)	B4–B7–B8	110.0(3)
B4–B7–B10	59.6(3)	H7–B7–B8	127(3)
H7–B7–B10	129(2)	B8–B7–B10	60.1(2)
B2–B8–B5	59.5(3)	B2–B8–B7	59.0(2)
B2–B8–H8	121(2)	B2–B8–B9	109.1(3)
B2–B8–B10	108.6(3)	B5–B8–B7	103.3(3)
B5–B8–H8	121(3)	B5–B8–B9	59.4(2)
B5–B8–B10	105.8(3)	B7–B8–H8	128(3)
B7–B8–B9	106.0(3)	B7–B8–B10	59.3(2)
H8–B8–B9	119(3)	H8–B8–B10	124(2)
B9–B8–B10	60.0(3)	B3–B9–B5	58.8(3)
B3–B9–B6	58.1(3)	B3–B9–B8	109.7(3)
B3–B9–H9	125(3)	B3–B9–B10	109.9(3)
B5–B9–B6	101.0(3)	B5–B9–B8	60.2(2)
B5–B9–H9	129(3)	B5–B9–B10	106.3(3)
B6–B9–B8	105.4(3)	B6–B9–H9	124(3)
B6–B9–B10	60.3(3)	B8–B9–H9	119(3)
B8–B9–B10	59.8(3)	H9–B9–B10	115(3)
B4–B10–B6	58.0(3)	B4–B10–B7	58.8(2)
B4–B10–B8	109.8(3)	B4–B10–B9	109.8(3)
B4–B10–H10	121(2)	B6–B10–B7	101.5(3)
B6–B10–B8	105.7(3)	B6–B10–B9	60.3(3)
B6–B10–H10	122(3)	B7–B10–B8	60.6(2)
B7–B10–B9	107.2(3)	B7–B10–H10	128(3)
B8–B10–B9	60.2(2)	B8–B10–H10	123(2)
B9–B10–H10	118(3)	Ru1–C1–O1	176.8(4)
Pt1–P1–C11	115.78(13)	Pt1–P1–C17	117.71(15)
Pt1–P1–C18	112.15(14)	C11–P1–C17	102.85(19)
C11–P1–C18	105.0(2)	C17–P1–C18	101.6(2)
P1–C11–C12	122.9(3)	P1–C11–C16	118.4(3)
C12–C11–C16	118.7(4)	C11–C12–H12	119.6
C11–C12–C13	120.8(4)	H12–C12–C13	119.6
C12–C13–H13	120.1	C12–C13–C14	119.9(4)
H13–C13–C14	120.1	C13–C14–H14	120.0
C13–C14–C15	120.1(4)	H14–C14–C15	120.0
C14–C15–H15	119.7	C14–C15–C16	120.6(4)
H15–C15–C16	119.7	C11–C16–C15	120.0(4)
C11–C16–H16	120.0	C15–C16–H16	120.0
P1–C17–H17A	109.5	P1–C17–H17B	109.5
P1–C17–H17C	109.5	H17A–C17–H17B	109.5

H17A–C17–H17C	109.5	H17B–C17–H17C	109.5
P1–C18–H18A	109.5	P1–C18–H18B	109.5
P1–C18–H18C	109.5	H18A–C18–H18B	109.5
H18A–C18–H18C	109.5	H18B–C18–H18C	109.5
Pt1–P2–C21	118.21(14)	Pt1–P2–C27	113.82(18)
Pt1–P2–C28	113.1(2)	C21–P2–C27	101.6(2)
C21–P2–C28	105.2(2)	C27–P2–C28	103.2(3)
P2–C21–C22	123.6(3)	P2–C21–C26	117.7(3)
C22–C21–C26	118.8(4)	C21–C22–H22	119.8
C21–C22–C23	120.4(4)	H22–C22–C23	119.8
C22–C23–H23	119.9	C22–C23–C24	120.2(4)
H23–C23–C24	119.9	C23–C24–H24	120.0
C23–C24–C25	120.0(4)	H24–C24–C25	120.0
C24–C25–H25	120.0	C24–C25–C26	120.1(5)
H25–C25–C26	120.0	C21–C26–C25	120.4(4)
C21–C26–H26	119.8	C25–C26–H26	119.8
P2–C27–H27A	109.5	P2–C27–H27B	109.5
P2–C27–H27C	109.5	H27A–C27–H27B	109.5
H27A–C27–H27C	109.5	H27B–C27–H27C	109.5
P2–C28–H28A	109.5	P2–C28–H28B	109.5
P2–C28–H28C	109.5	H28A–C28–H28B	109.5
H28A–C28–H28C	109.5	H28B–C28–H28C	109.5
Ru1–P3–C311	116.05(13)	Ru1–P3–C321	115.82(15)
Ru1–P3–C331	113.33(13)	C311–P3–C321	105.79(17)
C311–P3–C331	100.72(18)	C321–P3–C331	103.32(19)
P3–C311–C312	120.9(3)	P3–C311–C316	120.2(3)
C312–C311–C316	118.8(4)	C311–C312–H312	119.7
C311–C312–C313	120.6(4)	H312–C312–C313	119.7
C312–C313–H313	120.0	C312–C313–C314	120.0(4)
H313–C313–C314	120.0	C313–C314–H314	120.0
C313–C314–C315	120.0(4)	H314–C314–C315	120.0
C314–C315–H315	119.9	C314–C315–C316	120.1(4)
H315–C315–C316	119.9	C311–C316–C315	120.5(4)
C311–C316–H316	119.8	C315–C316–H316	119.8
P3–C321–C322	123.2(3)	P3–C321–C326	118.1(3)
C322–C321–C326	118.7(4)	C321–C322–H322	119.6
C321–C322–C323	120.8(4)	H322–C322–C323	119.6
C322–C323–H323	119.9	C322–C323–C324	120.1(4)
H323–C323–C324	119.9	C323–C324–H324	120.3
C323–C324–C325	119.3(4)	H324–C324–C325	120.3
C324–C325–H325	119.4	C324–C325–C326	121.3(4)
H325–C325–C326	119.4	C321–C326–C325	119.8(4)
C321–C326–H326	120.1	C325–C326–H326	120.1
P3–C331–C332	121.1(3)	P3–C331–C336	119.8(3)
C332–C331–C336	119.0(4)	C331–C332–H332	119.9
C331–C332–C333	120.2(4)	H332–C332–C333	119.9
C332–C333–H333	119.9	C332–C333–C334	120.3(4)
H333–C333–C334	119.9	C333–C334–H334	120.1
C333–C334–C335	119.9(4)	H334–C334–C335	120.1
C334–C335–H335	120.1	C334–C335–C336	119.8(4)
H335–C335–C336	120.1	C331–C336–C335	120.9(4)
C331–C336–H336	119.6	C335–C336–H336	119.6

Table S3 Bond lengths [Å] and angles [°] for [7,7-(PMe_2Ph)$_2$-9,9,9-(CO)(PPh_3)$_2$-*nido*-7,9-$PtOsB_9H_{11}$].CH_2Cl_2 (**6**) with s.u.s. in parentheses.

B1–H1	1.07(3)	B1–B2	1.745(5)
B1–B3	1.764(5)	B1–B4	1.775(5)
B1–B6	1.771(5)	B1–B11	1.797(4)
B2–H2	1.11(3)	B2–B3	1.763(4)
B2–B5	1.787(4)	B2–B6	1.858(4)
B2–Pt7	2.209(3)	B3–H3	1.08(3)
B3–B4	1.791(4)	B3–B5	1.767(5)
B3–B10	1.793(5)	B4–H4	1.10(3)
B4–Os9	2.266(3)	B4–B10	1.803(5)
B4–B11	1.816(4)	B5–H5	1.08(3)
B5–Pt7	2.287(3)	B5–B10	1.845(4)
B5–H510	1.27(3)	B6–H6	1.10(3)
B6–Pt7	2.230(3)	B6–B8	1.755(4)
B6–B11	1.782(4)	Pt7–B8	2.392(3)
Pt7–P1	2.3367(7)	Pt7–P2	2.3328(7)
B8–H8	1.06(3)	B8–Os9	2.379(3)
B8–B11	1.817(4)	B8–H89	1.31(3)
Os9–B10	2.356(3)	Os9–B11	2.314(3)
Os9–H89	1.81(4)	Os9–C9	1.860(3)
Os9–P3	2.3663(7)	Os9–P4	2.4115(6)
B10–H10	1.08(3)	B10–H510	1.28(3)
B11–H11	1.12(3)	C9–O9	1.158(4)
P1–C11	1.821(3)	P1–C17	1.813(3)
P1–C18	1.811(3)	C11–C12	1.395(4)
C11–C16	1.391(4)	C12–H12	0.950
C12–C13	1.381(4)	C13–H13	0.950
C13–C14	1.378(5)	C14–H14	0.950
C14–C15	1.379(5)	C15–H15	0.950
C15–C16	1.390(4)	C16–H16	0.950
C17–H17A	0.980	C17–H17B	0.980
C17–H17C	0.980	C18–H18A	0.980
C18–H18B	0.980	C18–H18C	0.980
P2–C21	1.793(11)	P2–C21'	1.830(7)
P2–C27	1.815(3)	P2–C28	1.811(3)
C21–C22	1.398(12)	C21–C26	1.389(12)
C22–H22	0.950	C22–C23	1.395(11)
C23–H23	0.950	C23–C24	1.401(13)
C24–H24	0.950	C24–C25	1.371(13)
C25–H25	0.950	C25–C26	1.392(12)
C26–H26	0.950	C21'–C22'	1.392(8)
C21'–C26'	1.415(9)	C22'–H22'	0.950
C22'–C23'	1.387(9)	C23'–H23'	0.950
C23'–C24'	1.390(10)	C24'–H24'	0.950
C24'–C25'	1.401(9)	C25'–H25'	0.950
C25'–C26'	1.400(8)	C26'–H26'	0.950
C27–H27A	0.980	C27–H27B	0.980
C27–H27C	0.980	C28–H28A	0.980
C28–H28B	0.980	C28–H28C	0.980
P3–C311	1.847(3)	P3–C321	1.843(3)
P3–C331	1.840(3)	C311–C312	1.397(4)
C311–C316	1.396(4)	C312–H312	0.950
C312–C313	1.393(4)	C313–H313	0.950

C313–C314	1.375(5)	C314–H314	0.950
C314–C315	1.381(5)	C315–H315	0.950
C315–C316	1.391(4)	C316–H316	0.950
C321–C322	1.389(5)	C321–C326	1.393(5)
C322–H322	0.950	C322–C323	1.393(4)
C323–H323	0.950	C323–C324	1.370(6)
C324–H324	0.950	C324–C325	1.382(6)
C325–H325	0.950	C325–C326	1.390(5)
C326–H326	0.950	C331–C332	1.400(4)
C331–C336	1.389(4)	C332–H332	0.950
C332–C333	1.377(4)	C333–H333	0.950
C333–C334	1.387(5)	C334–H334	0.950
C334–C335	1.376(5)	C335–H335	0.950
C335–C336	1.390(5)	C336–H336	0.950
P4–C411	1.857(3)	P4–C421	1.847(3)
P4–C431	1.840(3)	C411–C412	1.390(4)
C411–C416	1.393(4)	C412–H412	0.950
C412–C413	1.386(4)	C413–H413	0.950
C413–C414	1.379(4)	C414–H414	0.950
C414–C415	1.383(5)	C415–H415	0.950
C415–C416	1.385(4)	C416–H416	0.950
C421–C422	1.384(4)	C421–C426	1.399(4)
C422–H422	0.950	C422–C423	1.397(4)
C423–H423	0.950	C423–C424	1.378(5)
C424–H424	0.950	C424–C425	1.381(5)
C425–H425	0.950	C425–C426	1.388(4)
C426–H426	0.950	C431–C432	1.401(4)
C431–C436	1.388(4)	C432–H432	0.950
C432–C433	1.380(4)	C433–H433	0.950
C433–C434	1.381(4)	C434–H434	0.950
C434–C435	1.381(4)	C435–H435	0.950
C435–C436	1.385(4)	C436–H436	0.950
Cl1–C1	1.789(13)	C1–H1A	0.990
C1–H1B	0.990	C1–C2	1.479(17)
C2–H2A	0.990	C2–H2B	0.990
C2–Cl2	1.713(12)	Cl3–C3	1.806(15)
C3–H3A	0.990	C3–H3B	0.990
C3–C4	1.496(17)	C4–H4A	0.990
C4–H4B	0.990	C4–Cl4	1.726(15)

H1–B1–B2	119.0(17)	H1–B1–B3	117.5(16)
H1–B1–B4	120.7(17)	H1–B1–B6	122.5(16)
H1–B1–B11	120.3(17)	B2–B1–B3	60.34(18)
B2–B1–B4	109.3(2)	B2–B1–B6	63.80(18)
B2–B1–B11	113.1(2)	B3–B1–B4	60.80(19)
B3–B1–B6	111.5(2)	B3–B1–B11	112.3(2)
B4–B1–B6	108.1(2)	B4–B1–B11	61.12(18)
B6–B1–B11	59.93(18)	B1–B2–H2	120.5(16)
B1–B2–B3	60.36(19)	B1–B2–B5	109.3(2)
B1–B2–B6	58.80(18)	B1–B2–Pt7	119.43(19)
H2–B2–B3	122.2(16)	H2–B2–B5	121.3(16)
H2–B2–B6	120.4(16)	H2–B2–Pt7	107.1(16)
B3–B2–B5	59.69(18)	B3–B2–B6	107.6(2)
B3–B2–Pt7	121.44(19)	B5–B2–B6	110.7(2)
B5–B2–Pt7	68.90(14)	B6–B2–Pt7	65.86(13)

B1–B3–B2	59.29(18)	B1–B3–H3	124.1(17)
B1–B3–B4	59.91(18)	B1–B3–B5	109.3(2)
B1–B3–B10	109.1(2)	B2–B3–H3	122.8(17)
B2–B3–B4	107.8(2)	B2–B3–B5	60.83(18)
B2–B3–B10	110.1(2)	H3–B3–B4	121.8(18)
H3–B3–B5	118.0(18)	H3–B3–B10	117.9(17)
B4–B3–B5	110.4(2)	B4–B3–B10	60.41(18)
B5–B3–B10	62.43(18)	B1–B4–B3	59.29(18)
B1–B4–H4	118.3(17)	B1–B4–Os9	121.51(19)
B1–B4–B10	108.2(2)	B1–B4–B11	60.03(18)
B3–B4–H4	112.5(17)	B3–B4–Os9	123.4(2)
B3–B4–B10	59.87(18)	B3–B4–B11	110.1(2)
H4–B4–Os9	112.2(17)	H4–B4–B10	117.3(17)
H4–B4–B11	124.7(17)	Os9–B4–B10	69.70(14)
Os9–B4–B11	68.03(14)	B10–B4–B11	113.9(2)
B2–B5–B3	59.48(18)	B2–B5–H5	128.2(17)
B2–B5–Pt7	64.28(13)	B2–B5–B10	106.8(2)
B2–B5–H510	123.3(13)	B3–B5–H5	121.6(17)
B3–B5–Pt7	117.21(19)	B3–B5–B10	59.48(18)
B3–B5–H510	100.8(14)	H5–B5–Pt7	113.9(17)
H5–B5–B10	116.2(17)	H5–B5–H510	108(2)
Pt7–B5–B10	117.80(17)	Pt7–B5–H510	87.6(13)
B10–B5–H510	43.8(14)	B1–B6–B2	57.40(17)
B1–B6–H6	121.8(16)	B1–B6–Pt7	117.08(19)
B1–B6–B8	112.9(2)	B1–B6–B11	60.74(18)
B2–B6–H6	119.8(16)	B2–B6–Pt7	64.65(13)
B2–B6–B8	116.4(2)	B2–B6–B11	108.5(2)
H6–B6–Pt7	106.3(16)	H6–B6–B8	115.9(16)
H6–B6–B11	121.2(16)	Pt7–B6–B8	72.67(14)
Pt7–B6–B11	124.27(18)	B8–B6–B11	61.80(17)
B2–Pt7–B5	46.81(11)	B2–Pt7–B6	49.50(11)
B2–Pt7–B8	83.68(11)	B2–Pt7–P1	149.12(8)
B2–Pt7–P2	97.96(8)	B5–Pt7–B6	83.23(12)
B5–Pt7–B8	88.78(11)	B5–Pt7–P1	160.92(8)
B5–Pt7–P2	87.37(8)	B6–Pt7–B8	44.47(10)
B6–Pt7–P1	104.20(8)	B6–Pt7–P2	140.65(8)
B8–Pt7–P1	84.78(7)	B8–Pt7–P2	172.89(7)
P1–Pt7–P2	97.01(3)	B6–B8–Pt7	62.86(13)
B6–B8–H8	116.8(17)	B6–B8–Os9	116.29(18)
B6–B8–B11	59.82(17)	B6–B8–H89	134.3(15)
Pt7–B8–H8	107.9(18)	Pt7–B8–Os9	120.44(12)
Pt7–B8–B11	114.47(17)	Pt7–B8–H89	87.6(16)
H8–B8–Os9	119.6(17)	H8–B8–B11	124.2(18)
H8–B8–H89	105(2)	Os9–B8–B11	65.33(13)
Os9–B8–H89	48.8(16)	B11–B8–H89	111.4(16)
B4–Os9–B8	80.74(11)	B4–Os9–B10	45.88(12)
B4–Os9–B11	46.71(11)	B4–Os9–H89	99.5(11)
B4–Os9–C9	77.25(12)	B4–Os9–P3	123.15(9)
B4–Os9–P4	133.23(9)	B8–Os9–B10	85.80(10)
B8–Os9–B11	45.53(11)	B8–Os9–H89	33.0(11)
B8–Os9–C9	145.99(12)	B8–Os9–P3	123.71(8)
B8–Os9–P4	83.98(7)	B10–Os9–B11	81.00(11)
B10–Os9–H89	80.0(11)	B10–Os9–C9	96.87(11)
B10–Os9–P3	82.35(8)	B10–Os9–P4	169.65(8)
B11–Os9–H89	77.0(11)	B11–Os9–C9	101.21(12)

B11–Os9–P3	160.83(8)	B11–Os9–P4	92.91(8)
H89–Os9–C9	176.6(11)	H89–Os9–P3	90.8(11)
H89–Os9–P4	90.5(11)	C9–Os9–P3	90.16(9)
C9–Os9–P4	92.50(8)	P3–Os9–P4	102.06(2)
B3–B10–B4	59.72(18)	B3–B10–B5	58.09(17)
B3–B10–Os9	118.61(19)	B3–B10–H10	113.5(17)
B3–B10–H510	98.9(13)	B4–B10–B5	106.4(2)
B4–B10–Os9	64.43(13)	B4–B10–H10	129.7(18)
B4–B10–H510	123.6(13)	B5–B10–Os9	121.45(17)
B5–B10–H10	108.5(17)	B5–B10–H510	43.2(13)
Os9–B10–H10	120.9(17)	Os9–B10–H510	91.3(13)
H10–B10–H510	107(2)	B1–B11–B4	58.85(18)
B1–B11–B6	59.33(18)	B1–B11–B8	108.8(2)
B1–B11–Os9	118.02(19)	B1–B11–H11	115.4(16)
B4–B11–B6	105.9(2)	B4–B11–B8	111.9(2)
B4–B11–Os9	65.26(14)	B4–B11–H11	123.9(17)
B6–B11–B8	58.37(17)	B6–B11–Os9	118.32(18)
B6–B11–H11	116.9(17)	B8–B11–Os9	69.14(13)
B8–B11–H11	120.8(17)	Os9–B11–H11	116.6(16)
Os9–C9–O9	176.9(3)	Pt7–P1–C11	113.93(9)
Pt7–P1–C17	119.96(10)	Pt7–P1–C18	113.21(10)
C11–P1–C17	100.78(14)	C11–P1–C18	106.53(14)
C17–P1–C18	100.62(16)	P1–C11–C12	117.5(2)
P1–C11–C16	124.1(2)	C12–C11–C16	118.4(3)
C11–C12–H12	119.3	C11–C12–C13	121.3(3)
H12–C12–C13	119.3	C12–C13–H13	120.1
C12–C13–C14	119.8(3)	H13–C13–C14	120.1
C13–C14–H14	120.1	C13–C14–C15	119.8(3)
H14–C14–C15	120.1	C14–C15–H15	119.6
C14–C15–C16	120.7(3)	H15–C15–C16	119.6
C11–C16–C15	120.0(3)	C11–C16–H16	120.0
C15–C16–H16	120.0	P1–C17–H17A	109.5
P1–C17–H17B	109.5	P1–C17–H17C	109.5
H17A–C17–H17B	109.5	H17A–C17–H17C	109.5
H17B–C17–H17C	109.5	P1–C18–H18A	109.5
P1–C18–H18B	109.5	P1–C18–H18C	109.5
H18A–C18–H18B	109.5	H18A–C18–H18C	109.5
H18B–C18–H18C	109.5	Pt7–P2–C21	113.3(10)
Pt7–P2–C21'	107.4(6)	Pt7–P2–C27	117.60(12)
Pt7–P2–C28	119.88(12)	C21–P2–C27	99.3(15)
C21–P2–C28	102.2(6)	C21'–P2–C27	99.8(9)
C21'–P2–C28	108.7(4)	C27–P2–C28	101.45(18)
P2–C21–C22	116.6(10)	P2–C21–C26	121.1(10)
C22–C21–C26	122.1(10)	C21–C22–H22	121.2
C21–C22–C23	117.5(11)	H22–C22–C23	121.2
C22–C23–H23	120.1	C22–C23–C24	119.8(11)
H23–C23–C24	120.1	C23–C24–H24	118.9
C23–C24–C25	122.3(11)	H24–C24–C25	118.9
C24–C25–H25	120.8	C24–C25–C26	118.3(11)
H25–C25–C26	120.8	C21–C26–C25	119.9(11)
C21–C26–H26	120.1	C25–C26–H26	120.1
P2–C21'–C22'	126.8(7)	P2–C21'–C26'	114.5(6)
C22'–C21'–C26'	118.6(6)	C21'–C22'–H22'	118.9
C21'–C22'–C23'	122.3(8)	H22'–C22'–C23'	118.9
C22'–C23'–H23'	120.9	C22'–C23'–C24'	118.2(8)

H23'–C23'–C24'	120.9	C23'–C24'–H24'	119.1
C23'–C24'–C25'	121.9(7)	H24'–C24'–C25'	119.1
C24'–C25'–H25'	120.6	C24'–C25'–C26'	118.9(7)
H25'–C25'–C26'	120.6	C21'–C26'–C25'	120.1(7)
C21'–C26'–H26'	119.9	C25'–C26'–H26'	119.9
P2–C27–H27A	109.5	P2–C27–H27B	109.5
P2–C27–H27C	109.5	H27A–C27–H27B	109.5
H27A–C27–H27C	109.5	H27B–C27–H27C	109.5
P2–C28–H28A	109.5	P2–C28–H28B	109.5
P2–C28–H28C	109.5	H28A–C28–H28B	109.5
H28A–C28–H28C	109.5	H28B–C28–H28C	109.5
Os9–P3–C311	117.51(10)	Os9–P3–C321	120.73(9)
Os9–P3–C331	112.59(9)	C311–P3–C321	99.44(13)
C311–P3–C331	102.66(13)	C321–P3–C331	101.13(13)
P3–C311–C312	119.8(2)	P3–C311–C316	121.6(2)
C312–C311–C316	118.4(3)	C311–C312–H312	119.7
C311–C312–C313	120.6(3)	H312–C312–C313	119.7
C312–C313–H313	119.9	C312–C313–C314	120.2(3)
H313–C313–C314	119.9	C313–C314–H314	120.0
C313–C314–C315	119.9(3)	H314–C314–C315	120.0
C314–C315–H315	119.8	C314–C315–C316	120.4(3)
H315–C315–C316	119.8	C311–C316–C315	120.4(3)
C311–C316–H316	119.8	C315–C316–H316	119.8
P3–C321–C322	123.4(2)	P3–C321–C326	118.4(2)
C322–C321–C326	118.2(3)	C321–C322–H322	119.4
C321–C322–C323	121.3(3)	H322–C322–C323	119.4
C322–C323–H323	120.2	C322–C323–C324	119.7(3)
H323–C323–C324	120.2	C323–C324–H324	120.0
C323–C324–C325	120.1(3)	H324–C324–C325	120.0
C324–C325–H325	119.8	C324–C325–C326	120.4(3)
H325–C325–C326	119.8	C321–C326–C325	120.3(3)
C321–C326–H326	119.9	C325–C326–H326	119.9
P3–C331–C332	119.6(2)	P3–C331–C336	122.4(2)
C332–C331–C336	118.0(3)	C331–C332–H332	119.4
C331–C332–C333	121.2(3)	H332–C332–C333	119.4
C332–C333–H333	120.1	C332–C333–C334	119.9(3)
H333–C333–C334	120.1	C333–C334–H334	120.1
C333–C334–C335	119.8(3)	H334–C334–C335	120.1
C334–C335–H335	119.9	C334–C335–C336	120.3(3)
H335–C335–C336	119.9	C331–C336–C335	120.8(3)
C331–C336–H336	119.6	C335–C336–H336	119.6
Os9–P4–C411	119.53(9)	Os9–P4–C421	114.08(8)
Os9–P4–C431	117.96(9)	C411–P4–C421	99.10(12)
C411–P4–C431	100.82(12)	C421–P4–C431	102.30(12)
P4–C411–C412	120.6(2)	P4–C411–C416	122.1(2)
C412–C411–C416	117.3(3)	C411–C412–H412	119.3
C411–C412–C413	121.4(3)	H412–C412–C413	119.3
C412–C413–H413	119.7	C412–C413–C414	120.6(3)
H413–C413–C414	119.7	C413–C414–H414	120.5
C413–C414–C415	119.0(3)	H414–C414–C415	120.5
C414–C415–H415	119.8	C414–C415–C416	120.4(3)
H415–C415–C416	119.8	C411–C416–C415	121.4(3)
C411–C416–H416	119.3	C415–C416–H416	119.3
P4–C421–C422	120.8(2)	P4–C421–C426	120.7(2)
C422–C421–C426	118.5(3)	C421–C422–H422	119.6

C421–C422–C423	120.7(3)	H422–C422–C423	119.6
C422–C423–H423	120.0	C422–C423–C424	120.1(3)
H423–C423–C424	120.0	C423–C424–H424	120.0
C423–C424–C425	120.0(3)	H424–C424–C425	120.0
C424–C425–H425	120.0	C424–C425–C426	120.0(3)
H425–C425–C426	120.0	C421–C426–C425	120.8(3)
C421–C426–H426	119.6	C425–C426–H426	119.6
P4–C431–C432	123.7(2)	P4–C431–C436	118.3(2)
C432–C431–C436	117.7(3)	C431–C432–H432	119.7
C431–C432–C433	120.7(3)	H432–C432–C433	119.7
C432–C433–H433	119.6	C432–C433–C434	120.7(3)
H433–C433–C434	119.6	C433–C434–H434	120.3
C433–C434–C435	119.4(3)	H434–C434–C435	120.3
C434–C435–H435	120.0	C434–C435–C436	120.0(3)
H435–C435–C436	120.0	C431–C436–C435	121.5(3)
C431–C436–H436	119.2	C435–C436–H436	119.2
Cl1–C1–H1A	109.5	Cl1–C1–H1B	109.5
Cl1–C1–C2	110.8(13)	H1A–C1–H1B	108.1
H1A–C1–C2	109.5	H1B–C1–C2	109.5
C1–C2–H2A	108.6	C1–C2–H2B	108.6
C1–C2–Cl2	114.5(13)	H2A–C2–H2B	107.6
H2A–C2–Cl2	108.6	H2B–C2–Cl2	108.6
Cl3–C3–H3A	109.1	Cl3–C3–H3B	109.1
Cl3–C3–C4	112.4(13)	H3A–C3–H3B	107.9
H3A–C3–C4	109.1	H3B–C3–C4	109.1
C3–C4–H4A	110.1	C3–C4–H4B	110.1
C3–C4–Cl4	107.9(12)	H4A–C4–H4B	108.4
H4A–C4–Cl4	110.1	H4B–C4–Cl4	110.1

Table S4 Bond lengths [Å] and angles [°] for [5,5,5-$(PPh_3)_2$(CO)-*nido*-5-OsB_9H_{13}] (**7**) with s.u.s. in parentheses.

Os5–B1	2.294(4)	Os5–B2	2.334(4)
Os5–B6	2.247(4)	Os5–B10	2.385(4)
Os5–H56	1.59(5)	Os5–C1	1.878(4)
Os5–P1	2.3862(8)	Os5–P2	2.4043(9)
B1–H1	1.07(4)	B1–B2	1.814(6)
B1–B3	1.781(7)	B1–B4	1.817(6)
B1–B10	1.763(6)	B2–H2	1.06(4)
B2–B3	1.788(6)	B2–B6	1.746(6)
B2–B7	1.795(7)	B3–H3	1.12(5)
B3–B4	1.770(7)	B3–B7	1.753(7)
B3–B8	1.742(7)	B4–H4	1.26(4)
B4–B8	1.781(7)	B4–B9	1.708(7)
B4–B10	1.796(6)	B6–H6	1.09(4)
B6–B7	1.784(6)	B6–H56	1.47(5)
B6–H67	1.40(5)	B7–H7	1.08(5)
B7–B8	1.964(7)	B7–H67	1.19(5)
B8–H8	1.11(5)	B8–B9	1.787(7)
B8–H89	1.29(5)	B9–H9	1.12(5)
B9–B10	1.821(6)	B9–H89	1.26(5)
B9–H910	1.37(5)	B10–H10	1.06(4)
B10–H910	1.24(4)	C1–O1	1.152(4)
P1–C111	1.837(4)	P1–C121	1.838(3)
P1–C131	1.839(4)	C111–C112	1.388(5)

C111–C116	1.397(5)	C112–H112	0.950
C112–C113	1.389(6)	C113–H113	0.950
C113–C114	1.379(6)	C114–H114	0.950
C114–C115	1.386(6)	C115–H115	0.950
C115–C116	1.380(6)	C116–H116	0.950
C121–C122	1.391(5)	C121–C126	1.394(5)
C122–H122	0.950	C122–C123	1.388(5)
C123–H123	0.950	C123–C124	1.388(6)
C124–H124	0.950	C124–C125	1.378(6)
C125–H125	0.950	C125–C126	1.390(5)
C126–H126	0.950	C131–C132	1.396(5)
C131–C136	1.386(5)	C132–H132	0.950
C132–C133	1.383(5)	C133–H133	0.950
C133–C134	1.382(6)	C134–H134	0.950
C134–C135	1.385(6)	C135–H135	0.950
C135–C136	1.389(6)	C136–H136	0.950
P2–C211	1.842(4)	P2–C221	1.851(4)
P2–C231	1.851(3)	C211–C212	1.385(5)
C211–C216	1.397(5)	C212–H212	0.950
C212–C213	1.388(5)	C213–H213	0.950
C213–C214	1.376(6)	C214–H214	0.950
C214–C215	1.385(6)	C215–H215	0.950
C215–C216	1.388(6)	C216–H216	0.950
C221–C222	1.397(6)	C221–C226	1.387(5)
C222–H222	0.950	C222–C223	1.381(6)
C223–H223	0.950	C223–C224	1.377(7)
C224–H224	0.950	C224–C225	1.375(7)
C225–H225	0.950	C225–C226	1.395(6)
C226–H226	0.950	C231–C232	1.395(5)
C231–C236	1.399(5)	C232–H232	0.950
C232–C233	1.385(5)	C233–H233	0.950
C233–C234	1.372(7)	C234–H234	0.950
C234–C235	1.381(7)	C235–H235	0.950
C235–C236	1.393(6)	C236–H236	0.950
C2–H2A	1.000	C2–Cl1	1.697(14)
C2–Cl2	1.728(14)	C2–Cl3	1.671(14)
C2'–H2'	1.000	C2'–Cl1'	1.750(15)
C2'–Cl2'	1.704(15)	C2'–Cl3'	1.723(15)
C2"–H2"	1.000	C2"–Cl1"	1.718(16)
C2"–Cl2"	1.721(16)	C2"–Cl3"	1.707(16)

B1–Os5–B2	46.15(16)	B1–Os5–B6	82.65(16)
B1–Os5–B10	44.22(15)	B1–Os5–H56	103.8(17)
B1–Os5–C1	76.10(15)	B1–Os5–P1	141.51(12)
B1–Os5–P2	121.71(12)	B2–Os5–B6	44.75(16)
B2–Os5–B10	81.42(15)	B2–Os5–H56	82.3(17)
B2–Os5–C1	93.88(16)	B2–Os5–P1	102.02(11)
B2–Os5–P2	158.93(12)	B6–Os5–B10	94.34(15)
B6–Os5–H56	40.7(17)	B6–Os5–C1	134.25(16)
B6–Os5–P1	84.53(11)	B6–Os5–P2	126.24(11)
B10–Os5–H56	85.8(17)	B10–Os5–C1	97.67(15)
B10–Os5–P1	173.55(11)	B10–Os5–P2	80.58(11)
H56–Os5–C1	174.4(17)	H56–Os5–P1	89.2(17)
H56–Os5–P2	85.5(17)	C1–Os5–P1	87.59(11)
C1–Os5–P2	99.29(11)	P1–Os5–P2	94.94(3)

Os5–B1–H1	114(2)	Os5–B1–B2	68.09(19)
Os5–B1–B3	117.9(3)	Os5–B1–B4	123.5(3)
Os5–B1–B10	70.65(19)	H1–B1–B2	121(2)
H1–B1–B3	121(2)	H1–B1–B4	112(2)
H1–B1–B10	116(2)	B2–B1–B3	59.6(3)
B2–B1–B4	112.7(3)	B2–B1–B10	118.7(3)
B3–B1–B4	58.9(3)	B3–B1–B10	107.2(3)
B4–B1–B10	60.2(2)	Os5–B2–B1	65.76(19)
Os5–B2–H2	118(2)	Os5–B2–B3	115.7(3)
Os5–B2–B6	65.00(19)	Os5–B2–B7	113.1(3)
B1–B2–H2	120(2)	B1–B2–B3	59.3(3)
B1–B2–B6	114.8(3)	B1–B2–B7	106.1(3)
H2–B2–B3	117(2)	H2–B2–B6	119(2)
H2–B2–B7	121(2)	B3–B2–B6	111.3(3)
B3–B2–B7	58.6(3)	B6–B2–B7	60.5(2)
B1–B3–B2	61.1(3)	B1–B3–H3	124(2)
B1–B3–B4	61.6(3)	B1–B3–B7	109.4(3)
B1–B3–B8	109.0(3)	B2–B3–H3	115(2)
B2–B3–B4	116.3(3)	B2–B3–B7	60.9(3)
B2–B3–B8	117.4(3)	H3–B3–B4	118(2)
H3–B3–B7	115(2)	H3–B3–B8	118(2)
B4–B3–B7	118.5(3)	B4–B3–B8	60.9(3)
B7–B3–B8	68.4(3)	B1–B4–B3	59.5(3)
B1–B4–H4	115(2)	B1–B4–B8	105.7(3)
B1–B4–B9	111.1(3)	B1–B4–B10	58.4(2)
B3–B4–H4	114(2)	B3–B4–B8	58.7(3)
B3–B4–B9	111.2(3)	B3–B4–B10	106.3(3)
H4–B4–B8	125(2)	H4–B4–B9	127(2)
H4–B4–B10	126(2)	B8–B4–B9	61.6(3)
B8–B4–B10	106.8(3)	B9–B4–B10	62.6(3)
Os5–B6–B2	70.3(2)	Os5–B6–H6	127(2)
Os5–B6–B7	117.7(3)	Os5–B6–H56	45.0(18)
Os5–B6–H67	122(2)	B2–B6–H6	129(2)
B2–B6–B7	61.1(3)	B2–B6–H56	110.3(18)
B2–B6–H67	99(2)	H6–B6–B7	114(2)
H6–B6–H56	111(3)	H6–B6–H67	104(3)
B7–B6–H56	124.1(18)	B7–B6–H67	42(2)
H56–B6–H67	96(3)	B2–B7–B3	60.5(3)
B2–B7–B6	58.4(2)	B2–B7–H7	126(2)
B2–B7–B8	106.6(3)	B2–B7–H67	105(2)
B3–B7–B6	111.2(3)	B3–B7–H7	122(2)
B3–B7–B8	55.5(3)	B3–B7–H67	127(2)
B6–B7–H7	118(2)	B6–B7–B8	119.3(3)
B6–B7–H67	51(2)	H7–B7–B8	116(2)
H7–B7–H67	108(3)	B8–B7–H67	88(2)
B3–B8–B4	60.3(3)	B3–B8–B7	56.1(3)
B3–B8–H8	122(2)	B3–B8–B9	108.8(3)
B3–B8–H89	129(2)	B4–B8–B7	107.8(3)
B4–B8–H8	126(2)	B4–B8–B9	57.2(3)
B4–B8–H89	100(2)	B7–B8–H8	115(2)
B7–B8–B9	118.5(3)	B7–B8–H89	95(2)
H8–B8–B9	121(2)	H8–B8–H89	109(3)
B9–B8–H89	45(2)	B4–B9–B8	61.2(3)
B4–B9–H9	127(2)	B4–B9–B10	61.1(3)
B4–B9–H89	105(2)	B4–B9–H910	100.9(19)

B8–B9–H9	126(2)	B8–B9–B10	105.4(3)
B8–B9–H89	46(2)	B8–B9–H910	116(2)
H9–B9–B10	125(2)	H9–B9–H89	110(3)
H9–B9–H910	113(3)	B10–B9–H89	119(2)
B10–B9–H910	42.8(19)	H89–B9–H910	96(3)
Os5–B10–B1	65.12(19)	Os5–B10–B4	119.7(3)
Os5–B10–B9	123.3(3)	Os5–B10–H10	116(2)
Os5–B10–H910	88(2)	B1–B10–B4	61.4(2)
B1–B10–B9	108.4(3)	B1–B10–H10	128(2)
B1–B10–H910	126(2)	B4–B10–B9	56.4(2)
B4–B10–H10	117(2)	B4–B10–H910	102(2)
B9–B10–H10	110(2)	B9–B10–H910	49(2)
H10–B10–H910	106(3)	Os5–C1–O1	172.4(3)
Os5–P1–C111	114.36(11)	Os5–P1–C121	118.83(12)
Os5–P1–C131	115.64(12)	C111–P1–C121	102.29(16)
C111–P1–C131	99.85(16)	C121–P1–C131	103.30(16)
P1–C111–C112	123.3(3)	P1–C111–C116	118.0(3)
C112–C111–C116	118.7(3)	C111–C112–H112	119.8
C111–C112–C113	120.4(4)	H112–C112–C113	119.8
C112–C113–H113	119.8	C112–C113–C114	120.3(4)
H113–C113–C114	119.8	C113–C114–H114	120.2
C113–C114–C115	119.7(4)	H114–C114–C115	120.2
C114–C115–H115	119.9	C114–C115–C116	120.2(4)
H115–C115–C116	119.9	C111–C116–C115	120.6(4)
C111–C116–H116	119.7	C115–C116–H116	119.7
P1–C121–C122	119.6(3)	P1–C121–C126	121.7(3)
C122–C121–C126	118.6(3)	C121–C122–H122	119.6
C121–C122–C123	120.9(4)	H122–C122–C123	119.6
C122–C123–H123	120.1	C122–C123–C124	119.7(4)
H123–C123–C124	120.1	C123–C124–H124	120.0
C123–C124–C125	120.1(3)	H124–C124–C125	120.0
C124–C125–H125	119.9	C124–C125–C126	120.2(4)
H125–C125–C126	119.9	C121–C126–C125	120.5(3)
C121–C126–H126	119.7	C125–C126–H126	119.7
P1–C131–C132	120.6(3)	P1–C131–C136	121.3(3)
C132–C131–C136	118.0(3)	C131–C132–H132	119.6
C131–C132–C133	120.9(4)	H132–C132–C133	119.6
C132–C133–H133	119.8	C132–C133–C134	120.4(4)
H133–C133–C134	119.8	C133–C134–H134	120.2
C133–C134–C135	119.6(4)	H134–C134–C135	120.2
C134–C135–H135	120.1	C134–C135–C136	119.8(4)
H135–C135–C136	120.1	C131–C136–C135	121.3(4)
C131–C136–H136	119.3	C135–C136–H136	119.3
Os5–P2–C211	116.87(12)	Os5–P2–C221	108.71(12)
Os5–P2–C231	123.58(11)	C211–P2–C221	105.05(17)
C211–P2–C231	99.77(17)	C221–P2–C231	100.41(16)
P2–C211–C212	122.1(3)	P2–C211–C216	119.2(3)
C212–C211–C216	118.7(3)	C211–C212–H212	119.6
C211–C212–C213	120.9(4)	H212–C212–C213	119.6
C212–C213–H213	120.0	C212–C213–C214	120.0(4)
H213–C213–C214	120.0	C213–C214–H214	120.0
C213–C214–C215	120.0(4)	H214–C214–C215	120.0
C214–C215–H215	120.0	C214–C215–C216	120.1(4)
H215–C215–C216	120.0	C211–C216–C215	120.3(4)
C211–C216–H216	119.9	C215–C216–H216	119.9

P2–C221–C222	119.5(3)	P2–C221–C226	122.6(3)
C222–C221–C226	117.9(3)	C221–C222–H222	119.3
C221–C222–C223	121.4(4)	H222–C222–C223	119.3
C222–C223–H223	120.0	C222–C223–C224	120.0(4)
H223–C223–C224	120.0	C223–C224–H224	120.2
C223–C224–C225	119.6(4)	H224–C224–C225	120.2
C224–C225–H225	119.7	C224–C225–C226	120.6(4)
H225–C225–C226	119.7	C221–C226–C225	120.4(4)
C221–C226–H226	119.8	C225–C226–H226	119.8
P2–C231–C232	121.4(3)	P2–C231–C236	120.8(3)
C232–C231–C236	117.7(3)	C231–C232–H232	119.4
C231–C232–C233	121.2(4)	H232–C232–C233	119.4
C232–C233–H233	119.8	C232–C233–C234	120.4(4)
H233–C233–C234	119.8	C233–C234–H234	120.1
C233–C234–C235	119.8(4)	H234–C234–C235	120.1
C234–C235–H235	119.9	C234–C235–C236	120.3(4)
H235–C235–C236	119.9	C231–C236–C235	120.6(4)
C231–C236–H236	119.7	C235–C236–H236	119.7
H2A–C2–Cl1	107.9	H2A–C2–Cl2	107.9
H2A–C2–Cl3	107.9	Cl1–C2–Cl2	110.8(11)
Cl1–C2–Cl3	113.8(11)	Cl2–C2–Cl3	108.3(11)
H2'–C2'–Cl1'	111.3	H2'–C2'–Cl2'	111.3
H2'–C2'–Cl3'	111.3	Cl1'–C2'–Cl2'	112.3(13)
Cl1'–C2'–Cl3'	107.5(12)	Cl2'–C2'–Cl3'	102.7(12)
H2"–C2"–Cl1"	117.8	H2"–C2"–Cl2"	117.8
H2"–C2"–Cl3"	117.8	Cl1"–C2"–Cl2"	103.0(15)
Cl1"–C2"–Cl3"	97.4(13)	Cl2"–C2"–Cl3"	99.4(14)

DFT CALCULATIONS

1. Tables of the DFT B3LYP/6-31G*/LANL2DZ optimized geometries (Cartesian coordinates, in Angstroms). Energies (in Hartrees) in parenthesis.

Table S5 Asymmetric isomer, [6,6,6-H(PPh_3)$_2$-*nido*-6-IrB_9H_{13}] (**1**) (-2408.761959)

	x	**y**	**z**
B	-1.02495600	4.28809600	0.17720000
B	-0.11564300	4.38244900	-1.36659800
B	-0.92853200	2.69982500	0.87286700
B	0.43848300	5.32462700	0.05245700
B	0.15127600	4.29526600	1.47452400
B	1.59078700	4.43658200	-0.98529100
B	1.77672700	4.53929800	0.78758300
H	-2.04233900	4.86093100	0.42117900
H	-0.42558500	5.01724600	-2.32710500
H	-1.83910400	2.44601800	1.60028500
H	0.32733400	6.50905400	0.05760000
H	-0.04094200	4.66226900	2.59023700
H	2.43364300	4.92686200	-1.66644500
H	2.71453400	4.97744700	1.36995800
B	-1.06039900	2.92554600	-0.97781000
H	-2.07512500	2.81438100	-1.58722000
Ir	0.01633900	1.01094800	-0.43541800
P	-1.89242500	-0.30362800	-0.01471300
P	1.78727400	-0.56509800	-0.01402500
B	0.59732300	2.85478400	-1.73755600
H	0.89115700	2.62759100	-2.86979000
H	2.22136900	3.66332900	-0.12581600
H	1.24389300	3.55869700	1.52058500
H	0.02949500	1.85214700	1.19397000
H	1.34822900	2.02268700	-0.96600600
H	-0.04038800	0.39630600	-1.90593000
C	1.63401200	-1.95501700	1.21057400
C	2.14262100	-1.84802900	2.51547500
C	0.95228800	-3.13161700	0.85385400
C	1.96528800	-2.88150200	3.43795600
H	2.69213800	-0.96376200	2.81784700
C	0.78265000	-4.16455500	1.77601500
H	0.56368000	-3.25445000	-0.15035700
C	1.28396200	-4.04259600	3.07304800
H	2.37190200	-2.77793300	4.44052100
H	0.25425900	-5.06457100	1.47444400
H	1.14945800	-4.84763900	3.79037700
C	3.24628300	0.37762800	0.64212400
C	4.53938900	0.20802000	0.12451300
C	3.06088600	1.28831900	1.69703400
C	5.61524300	0.92702000	0.65050100

H	4.71414800	-0.48110900	-0.69374400
C	4.14007400	1.99371900	2.23191500
H	2.06716900	1.44816500	2.10488800
C	5.42144600	1.81727800	1.70658700
H	6.60735500	0.78721200	0.22976900
H	3.97355500	2.69170100	3.04735600
H	6.25993500	2.37585200	2.11300700
C	2.48847600	-1.40057300	-1.51220000
C	3.19413500	-2.61309000	-1.43272700
C	2.38627700	-0.76089600	-2.75818000
C	3.76359200	-3.17997100	-2.57443700
H	3.30091900	-3.11985200	-0.47954900
C	2.96316000	-1.32648300	-3.89671900
H	1.85527100	0.18166900	-2.83857200
C	3.64769600	-2.53982900	-3.80972400
H	4.29991700	-4.12186000	-2.49499400
H	2.87355500	-0.81555000	-4.85147000
H	4.09123400	-2.98229400	-4.69770100
C	-1.83154700	-2.01788700	-0.72525000
C	-2.43033900	-3.10632400	-0.07226200
C	-1.21706000	-2.23885600	-1.96960600
C	-2.41053700	-4.37987100	-0.64468800
H	-2.90640300	-2.96889700	0.89188400
C	-1.20164500	-3.51200600	-2.54273100
H	-0.74094300	-1.41544800	-2.49010100
C	-1.79589900	-4.58818800	-1.88039300
H	-2.87710100	-5.20945600	-0.11988100
H	-0.71832600	-3.65955700	-3.50455700
H	-1.78038100	-5.57998100	-2.32427000
C	-2.38360700	-0.56719100	1.74692800
C	-3.71263800	-0.84880200	2.10847600
C	-1.40741500	-0.52358700	2.75153600
C	-4.04973900	-1.08653800	3.44160200
H	-4.48886900	-0.87357400	1.35073300
C	-1.74544100	-0.76413900	4.08391200
H	-0.38134700	-0.29313200	2.49135900
C	-3.06682300	-1.04548000	4.43258800
H	-5.08275700	-1.29760600	3.70469000
H	-0.97410100	-0.72541600	4.84800000
H	-3.33156600	-1.22602700	5.47098500
C	-3.44527100	0.36080600	-0.78242700
C	-4.10636200	1.44853500	-0.18824100
C	-3.96491000	-0.17806700	-1.96758000
C	-5.26452800	1.97187100	-0.75968200
H	-3.71125500	1.89661700	0.71615200
C	-5.12059900	0.35540000	-2.54330400
H	-3.47874500	-1.01961100	-2.44765900
C	-5.77525200	1.42850000	-1.94054800
H	-5.75985600	2.81468500	-0.28576400
H	-5.50751200	-0.07570600	-3.46277300
H	-6.67483900	1.84211100	-2.38838000

Table S6. **S**ymmetric isomer of [6,6,6-H(PPh_3)$_2$-*nido*-6-IrB_9H_{13}] (-2408.752057)

	x	**y**	**z**
B	0.56929400	4.31145700	1.10311500
B	-1.19790200	4.14561800	1.11563100
B	1.27468000	2.89401700	0.37259700
B	-0.42779800	5.42558500	0.11748900
B	1.06333300	4.68514900	-0.53551400
B	-1.77380400	4.43570800	-0.51756000
B	-0.39744600	4.96995800	-1.53307100
H	1.25661200	4.80406400	1.94408100
H	-1.95441000	4.50358700	1.96533600
H	2.39617300	2.67000200	0.68370900
H	-0.52830400	6.56661500	0.43979300
H	2.05960000	5.26325000	-0.83216800
H	-2.86394900	4.82371800	-0.79193500
H	-0.45750300	5.64216400	-2.51118800
B	-0.17030600	2.73364100	1.42029000
H	-0.12430300	2.37971500	2.56108200
Ir	-0.03649000	1.08964000	-0.32868600
P	-1.81413900	-0.49241700	-0.05710500
P	1.85597600	-0.32175900	-0.02475600
B	-1.63401200	2.63331000	0.36936300
H	-2.70099200	2.18958800	0.65253300
H	-1.27117700	3.98107900	-1.66010100
H	0.62826700	4.13276200	-1.66048600
H	1.09841200	2.32546800	-0.84910600
H	-1.31772300	2.17031400	-0.85608000
H	-0.00174600	0.48776900	-1.82851900
C	2.20125200	-1.67267500	-1.25356500
C	3.41398000	-2.38388800	-1.16568100
C	1.34309000	-1.94969500	-2.32236700
C	3.73569100	-3.36389700	-2.10259100
H	4.12108700	-2.15737600	-0.37373200
C	1.66945000	-2.92649000	-3.26706500
H	0.41878000	-1.39635100	-2.42362600
C	2.86193000	-3.63918900	-3.15790500
H	4.67637700	-3.90112600	-2.01641900
H	0.98560100	-3.12489200	-4.08740400
H	3.11718300	-4.39675400	-3.89411500
C	1.89109400	-1.12627400	1.63959100
C	1.63656300	-0.30874900	2.75458200
C	2.16243500	-2.48774900	1.84533900
C	1.67292400	-0.84019800	4.04419200
H	1.40354300	0.74154700	2.61271600
C	2.18394900	-3.01763900	3.13782300
H	2.34946500	-3.14173600	1.00118500
C	1.94420200	-2.19593500	4.23985000
H	1.47904100	-0.19225200	4.89440500
H	2.39105900	-4.07511500	3.27983900
H	1.96394600	-2.61012600	5.24428800
C	3.49597200	0.53352300	-0.13980600
C	4.41674600	0.56415700	0.91330000
C	3.83576900	1.13409800	-1.36281900
C	5.65500400	1.19199100	0.74816700

H	4.17397500	0.10930200	1.86742900
C	5.06952400	1.75966800	-1.52354800
H	3.13095600	1.11919600	-2.18976200
C	5.98355000	1.79167600	-0.46630700
H	6.35829900	1.21341600	1.57632000
H	5.31648000	2.22606500	-2.47330800
H	6.94444600	2.28336600	-0.59083500
C	-1.56189400	-2.23703800	-0.64257400
C	-0.83999600	-3.12720600	0.16950900
C	-2.08490200	-2.70793900	-1.85568900
C	-0.63801800	-4.44865700	-0.22639200
H	-0.44595100	-2.79457200	1.12369800
C	-1.88021000	-4.03262700	-2.25087800
H	-2.66618400	-2.05004900	-2.49215300
C	-1.15511900	-4.90597600	-1.44015900
H	-0.07981600	-5.12196700	0.41859300
H	-2.29998100	-4.38085400	-3.19098700
H	-1.00102400	-5.93698500	-1.74674000
C	-2.46716600	-0.81535600	1.64330400
C	-3.32801100	-1.90540600	1.87576200
C	-2.13013400	0.02080700	2.71433100
C	-3.84792900	-2.13883700	3.14775300
H	-3.59208000	-2.57581400	1.06397400
C	-2.65007400	-0.21974100	3.98913600
H	-1.46605400	0.86028700	2.55537000
C	-3.50939200	-1.29498500	4.20923200
H	-4.51423600	-2.98202300	3.30934900
H	-2.37891200	0.44138300	4.80751300
H	-3.91313500	-1.47916400	5.20132900
C	-3.28515700	0.04697500	-1.04921100
C	-4.58974700	0.01396300	-0.53799100
C	-3.08965600	0.49323600	-2.36790100
C	-5.67188600	0.40770200	-1.32842300
H	-4.76960600	-0.30078700	0.48334900
C	-4.17371400	0.87422400	-3.15903100
H	-2.08456100	0.55846900	-2.77214000
C	-5.46961500	0.83381200	-2.64064600
H	-6.67423800	0.38720300	-0.90939100
H	-4.00143600	1.21563500	-4.17617800
H	-6.31299900	1.14200000	-3.25244600

Table S7 Asymmetric isomer, [6,6,6-H(PPh_3)$_2$-*nido*-6-RhB_9H_{13}] (**2**) (-2413.541592)

	x	**y**	**z**
B	-1.17308900	4.34338100	0.08832100
B	-0.27244100	4.43353100	-1.46759300
B	-1.01959500	2.79749600	0.85603800
B	0.24882900	5.43564700	-0.07734900
B	0.00821400	4.44738600	1.37802500
B	1.43084900	4.56894900	-1.09844600
B	1.62062400	4.71842800	0.67294600
H	-2.21498400	4.88366700	0.30070200
H	-0.62878900	5.03123800	-2.43560800
H	-1.94358900	2.54364500	1.56787600

H	0.08742500	6.61385700	-0.10775700
H	-0.18639300	4.84248000	2.48372400
H	2.25353200	5.07986300	-1.78910300
H	2.54469600	5.20911200	1.23518600
B	-1.14353600	2.94232000	-1.02578700
H	-2.15707000	2.75409600	-1.61799400
Rh	-0.03148900	1.09209800	-0.45757200
P	-1.92874700	-0.25789000	-0.04431700
P	1.83650500	-0.46490900	-0.04058800
B	0.51144600	2.93729800	-1.81077900
H	0.79039800	2.70854800	-2.94756600
H	2.08925700	3.83645200	-0.22248900
H	1.12830200	3.74664200	1.43972600
H	-0.06176200	2.01045100	1.16904500
H	1.24385300	2.14668800	-1.04504000
H	-0.11207600	0.49402100	-1.89456500
C	1.76983400	-1.86053800	1.18220500
C	2.33785900	-1.75611700	2.46223400
C	1.08312500	-3.04158000	0.84863100
C	2.21627500	-2.79917500	3.38344200
H	2.88908200	-0.86613700	2.74466800
C	0.96991000	-4.08352300	1.76882500
H	0.64641900	-3.15965600	-0.13668800
C	1.53189000	-3.96545600	3.04159500
H	2.66837200	-2.69859800	4.36667600
H	0.43734700	-4.98725000	1.48603400
H	1.44060800	-4.77728000	3.75808600
C	3.24731800	0.55864000	0.59175400
C	4.54289900	0.46206900	0.06190900
C	3.01612900	1.46487600	1.64166000
C	5.57852600	1.24790200	0.57251800
H	4.74909800	-0.22227900	-0.75343700
C	4.05667400	2.23659800	2.16174600
H	2.01730600	1.56962300	2.05633400
C	5.34128900	2.13246800	1.62489000
H	6.57368200	1.16439800	0.14404500
H	3.85725500	2.92941000	2.97424900
H	6.14879700	2.74276800	2.01948600
C	2.54581700	-1.26054400	-1.55381700
C	3.29529900	-2.44767300	-1.49932300
C	2.38712400	-0.61859400	-2.79308200
C	3.85723800	-2.98607800	-2.65839600
H	3.44122700	-2.95669800	-0.55241500
C	2.95695200	-1.15557700	-3.94889600
H	1.81751600	0.30307200	-2.85534100
C	3.68851200	-2.34285200	-3.88604400
H	4.42933900	-3.90819100	-2.59866300
H	2.82419300	-0.64365800	-4.89808500
H	4.12656200	-2.76329600	-4.78734400
C	-1.79985300	-1.97298400	-0.74052100
C	-2.36115900	-3.07734600	-0.08040300
C	-1.16825400	-2.18099700	-1.97818300
C	-2.28806800	-4.35414900	-0.64090800
H	-2.85079500	-2.94778400	0.87819700
C	-1.09941600	-3.45773000	-2.53938400

H	-0.72040600	-1.34362100	-2.50252200
C	-1.65652400	-4.54960300	-1.87048000
H	-2.72674300	-5.19647700	-0.11238100
H	-0.60277800	-3.59545200	-3.49582900
H	-1.59921200	-5.54421800	-2.30448700
C	-2.37218100	-0.53165700	1.72716000
C	-3.68912700	-0.80444600	2.13455400
C	-1.35714900	-0.50770400	2.69376200
C	-3.97709800	-1.05041300	3.47798500
H	-4.49259500	-0.81663500	1.40549300
C	-1.64604400	-0.75832000	4.03540600
H	-0.33935500	-0.28601600	2.39449600
C	-2.95686400	-1.02855900	4.43103800
H	-5.00128100	-1.25422700	3.77870300
H	-0.84565000	-0.73654700	4.76969000
H	-3.18407900	-1.21634800	5.47700000
C	-3.51269200	0.33959200	-0.79618200
C	-4.18353700	1.43395100	-0.22491100
C	-4.04896700	-0.25503500	-1.94712600
C	-5.36868900	1.90813100	-0.78378300
H	-3.77462800	1.92530200	0.65056300
C	-5.23153300	0.23018600	-2.51073200
H	-3.55390100	-1.10160700	-2.40930700
C	-5.89624500	1.30945200	-1.93003500
H	-5.87165700	2.75650500	-0.32821200
H	-5.63142900	-0.24314500	-3.40348900
H	-6.81655900	1.68538200	-2.36884700

Table S8 Symmetric isomer, [6,6,6-H(PPh_3)$_2$-*nido*-6-RhB_9H_{13}] (**1**) (-2413.528223)

	x	**y**	**z**
B	0.62641100	4.42842100	1.01388500
B	-1.13923100	4.29699000	0.99976600
B	1.31196800	2.96892300	0.33272600
B	-0.32714300	5.52180400	-0.03370000
B	1.16135400	4.72168700	-0.63085200
B	-1.68211300	4.52965400	-0.65720100
B	-0.27697100	5.00993700	-1.66794100
H	1.30988500	4.93523700	1.84971800
H	-1.90269500	4.69902200	1.82331300
H	2.41895600	2.71525400	0.67980900
H	-0.41123900	6.67679600	0.24087900
H	2.17484300	5.26822600	-0.92991600
H	-2.75956600	4.92715200	-0.96692300
H	-0.30664300	5.66274900	-2.66080000
B	-0.14706200	2.87366600	1.35681800
H	-0.12852200	2.53564400	2.50448100
Rh	-0.01971500	1.15858200	-0.35229800
P	-1.85055700	-0.39188900	-0.07770300
P	1.88025000	-0.26865300	-0.04468800
B	-1.59460100	2.76565700	0.28706700
H	-2.66825200	2.34402700	0.58479500
H	-1.16469700	4.04175900	-1.78628900
H	0.72894100	4.15512900	-1.75630400

H	1.13335800	2.39366900	-0.84828200
H	-1.27894100	2.27701400	-0.89037600
H	0.01338200	0.53008100	-1.80897600
C	2.19013300	-1.66338600	-1.22858200
C	3.38310900	-2.40456200	-1.12191800
C	1.32107000	-1.94521500	-2.28740100
C	3.67508700	-3.41776600	-2.03285500
H	4.09704500	-2.17616600	-0.33654400
C	1.61799500	-2.95576000	-3.20574500
H	0.41126000	-1.36912000	-2.40004800
C	2.79123900	-3.69705500	-3.07886600
H	4.60073300	-3.97844000	-1.93427600
H	0.92685400	-3.15835000	-4.01886000
H	3.02391400	-4.48100300	-3.79462700
C	1.91172200	-1.00879000	1.64648500
C	1.71097700	-0.13856200	2.73279100
C	2.11374300	-2.37467900	1.89822400
C	1.73372200	-0.62507000	4.04008500
H	1.52815300	0.91646500	2.55451300
C	2.12273300	-2.85780700	3.20909600
H	2.25880700	-3.06675900	1.07623200
C	1.93736300	-1.98539200	4.28224800
H	1.58221600	0.06184300	4.86800200
H	2.27736700	-3.91864200	3.38801800
H	1.94624600	-2.36368900	5.30087600
C	3.52064000	0.57289400	-0.20625800
C	4.47096200	0.59562400	0.82099800
C	3.83071900	1.16997000	-1.43857400
C	5.70988700	1.21098400	0.61991500
H	4.25050500	0.14483900	1.78255400
C	5.06593200	1.78249600	-1.63508100
H	3.10151600	1.16400300	-2.24417600
C	6.00974700	1.80623500	-0.60430500
H	6.43647600	1.22659600	1.42783800
H	5.28985300	2.24689700	-2.59147200
H	6.97121300	2.28894800	-0.75629800
C	-1.62520500	-2.15014500	-0.62780200
C	-0.91006400	-3.03216500	0.19949700
C	-2.15500800	-2.63749700	-1.83146000
C	-0.72546900	-4.36346400	-0.17067000
H	-0.50731200	-2.68440400	1.14502000
C	-1.96663000	-3.97198500	-2.20106100
H	-2.72896400	-1.98420800	-2.47943000
C	-1.25099000	-4.83812000	-1.37432200
H	-0.17350900	-5.03098500	0.48562300
H	-2.39181800	-4.33336300	-3.13375800
H	-1.10983700	-5.87665400	-1.66103200
C	-2.52409800	-0.66044800	1.62285700
C	-3.39422200	-1.73702100	1.88167100
C	-2.19003700	0.20868600	2.66883200
C	-3.92601700	-1.92577000	3.15621800
H	-3.65670800	-2.43048500	1.08898300
C	-2.72195300	0.01197800	3.94611100
H	-1.52016600	1.03963500	2.48722000
C	-3.58988800	-1.05072300	4.19290400

H	-4.59991100	-2.75852000	3.33919200
H	-2.45341000	0.69721600	4.74525100
H	-4.00264000	-1.20077800	5.18703900
C	-3.28991300	0.16607700	-1.10053000
C	-4.60316800	0.16113900	-0.61045800
C	-3.06249700	0.59862000	-2.41814400
C	-5.66358300	0.57000700	-1.42209700
H	-4.80526900	-0.14499500	0.40958800
C	-4.12524300	0.99517900	-3.23022300
H	-2.04913000	0.64093100	-2.80528900
C	-5.43014300	0.98368200	-2.73330200
H	-6.67341100	0.57114000	-1.02092500
H	-3.92934700	1.32676900	-4.24631500
H	-6.25669600	1.30462900	-3.36127200

Table S9 Asymmetric isomer, [6,6,6-$CO(PPh_3)_2$-*nido*-6-RuB_9H_{13}] (**3**) (-2510.678579)

	x	**y**	**z**
B	-0.59108800	4.39980300	0.15572300
B	0.36996300	4.48482400	-1.35302600
B	-0.71604800	2.75679600	0.70922400
B	0.99447500	5.24390800	0.14487700
B	0.52564900	4.16654000	1.47978800
B	2.05851900	4.28083200	-0.92102000
B	2.19099200	4.23811900	0.86140700
H	-1.54161700	5.07244600	0.41617000
H	0.17591600	5.21540300	-2.27455600
H	-1.65682000	2.56635500	1.41585500
H	1.03827800	6.42952700	0.23209600
H	0.33218700	4.47522200	2.61268100
H	2.98496100	4.70079700	-1.53810300
H	3.15681800	4.50683300	1.49736200
B	-0.75531300	3.12720900	-1.08962500
H	-1.74868700	3.19017800	-1.74363000
P	-2.01828500	-0.15634600	-0.00652500
P	1.81756100	-0.59580300	-0.05790000
B	0.91025600	2.91214200	-1.80522700
H	1.18309200	2.74248600	-2.95503000
H	2.54988200	3.37720000	-0.09855800
H	1.51084600	3.28937200	1.50910600
H	0.13106500	1.80472300	0.95885800
H	1.48410600	1.95213100	-1.10193800
C	1.57520900	-2.25126000	0.74912300
C	1.98153100	-2.53536800	2.06230100
C	0.97110500	-3.27369300	-0.00184700
C	1.77769200	-3.80464000	2.61120200
H	2.47248000	-1.77556100	2.65979800
C	0.77925400	-4.54183400	0.54352700
H	0.65796100	-3.08463900	-1.02292300
C	1.17773700	-4.81096500	1.85517600
H	2.10207900	-4.00474000	3.62902600
H	0.31087000	-5.31568100	-0.05713500
H	1.02463300	-5.79862400	2.28163900
C	2.93582500	0.27471500	1.14248700

C	4.30440300	0.45313200	0.89072800
C	2.40518000	0.76805500	2.34842200
C	5.12035600	1.10075300	1.82232700
H	4.74101500	0.08749100	-0.03176200
C	3.22575300	1.39830200	3.28443700
H	1.34504400	0.66480400	2.56105200
C	4.58710600	1.56878300	3.02267100
H	6.17615800	1.23618800	1.60420900
H	2.79548800	1.76990000	4.21027600
H	5.22328200	2.07199100	3.74531100
C	2.96586100	-1.03936900	-1.44861000
C	3.77565700	-2.18760800	-1.38864900
C	3.08331700	-0.19328500	-2.56270700
C	4.66619200	-2.48496700	-2.42057000
H	3.71276500	-2.85358700	-0.53491100
C	3.97845000	-0.49164300	-3.59237200
H	2.48342300	0.70607100	-2.63358700
C	4.76859400	-1.63924400	-3.52706000
H	5.28013600	-3.37947700	-2.35731700
H	4.05020900	0.17605000	-4.44630100
H	5.46013700	-1.87379300	-4.33176900
C	-2.19976400	-1.96039500	-0.42643400
C	-2.73582000	-2.87670000	0.49124900
C	-1.89291400	-2.41445300	-1.72079600
C	-2.95299800	-4.20780200	0.12807800
H	-2.99275600	-2.55492200	1.49381100
C	-2.11994400	-3.74238800	-2.08616600
H	-1.49273400	-1.73358400	-2.46194600
C	-2.64896600	-4.64544200	-1.16114100
H	-3.36827200	-4.89928900	0.85635900
H	-1.88501200	-4.06703000	-3.09633300
H	-2.82829500	-5.67880800	-1.44603900
C	-2.34819000	-0.14608500	1.81416300
C	-3.56472200	0.27667000	2.36635000
C	-1.33974200	-0.60870100	2.67464200
C	-3.75936100	0.25408300	3.75001200
H	-4.36090200	0.63155100	1.72202000
C	-1.53969700	-0.64091300	4.05408600
H	-0.40119600	-0.96567400	2.26423400
C	-2.74962100	-0.20148000	4.59718200
H	-4.70501200	0.59566400	4.16209400
H	-0.74966700	-1.00880900	4.70338900
H	-2.90362800	-0.21668400	5.67270300
C	-3.57592600	0.53600000	-0.75260500
C	-3.89848900	1.89114800	-0.55999600
C	-4.45774200	-0.26018300	-1.50187700
C	-5.06857600	2.42777000	-1.09643900
H	-3.23829200	2.53105000	0.00975700
C	-5.62183100	0.28485300	-2.04853600
H	-4.24916800	-1.31019700	-1.66473000
C	-5.93225500	1.62896000	-1.84772500
H	-5.29438500	3.47787600	-0.93389400
H	-6.28574100	-0.35011600	-2.62916300
H	-6.83829200	2.05175900	-2.27351900
Ru	0.04321600	1.00153300	-0.67746000

C	-0.17027400	0.40139900	-2.44567400
O	-0.33554700	0.10935200	-3.55429900

Table S10 Symmetric isomer, [6,6,6-CO(PPh_3)$_2$-*nido*-6-RuB_9H_{13}] (**3**) (-2510.670697)

	x	**y**	**z**
B	-1.00356800	-4.23396200	0.86605200
B	0.77321200	-4.27358000	0.90896000
B	-1.53426000	-2.80153400	0.03914300
B	-0.11738600	-5.50504900	-0.04009400
B	-1.50585800	-4.64559600	-0.76350600
B	1.34267000	-4.70968500	-0.68925300
B	-0.06439300	-5.12171400	-1.71287000
H	-1.75034500	-4.60443500	1.71835000
H	1.45859500	-4.67291700	1.79968200
H	-2.64264900	-2.44423400	0.28269700
H	-0.15222000	-6.63418600	0.33330100
H	-2.55342300	-5.12455100	-1.06105800
H	2.38346600	-5.23252000	-0.93063400
H	-0.05511900	-5.82970600	-2.66702000
B	-0.08580700	-2.72453400	1.11264500
H	-0.09124100	-2.29875200	2.22625800
P	1.89105900	0.27452500	0.07943900
P	-1.90165700	0.35884200	-0.06170300
B	1.40343300	-2.86104400	0.11652700
H	2.50798200	-2.56159200	0.43668300
H	0.91272800	-4.22778500	-1.84583100
H	-0.99407800	-4.18745400	-1.89617400
H	-1.20290700	-2.31736200	-1.14005700
H	1.18173100	-2.35466000	-1.08240300
C	-1.58556700	2.18160700	0.09716400
C	-1.79970000	2.88109000	1.29446400
C	-1.17928700	2.90075900	-1.03902000
C	-1.60638700	4.26435600	1.35400200
H	-2.13450000	2.35233600	2.17994000
C	-1.00177000	4.28183000	-0.98123700
H	-1.01804400	2.38458700	-1.98031100
C	-1.21117900	4.96821800	0.21712500
H	-1.78049600	4.78921200	2.28967000
H	-0.69001300	4.81951100	-1.87147700
H	-1.07036400	6.04476900	0.26133500
C	-2.81140100	-0.02031100	1.50469800
C	-4.21228800	-0.05919400	1.56641400
C	-2.07424800	-0.24945900	2.67682400
C	-4.85916800	-0.31605800	2.77670900
H	-4.80525400	0.09719700	0.67276300
C	-2.72470800	-0.49455700	3.88626600
H	-0.99164700	-0.25790100	2.64681100
C	-4.11914100	-0.53056800	3.93986100
H	-5.94488500	-0.35326000	2.80486800
H	-2.13605000	-0.67496800	4.78142900
H	-4.62516900	-0.73412400	4.87974500
C	-3.23589200	0.37770100	-1.35850600
C	-4.11188400	1.47455000	-1.46038500

C	-3.41749700	-0.70142200	-2.23586900
C	-5.13080500	1.48987700	-2.41289600
H	-3.99900300	2.32524100	-0.79686700
C	-4.43734600	-0.68422400	-3.18976800
H	-2.76631200	-1.56345200	-2.18013900
C	-5.29560400	0.41067500	-3.28323200
H	-5.79343000	2.34900500	-2.47472400
H	-4.55504800	-1.53124500	-3.85985400
H	-6.08628700	0.42467700	-4.02847600
C	2.07288600	2.03922500	-0.49725100
C	2.45704400	3.09682900	0.33895500
C	2.00320100	2.27449800	-1.88084400
C	2.74075700	4.35794500	-0.19212500
H	2.55364100	2.94565900	1.40744700
C	2.29907200	3.52910000	-2.41091700
H	1.73764900	1.47157300	-2.55946200
C	2.66477800	4.57957500	-1.56629600
H	3.03392400	5.16342300	0.47607900
H	2.24806100	3.68223300	-3.48566700
H	2.89776700	5.55809400	-1.97764400
C	2.03721400	0.34181800	1.91809100
C	2.84060600	-0.57354700	2.61703500
C	1.24299400	1.23702000	2.65501600
C	2.86889900	-0.57222500	4.01219200
H	3.43683400	-1.29881700	2.07632100
C	1.27942200	1.24005000	4.05065700
H	0.59158900	1.93903400	2.14455800
C	2.09476700	0.33697500	4.73427900
H	3.49536400	-1.29110200	4.53270200
H	0.66410300	1.94744800	4.60030000
H	2.12072000	0.33659700	5.82051000
C	3.56043800	-0.27959700	-0.52431300
C	3.67910100	-1.01990700	-1.70785100
C	4.72976200	0.16706000	0.11205200
C	4.93591200	-1.32614300	-2.23235500
H	2.78925700	-1.36860900	-2.21943800
C	5.98526700	-0.14827200	-0.40722200
H	4.66489500	0.76449900	1.01585300
C	6.09235600	-0.89741800	-1.58054400
H	5.00710400	-1.90754500	-3.14745000
H	6.87955400	0.19694300	0.10469200
H	7.07067400	-1.14216900	-1.98504100
Ru	-0.00636300	-1.11510100	-0.63065700
C	0.00397000	-0.43775900	-2.40183200
O	-0.00573200	-0.21897800	-3.54293700

Table S11 Asymmetric isomer, [6,6,6-$CO(PPh_3)_2$-*nido*-6-OsB_9H_{13}] (**4**) (-2507.866089)

	x	**y**	**x**
B	-0.50410600	4.31643700	0.31720800
B	0.42926300	4.42613600	-1.20408600
B	-0.65665300	2.65597600	0.81291900
B	1.09746900	5.12630900	0.30342300
B	0.63037800	4.01447800	1.61172600

B	2.12018000	4.17368900	-0.81078200
B	2.28639700	4.07889300	0.96680100
H	-1.43455900	4.99681700	0.62523100
H	0.24174900	5.18480600	-2.10397900
H	-1.57789900	2.45557900	1.54073200
H	1.16785300	6.30736600	0.42692900
H	0.46022300	4.29087600	2.75655000
H	3.04022900	4.59129500	-1.43863800
H	3.26796500	4.31056100	1.59305400
B	-0.72483400	3.09264300	-0.96314100
H	-1.72771600	3.20021400	-1.59540100
P	-2.00240400	-0.20229300	0.03828500
P	1.78353900	-0.66606700	-0.01803100
B	0.91428600	2.84957200	-1.70884900
H	1.17523600	2.69721500	-2.86277400
H	2.61489500	3.24092000	-0.02410300
H	1.60127700	3.12174900	1.59920900
H	0.18831700	1.67143400	1.04556400
H	1.52446600	1.85633500	-1.02576000
C	1.49294500	-2.34470500	0.72471100
C	1.85570400	-2.68039600	2.03835200
C	0.90517400	-3.33301100	-0.08229100
C	1.62244700	-3.96650300	2.53399600
H	2.33600800	-1.94865500	2.67817100
C	0.68401400	-4.61781500	0.40994800
H	0.62773300	-3.10377900	-1.10526700
C	1.03765500	-4.93818500	1.72305100
H	1.91253000	-4.20688600	3.55345300
H	0.22823300	-5.36473400	-0.23291200
H	0.86219700	-5.93911500	2.10793500
C	2.90125400	0.13967400	1.23013400
C	4.27365700	0.31027300	0.99445100
C	2.37064600	0.59148500	2.45243300
C	5.09264600	0.90869900	1.95618700
H	4.71217200	-0.02199200	0.06056300
C	3.19336700	1.17261700	3.41768000
H	1.30823500	0.49639700	2.65575800
C	4.55865700	1.33492300	3.17134300
H	6.15117800	1.03927500	1.74878900
H	2.76181000	1.51247100	4.35501300
H	5.19691800	1.79958800	3.91756600
C	2.95295600	-1.09727500	-1.39711100
C	3.76804900	-2.24103300	-1.31852700
C	3.08866200	-0.25327700	-2.51003500
C	4.68130800	-2.53581400	-2.33076600
H	3.69192100	-2.90531100	-0.46454500
C	4.00534900	-0.54992300	-3.52138600
H	2.48455000	0.64134500	-2.59705700
C	4.80070000	-1.69235700	-3.43744800
H	5.29866200	-3.42677300	-2.25276100
H	4.08948000	0.11562400	-4.37580900
H	5.50941500	-1.92490400	-4.22766600
C	-2.23590600	-1.99364900	-0.41441800
C	-2.79182400	-2.90959300	0.49148000
C	-1.95058400	-2.43483400	-1.71844900

C	-3.04817400	-4.22828800	0.10879900
H	-3.03290900	-2.59849100	1.50120300
C	-2.21766800	-3.74981900	-2.10303700
H	-1.53765500	-1.75451900	-2.45288200
C	-2.76537200	-4.65308200	-1.18922700
H	-3.47710200	-4.91962400	0.82926100
H	-1.99914600	-4.06394200	-3.12021100
H	-2.97538500	-5.67626200	-1.48959000
C	-2.34868400	-0.21795200	1.85681300
C	-3.57261900	0.18905100	2.40487200
C	-1.35053500	-0.69900400	2.71840400
C	-3.78209500	0.13711700	3.78559100
H	-4.36349100	0.55466200	1.76025000
C	-1.56462700	-0.76079700	4.09472700
H	-0.40969200	-1.04880600	2.30855300
C	-2.78062200	-0.33403900	4.63405800
H	-4.73301800	0.46787000	4.19435200
H	-0.78142300	-1.14226100	4.74446800
H	-2.94619700	-0.37199100	5.70729900
C	-3.53851100	0.54825200	-0.70128000
C	-3.85752900	1.89175100	-0.43431100
C	-4.40611200	-0.19250700	-1.51994200
C	-5.00965700	2.46975500	-0.96615400
H	-3.20964900	2.49071900	0.19151700
C	-5.55176100	0.39453200	-2.06267700
H	-4.20154100	-1.23259500	-1.74032800
C	-5.85865700	1.72594600	-1.78757600
H	-5.23298700	3.50959900	-0.74477500
H	-6.20408900	-0.19852900	-2.69811400
H	-6.75045800	2.18169000	-2.20939800
Os	0.05893800	0.92629400	-0.62279500
C	-0.12900200	0.30254100	-2.38248800
O	-0.27100500	-0.01067400	-3.49454700

Table S12 [1,1,1-(CO)H(PPh_3)-*isocloso*-1-RuB_9H_8-μ-(1,2)-{$Pt(PMe_2Ph)_2$}] (**6**) (-2896.913038)

	x	**y**	**z**
Pt	-1.34680400	-0.79062800	-0.34213500
Ru	1.55691900	-1.53722600	-0.54189700
H	0.24207900	-0.19542200	-0.79685900
B	-0.19343700	-2.41232700	0.18867900
B	1.95792700	-3.49446800	-1.50371500
H	2.36101000	-3.65208100	-2.61162000
B	2.52396000	-2.44400600	1.23188500
H	3.31788300	-1.91351400	1.94101300
B	0.28995700	-3.56644700	-1.03277700
H	-0.48828000	-3.75934100	-1.91879700
B	2.90554800	-3.52787300	-0.05512900
H	4.06953900	-3.74659600	-0.23078600
B	0.84035900	-2.59262100	1.57215500
H	0.45124500	-2.10739700	2.59295200
B	0.16889100	-4.02510500	0.70697800
H	-0.64935500	-4.77768800	1.15300900

B	1.51088600	-4.66725100	-0.31579000
H	1.60924200	-5.83523000	-0.54079700
B	1.85532700	-4.04731200	1.33698600
H	2.18558100	-4.81525600	2.18917100
C	2.04479700	-1.05599700	-2.37132700
O	2.30033700	-0.79768800	-3.46401800
P	-2.19833600	1.22280200	-1.44896800
C	-2.39375600	2.76608500	-0.45360300
C	-2.88864300	3.95846300	-1.00499900
H	-3.18568900	3.99720900	-2.05001600
C	-3.00342400	5.10967200	-0.22519100
H	-3.38944700	6.02495000	-0.66637100
C	-2.62263900	5.08663400	1.11954900
H	-2.71198500	5.98401400	1.72604200
C	-2.12801800	3.90761100	1.67963800
H	-1.82560200	3.88284200	2.72326900
C	-2.01613200	2.75556500	0.89690500
H	-1.62456700	1.83761500	1.32752200
C	-3.82509400	1.06953600	-2.32537100
H	-3.77006000	0.20980000	-3.00161000
H	-4.05956400	1.96301400	-2.91383300
H	-4.62752600	0.89348300	-1.60568900
C	-1.10753900	1.75571200	-2.84536000
H	-0.11646700	2.00487200	-2.46025500
H	-1.51557500	2.62030600	-3.38016900
H	-1.00489700	0.91857200	-3.54361900
P	-3.21109500	-1.87787400	0.48321800
C	-4.80361100	-0.94785900	0.54978900
C	-5.95682300	-1.36614000	-0.12998700
H	-5.94283600	-2.27017300	-0.73017700
C	-7.13988900	-0.62620900	-0.04699400
H	-8.02319800	-0.96454800	-0.58205000
C	-7.18810400	0.53801400	0.71988900
H	-8.10854300	1.11171900	0.78498000
C	-6.04535800	0.96419800	1.40250500
H	-6.07183800	1.87232000	1.99854900
C	-4.86332800	0.23004700	1.31400700
H	-3.97716100	0.58471500	1.83358300
C	-3.05060400	-2.45951300	2.22998200
H	-2.19277900	-3.13234800	2.30247800
H	-3.96222300	-2.97695500	2.54692200
H	-2.87365900	-1.60609000	2.89012500
C	-3.61222900	-3.43159600	-0.42271800
H	-3.82032400	-3.21692800	-1.47471100
H	-4.46511100	-3.95298000	0.02457000
H	-2.72977000	-4.07471000	-0.37936900
P	2.83169000	0.46775000	0.27012400
C	4.66947700	0.44222800	0.06699800
C	5.33669200	-0.76849100	-0.16486800
H	4.77660900	-1.69372600	-0.22094800
C	6.72471800	-0.79140500	-0.32601500
H	7.22436700	-1.73900200	-0.50698400
C	7.46122800	0.39059300	-0.25827300
H	8.54032700	0.37060400	-0.38604600
C	6.80538600	1.60380400	-0.03217100

H	7.37092300	2.53069000	0.01545900
C	5.42030800	1.63157600	0.12498700
H	4.92158500	2.58321800	0.28220700
C	2.52843300	0.89590600	2.04125200
C	3.54330400	1.33152600	2.90497000
H	4.56627600	1.40510800	2.55325500
C	3.25051600	1.66074000	4.23002000
H	4.04985900	1.98874000	4.88919600
C	1.94332200	1.56273100	4.70785000
H	1.71906700	1.81615800	5.74060500
C	0.92882800	1.11969800	3.85697900
H	-0.08785000	1.01671000	4.22748900
C	1.21902000	0.77815600	2.53562600
H	0.43384200	0.39331900	1.89115800
C	2.41301000	2.04578400	-0.62022400
C	1.61174100	3.04327300	-0.04743300
H	1.23181100	2.92414500	0.96094200
C	1.29965100	4.20468000	-0.76034900
H	0.67274700	4.96164100	-0.29721300
C	1.78765000	4.38884900	-2.05381900
H	1.54965400	5.29433000	-2.60565200
C	2.58656800	3.40067100	-2.63566000
H	2.97519700	3.53318900	-3.64186900
C	2.89391700	2.23902400	-1.92760600
H	3.52782600	1.49064200	-2.39275600

Table S13 [7,7-$(PMe_2Ph)_2$-9,9,9-$(CO)(PPh_3)_2$-*nido*-7,9-$PtOsB_9H_{11}$] (**7**). (-3931.277498)

	x	**y**	**z**
B	-1.26459500	-0.06378600	-3.43509500
H	-1.55029400	0.37008200	-4.50994300
B	-2.46243500	-0.94182100	-2.51601900
H	-3.56596000	-1.12303500	-2.95035500
B	-1.08799800	-1.80362700	-3.16775600
H	-1.20354400	-2.59838300	-4.05126000
B	0.33754800	-0.72098800	-3.07592100
H	1.08143600	-0.84798200	-4.00208800
B	-1.64070500	-2.21168700	-1.55146400
H	-2.03868900	-3.29900400	-1.28129600
B	-1.88395500	0.74023200	-1.97954200
H	-2.60845100	1.68762600	-2.06845400
Pt	-2.69381300	-0.55186600	-0.30816000
B	-0.69653700	0.78939900	-0.66663900
H	-0.73538100	1.74251500	0.05272200
Os	1.43521500	-0.19229100	-1.11853400
B	0.16451900	-2.06857700	-1.90921400
H	0.70189200	-3.13079600	-1.91448400
B	-0.16556200	0.89157800	-2.39704100
H	0.15789100	1.93736900	-2.86749900
H	-0.55998800	-2.03016300	-0.81234000
H	-0.00403300	-0.11769400	0.01382500
C	2.81937000	-0.18860200	-2.38037900
O	3.64479600	-0.14885700	-3.20495200
P	-3.21749900	1.05907800	1.42056600

C	-3.36849100	2.80074300	0.84922100
C	-4.34414900	3.09736600	-0.11646700
H	-4.95573700	2.30099200	-0.53177200
C	-4.52771700	4.40579200	-0.56026400
H	-5.28536200	4.61905400	-1.30930400
C	-3.72991100	5.43582400	-0.05577400
H	-3.86897100	6.45501900	-0.40624300
C	-2.75058400	5.14874400	0.89533800
H	-2.12128800	5.94329800	1.28762800
C	-2.56995300	3.83893800	1.34810700
H	-1.79597200	3.63735300	2.08103200
C	-4.79140300	0.90644400	2.39532600
H	-5.65558700	0.95197300	1.72964000
H	-4.85939300	1.71955400	3.12558400
H	-4.81435100	-0.05049000	2.92521200
C	-1.98314800	1.08825500	2.78825900
H	-1.97805400	0.09922400	3.25745300
H	-2.23452400	1.83727600	3.54614200
H	-0.98577400	1.28809700	2.39536400
P	-4.43908400	-2.14649600	0.21326000
C	-6.10167900	-1.35958700	0.07225900
C	-7.16075300	-1.63164300	0.95050400
H	-7.02468400	-2.31505600	1.78343800
C	-8.40666900	-1.02588100	0.76996900
H	-9.21592300	-1.24360500	1.46206200
C	-8.61264700	-0.14808100	-0.29543000
H	-9.58295100	0.32026900	-0.43632000
C	-7.56633000	0.12426300	-1.18032000
H	-7.71966800	0.80254000	-2.01537700
C	-6.31733400	-0.47125700	-0.99625700
H	-5.50423800	-0.24933000	-1.68273900
C	-4.66147400	-3.60444800	-0.90544500
H	-4.64274100	-3.27173900	-1.94612400
H	-5.62122000	-4.08500000	-0.68925800
H	-3.84808200	-4.31796800	-0.75970100
C	-4.42319000	-2.98183500	1.86594200
H	-5.21523900	-3.73304500	1.95627700
H	-4.52317800	-2.25450200	2.67642300
H	-3.45312600	-3.47742100	1.96938100
P	2.47579000	-1.94200700	0.21286600
C	3.47121900	-3.21559300	-0.72260300
C	4.32126700	-4.09571200	-0.02644600
H	4.40203500	-4.03254700	1.05381800
C	5.07333900	-5.05291400	-0.70650200
H	5.72333100	-5.72123000	-0.14755700
C	4.99683800	-5.14593500	-2.09813500
H	5.58840400	-5.88671200	-2.62985100
C	4.15757200	-4.28145000	-2.79919600
H	4.08650300	-4.34282500	-3.88154000
C	3.39766000	-3.32709100	-2.11786100
H	2.74048900	-2.67792500	-2.67911800
C	3.71255600	-1.61171800	1.57971500
C	3.47606700	-1.87626600	2.93764400
H	2.52870700	-2.29624000	3.25630000
C	4.46064800	-1.62261500	3.89814100

H	4.25584400	-1.83941100	4.94371500
C	5.70079500	-1.11245600	3.51775300
H	6.46734600	-0.92092900	4.26403700
C	5.95253700	-0.85574700	2.16769000
H	6.91326500	-0.45797300	1.85485400
C	4.96807500	-1.09964700	1.21196600
H	5.18476000	-0.90027100	0.16809500
C	1.22167300	-2.96892800	1.13131100
C	0.33090500	-2.32922800	2.00894500
H	0.34771900	-1.24776500	2.10283500
C	-0.58047000	-3.06583800	2.76596000
H	-1.24361400	-2.55272200	3.45825800
C	-0.64127200	-4.45612800	2.63641100
H	-1.34887500	-5.03205900	3.22762500
C	0.21467300	-5.09825100	1.74196600
H	0.16789900	-6.17711800	1.61982300
C	1.14338400	-4.36240100	1.00107400
H	1.80446700	-4.88083700	0.31649600
P	2.36766700	1.89951300	-0.11520600
C	4.21205100	2.05167200	0.16789400
C	5.11257400	1.65095100	-0.83460300
H	4.75204600	1.20521900	-1.75209200
C	6.48790000	1.83951700	-0.68343500
H	7.15886100	1.52731500	-1.47939200
C	6.99575000	2.42664700	0.47701700
H	8.06608900	2.57530200	0.59429500
C	6.11381400	2.82700800	1.48051600
H	6.49234200	3.28801400	2.38923300
C	4.73753000	2.64684900	1.32587200
H	4.07777600	2.97743300	2.11880600
C	2.07184400	3.45574200	-1.10528200
C	3.12158000	4.16100500	-1.71419800
H	4.14511800	3.82346000	-1.61024000
C	2.87200600	5.31550500	-2.46066000
H	3.70362500	5.83850500	-2.92571100
C	1.57179400	5.79703900	-2.60151600
H	1.37933100	6.69725100	-3.17941000
C	0.51889200	5.10814800	-1.99734800
H	-0.50311100	5.46182400	-2.10214400
C	0.76327800	3.94473300	-1.26864200
H	-0.07280100	3.41699000	-0.82904800
C	1.75260400	2.37203800	1.57830600
C	1.35034600	3.67034500	1.92619800
H	1.31608700	4.44814800	1.17210900
C	1.00218600	3.97966100	3.24496500
H	0.69678900	4.99312600	3.49341800
C	1.06460600	3.00341600	4.24069700
H	0.80559900	3.25011400	5.26708100
C	1.47555500	1.71074900	3.90791400
H	1.54497500	0.94254400	4.67367800
C	1.80780400	1.39886500	2.58874200
H	2.14729200	0.39777700	2.35071700

2. Tables of the DFT B3LYP/6-31G*/LANL2DZ optimized geometries found for the PH_3-ligated models in the relaxed potential energy scan (PES) upon the rotation of the {$M(X)(PH_3)_2$} ligand sphere (Cartesian coordinates, in Angstroms). Energies (in Hartrees) in parentheses.

2.1 [6,6,6-$H(PH_3)_2$-*nido*-6-RhB_9H_{13}] model

Table S14 Low-energy asymmetric conformer

	x	y	z
B	2.30143200	1.35694300	0.28031000
B	2.47664600	0.37245000	-1.22369000
B	0.78721600	1.10780100	1.06717300
B	3.50735300	0.02464700	0.19925300
B	2.50428500	0.27029800	1.64628500
B	2.74740600	-1.28579300	-0.74189600
B	2.90181000	-1.35618000	1.03677300
H	2.74420700	2.45366200	0.42067200
H	3.05447700	0.71744700	-2.20633300
H	0.40516300	2.04916800	1.69872200
H	4.66684100	0.28125100	0.15200100
H	2.88293200	0.57039000	2.73231800
H	3.31455000	-2.11246500	-1.37958800
H	3.46259500	-2.20923200	1.64282000
B	0.91319800	1.14243800	-0.83131800
H	0.62008000	2.11254700	-1.46079600
Rh	-0.80775300	-0.10487600	-0.21560800
P	-2.11365100	1.75878700	0.14055600
P	-2.43940600	-1.73356300	0.39408900
B	1.05008700	-0.54192800	-1.54215500
H	0.86974600	-0.90201500	-2.66095100
H	2.05358200	-1.93487100	0.17237900
H	1.90598700	-0.90240400	1.79023700
H	0.10741500	0.07677300	1.40518700
H	0.29074400	-1.33059700	-0.76018400
H	-1.47311300	-0.19575400	-1.63861300
H	-2.55338000	-2.19705300	1.72703400
H	-3.81771300	-1.50512600	0.16734300
H	-2.36320000	-2.99665400	-0.23337100
H	-2.29809200	2.26036200	1.44656800
H	-1.71148500	2.93947500	-0.51239400
H	-3.46378300	1.71278400	-0.27403900

Table S15 High-energy asymmetric conformer

	x	y	z
B	2.13603300	0.60545400	1.36545900
B	2.41634400	1.23308300	-0.32092900
B	0.67968200	-0.27185900	1.52131900
B	3.50321900	-0.01129600	0.44072100
B	2.43572600	-1.12911300	1.31272900
B	3.01133900	-0.07158700	-1.28940100

B	3.14201000	-1.52325200	-0.32116800
H	2.42619900	1.20351600	2.35313100
H	2.90501900	2.29168900	-0.56447200
H	0.18469800	-0.25233400	2.60862100
H	4.60544100	0.29385200	0.76340700
H	2.78101300	-1.82458300	2.21303600
H	3.69545600	0.05564900	-2.25178600
H	3.82363100	-2.47171300	-0.53221700
B	0.78723300	1.21939400	0.37115300
H	0.43012200	2.31565500	0.68921700
Rh	-0.80433600	-0.10997000	-0.42752600
P	-1.97840200	1.66133800	0.41242100
P	-2.61498800	-1.55051900	0.14973500
B	1.11700200	0.74168500	-1.39606300
H	0.97893600	1.43450800	-2.35334200
H	2.44300000	-1.25826200	-1.41106900
H	2.04144100	-1.93419200	0.34301300
H	0.10156400	-1.14430300	0.80749800
H	0.56135900	-0.43370600	-1.60789500
H	-1.55675700	0.26988400	-1.76387500
H	-2.61331200	-1.90107500	1.51799700
H	-3.92732300	-1.02768300	0.08353300
H	-2.91245700	-2.83393700	-0.37206900
H	-1.85535000	2.04160100	1.76298700
H	-1.76782000	2.89760400	-0.22075300
H	-3.39183600	1.60165700	0.32229700

Table S16 Intermediate-energy symmetric conformer

	x	**y**	**z**
B	2.24376800	-0.83689400	1.21680200
B	2.24716400	0.94057800	1.13149300
B	0.81893700	-1.45197000	0.41705900
B	3.48879800	0.00601200	0.24191700
B	2.65666300	-1.45512700	-0.37886100
B	2.65445000	1.39415100	-0.52480700
B	3.11970600	-0.08279900	-1.43249300
H	2.63329300	-1.51590700	2.11494400
H	2.64297800	1.69973900	1.95986800
H	0.43583900	-2.53969500	0.73528400
H	4.61722300	0.02450400	0.61600800
H	3.15308800	-2.51570100	-0.58218000
H	3.15401100	2.42458200	-0.84288400
H	3.84850800	-0.12671100	-2.36870200
B	0.72761100	0.06550000	1.40725500
H	0.26296600	0.12088000	2.50574000
Rh	-0.79461800	-0.00508100	-0.33928900
P	-2.23017100	1.73345700	0.14241200
P	-2.24285900	-1.73789600	0.12379900
B	0.82966400	1.49572700	0.28255600
H	0.46003600	2.60793400	0.52374500
H	2.21422600	0.85807000	-1.65835100
H	2.22221900	-1.04729300	-1.56586500
H	0.37406400	-1.22337300	-0.82846200

H	0.36307700	1.18576300	-0.92818500
H	-1.55742400	-0.01534800	-1.77080900
H	-2.33183700	-2.22504100	1.44490200
H	-3.61891700	-1.56362700	-0.14480700
H	-2.02347700	-2.94799900	-0.56056000
H	-2.25976200	2.24686200	1.45565700
H	-2.05446300	2.92928400	-0.57862700
H	-3.61618200	1.54241600	-0.05647100

2.2 [6,6,6-H(PMe_3)$_2$-*nido*-6-IrB_9H_{13}]

Table S17 Low-energy asymmetric conformer

	x	**y**	**z**
B	-3.06283400	-1.37032000	0.37007900
B	-3.29797000	-0.39259100	-1.11424700
B	-1.45793700	-1.16021900	1.00309000
B	-4.22176800	0.00709300	0.36751200
B	-3.11813200	-0.27974900	1.73824400
B	-3.47086600	1.28000300	-0.62786000
B	-3.51905200	1.35728600	1.16311500
H	-3.53109100	-2.44732800	0.57692100
H	-3.94841400	-0.70420500	-2.06339700
H	-1.07735300	-2.08969000	1.65312800
H	-5.39185300	-0.20270300	0.40871500
H	-3.42412700	-0.57246800	2.84999100
H	-4.05023900	2.12471400	-1.23229700
H	-4.01498800	2.22592500	1.80479500
B	-1.74925500	-1.22494600	-0.82820200
H	-1.57251800	-2.20351200	-1.48675200
Ir	0.07615300	0.01532900	-0.29211700
P	1.54854800	-1.72765500	0.12609300
P	1.55715000	1.79154900	0.15154200
B	-1.84990200	0.46176400	-1.51781800
H	-1.71235300	0.81570000	-2.64595600
H	-2.71434200	1.91545900	0.24900300
H	-2.48309500	0.87945800	1.84231000
H	-0.72111700	-0.11550600	1.36083500
H	-1.05759400	1.26913200	-0.77275900
H	0.69384900	0.09022000	-1.77506100
C	1.98634000	-2.08349100	1.88271100
H	1.06793100	-2.26371800	2.44659200
H	2.63375400	-2.96458400	1.95295100
H	2.50096400	-1.22520500	2.32340300
C	0.97750300	-3.36024600	-0.50142500
H	1.74171200	-4.12588500	-0.32674100
H	0.04851300	-3.63937800	0.00044600
H	0.76929600	-3.27992500	-1.57139000
C	3.19920100	-1.56719900	-0.68632800
H	3.72965000	-0.68899200	-0.30719900
H	3.81259200	-2.45586400	-0.50152700
H	3.05666100	-1.44640300	-1.76403500
C	2.71245000	1.70917200	1.59755700
H	3.45113500	0.91515100	1.45158100

H	3.24305100	2.65815700	1.73518900
H	2.14040600	1.48420600	2.50292100
C	2.67653000	2.32878900	-1.21660500
H	3.24568800	3.22359900	-0.94068900
H	3.37351000	1.52465700	-1.47032900
H	2.07147400	2.54154700	-2.10272400
C	0.63194500	3.34781200	0.52057600
H	1.31863800	4.17654100	0.72688600
H	0.00075200	3.60720700	-0.33443600
H	-0.01496000	3.19433200	1.38965600

Table S18 High-energy asymmetric conformer

	x	**y**	**z**
B	-2.84487700	-0.64317800	1.43107000
B	-3.20614700	-1.20557800	-0.23841200
B	-1.33793500	0.15241000	1.55576000
B	-4.21034800	0.08060800	0.59406200
B	-3.03040200	1.11793900	1.41398400
B	-3.79999800	0.11985900	-1.15985500
B	-3.81872500	1.56589700	-0.19259200
H	-3.13096200	-1.23510200	2.42519000
H	-3.74875600	-2.23179700	-0.51434100
H	-0.81870600	0.10265400	2.63195500
H	-5.31416600	-0.16870000	0.95974100
H	-3.30775300	1.82624100	2.32957500
H	-4.51821200	0.01517000	-2.10049000
H	-4.46059100	2.55285800	-0.35167600
B	-1.55082300	-1.28821200	0.38948300
H	-1.23584800	-2.40080200	0.68120500
Ir	0.07306900	0.03215000	-0.45745100
P	1.46281000	-1.69640500	0.20001500
P	1.65679500	1.70528800	0.07009200
B	-1.87455100	-0.72833000	-1.32078500
H	-1.82191600	-1.29915700	-2.36418400
H	-3.19216400	1.28950300	-1.31475700
H	-2.66333700	1.91317100	0.42160500
H	-0.75605300	1.04593100	0.85307300
H	-1.31127600	0.53322200	-1.49701100
H	0.75804300	-0.25083200	-1.88688900
C	1.46168600	-2.23787700	1.96312400
H	0.44421100	-2.49957900	2.25920100
H	2.11773000	-3.10552200	2.09688900
H	1.80589600	-1.42239600	2.60508700
C	1.09139000	-3.23763600	-0.74263200
H	1.74014900	-4.05552600	-0.40865700
H	0.04580000	-3.51418300	-0.60381600
H	1.26253600	-3.04531000	-1.80552800
C	3.27290700	-1.54524400	-0.15646400
H	3.74577700	-0.77706400	0.46061100
H	3.76933400	-2.50076500	0.04505300
H	3.41345900	-1.28960700	-1.21052000
C	2.29767300	1.61313500	1.80133100
H	2.93132200	0.73276400	1.93737800

H	2.88043500	2.50729000	2.04919000
H	1.44818300	1.53036600	2.48583200
C	3.17897500	1.99943500	-0.93914000
H	3.75889100	2.83767700	-0.53637000
H	3.81131800	1.10947600	-0.96572100
H	2.87663900	2.23193600	-1.96471600
C	0.89970000	3.39343600	0.06128500
H	1.62400600	4.15960800	0.36127500
H	0.53114600	3.61688600	-0.94418000
H	0.04955000	3.41419300	0.74953200

Table S19 Intermediate-energy symmetric conformer

	x	**x**	**z**
B	-2.98010700	0.87632400	1.22403800
B	-2.98685900	-0.89920000	1.19898100
B	-1.55634100	1.45733300	0.40956300
B	-4.23631100	0.00641600	0.28534400
B	-3.40098000	1.43665400	-0.38665500
B	-3.40875900	-1.41032700	-0.42860800
B	-3.86818400	0.02897700	-1.38772100
H	-3.36348400	1.59141000	2.09804700
H	-3.37575100	-1.63603200	2.05216300
H	-1.21708600	2.55981000	0.71325100
H	-5.36379400	0.00442900	0.66488500
H	-3.89899700	2.48898700	-0.63111700
H	-3.91619300	-2.45039400	-0.70427700
H	-4.59124300	0.04463000	-2.33006800
B	-1.46413000	-0.02172800	1.45313300
H	-1.03568500	-0.04133400	2.56799800
Ir	0.09439300	0.00207300	-0.31688000
P	1.52146800	-1.80793300	0.06769000
P	1.53114100	1.80369600	0.06869400
B	-1.57087000	-1.46930400	0.36494400
H	-1.23916800	-2.58166000	0.63959200
H	-2.95914800	-0.92205300	-1.57521500
H	-2.95452200	0.98050200	-1.54826000
H	-1.07689800	1.22264000	-0.84032600
H	-1.08012300	-1.20493000	-0.87062300
H	0.80760000	0.00488000	-1.78965500
C	1.54333200	-2.43939100	1.80027000
H	0.52889100	-2.70879400	2.10017100
H	2.20239300	-3.31022500	1.89181300
H	1.89489500	-1.64695700	2.46781600
C	1.09939700	-3.28384200	-0.95589600
H	1.73680300	-4.13255200	-0.68465500
H	0.05279000	-3.55575200	-0.81172800
H	1.25604800	-3.03701300	-2.01034100
C	3.33053000	-1.67967200	-0.29459100
H	3.83601800	-1.05628400	0.44578500
H	3.77428500	-2.68033200	-0.25667100
H	3.49184100	-1.25619700	-1.28887000
C	1.60332700	2.39858700	1.81289700
H	1.96750600	1.59039100	2.45429900

H	2.26917700	3.26408500	1.90586300
H	0.59836100	2.66713600	2.14475600
C	3.32664400	1.68315700	-0.35799600
H	3.77294000	2.68234200	-0.31195800
H	3.85902700	1.04044100	0.34537400
H	3.44934200	1.28469500	-1.36830500
C	1.08092600	3.30133100	-0.91061200
H	1.72830400	4.14279000	-0.64044200
H	1.20650000	3.07623300	-1.97405200
H	0.03972200	3.57232900	-0.73078300

2.3 [6,6,6-(CO)(PH_3)$_2$-*nido*-6-RuB_9H_{13}] model

Table S20 Low-energy asymmetric conformer

	x	**y**	**z**
B	2.52714700	-1.34157800	0.33793800
B	1.02978100	-0.83831000	1.17263500
B	2.52987100	0.10840100	1.39684500
B	3.69054800	0.00005600	0.04191300
B	1.05330800	-1.41582300	-0.57146200
B	1.06231100	0.99806100	1.23407200
B	2.79805000	1.50627300	0.36580600
B	3.15215900	0.93733500	-1.29841800
C	-1.73145900	0.58387100	1.48976100
O	-2.34340100	0.86116200	2.42645500
Ru	-0.69252700	0.06085600	-0.01471000
H	2.99629000	-2.40301400	0.60664700
H	0.71148100	-1.53240500	2.08954900
H	3.01084900	0.18153700	2.48388100
H	4.84600900	-0.15670500	0.27223900
H	0.74077300	-2.50590800	-0.95201100
H	0.76113000	1.69385600	2.15287800
H	3.27231600	2.54207600	0.70422900
H	3.75905700	1.54740300	-2.11654600
H	0.43054800	-0.52857500	-1.31688100
H	0.39033400	1.44599500	0.17004800
H	2.20602800	1.73954800	-0.79208700
H	2.25079700	0.18800500	-1.93062200
P	-1.92572300	-1.91549600	-0.29879100
H	-1.65751100	-2.98134100	0.58414700
H	-3.33584700	-1.88557300	-0.17375600
H	-1.83599100	-2.60943100	-1.52337200
P	-1.98614500	1.41099200	-1.49413200
H	-3.32611400	1.13642800	-1.86885700
H	-2.18432100	2.76482700	-1.13861600
H	-1.48445400	1.63482400	-2.79711200
B	2.83847800	-0.81322200	-1.30077900
H	3.32553000	-1.48014300	-2.15565600

Table S21 High-energy asymmetric conformer

	x	y	z
B	2.43878200	-0.88632400	1.09943600
B	0.98462100	0.13272200	1.29999600
B	2.54853300	0.90712700	0.99300400
B	3.71448000	-0.17248100	0.11697400
B	0.99577900	-1.49281900	0.39296600
B	1.12941200	1.53221600	0.14050500
B	3.04143000	1.33649500	-0.60805000
B	3.30725700	-0.11175200	-1.56135900
C	-1.78466500	1.65991600	-0.47200800
O	-2.39467300	2.63038600	-0.61106900
Ru	-0.69798300	0.11762500	-0.20980000
H	2.81124400	-1.53975200	2.02252100
H	0.65254700	0.24594500	2.44464600
H	2.99092000	1.61748500	1.84047100
H	4.84225400	-0.24610100	0.48465000
H	0.60084900	-2.53172400	0.83421900
H	0.87214500	2.67720500	0.34341300
H	3.61336300	2.34014500	-0.88358000
H	3.99161800	-0.23753800	-2.52312900
H	0.43096200	-1.25559600	-0.72086400
H	0.63190200	1.15795300	-1.02396900
H	2.51391000	0.91998900	-1.75085100
H	2.28645900	-0.97725300	-1.66041800
P	-1.73208400	-0.38841400	1.79550200
H	-1.73176500	0.62732400	2.76839400
H	-3.12207000	-0.68205700	1.79952900
H	-1.27822900	-1.47676500	2.56360400
P	-2.21530000	-1.42140700	-1.20894900
H	-3.56889800	-1.42565800	-0.79399600
H	-2.45822900	-1.59193500	-2.59473100
H	-1.90767000	-2.76512700	-0.90200000
B	2.73224000	-1.50640400	-0.52962500
H	3.15342400	-2.58123100	-0.81363100

Table S22 Intermediate-energy asymmetric conformer

	x	y	z
B	2.49831800	-0.91283400	1.06393200
B	0.99241100	-0.02418200	1.41190300
B	2.49836700	0.87591300	1.09522000
B	3.67806900	-0.00192900	0.07174400
B	1.03011100	-1.49854700	0.34371100
B	1.02950500	1.48209400	0.39176800
B	2.81299100	1.43774800	-0.53650600
B	3.17570900	0.03099000	-1.57530200
C	-1.74552100	0.00975800	-1.77125200
O	-2.25619800	0.01413000	-2.80702300
Ru	-0.69510200	0.00073400	-0.14701100
H	2.94940200	-1.63437300	1.89757100
H	0.62147000	-0.04268800	2.54902700
H	2.94788200	1.56856300	1.95386600

H	4.82918100	-0.00786800	0.36831500
H	0.71398300	-2.60953500	0.65620200
H	0.71111000	2.58299600	0.73615300
H	3.29569400	2.48614800	-0.81951100
H	3.81094500	0.04772600	-2.57786300
H	0.42127500	-1.22656900	-0.80466400
H	0.42681700	1.24316900	-0.76788900
H	2.25687300	0.99144100	-1.64987400
H	2.25399900	-0.92613200	-1.68366400
P	-1.94380000	1.71237600	0.85000300
H	-1.86406200	3.01066600	0.30666800
H	-3.35323800	1.59852300	0.92629700
H	-1.68117100	2.01416300	2.20205800
P	-1.94045700	-1.71739400	0.84162900
H	-3.34789200	-1.59574300	0.93982900
H	-1.87761000	-3.01010300	0.28261500
H	-1.65949500	-2.03578900	2.18609700
B	2.80930800	-1.41544100	-0.58881500
H	3.29194900	-2.45228800	-0.91180300

[i] Sheldrick, G. M., 2008, CELL_NOW, University of Göttingen
[ii] Sheldrick, G. M., 2008, TWINABS, University of Gottingen