General Procedures. All manipulations were carried out under an inert atmosphere either in a nitrogen-filled glove box or under argon using standard Schlenk techniques. All solvents used were reagent grade or better. THF, acetone, pentane and benzene were distilled over Na/benzophenone ketyl; methanol was distilled over CaH_2. All solvents were degassed and stored under high purity nitrogen after distillation. All deuterated solvents were degassed and stored under high purity nitrogen on molecular sieves (3Å). ^1H, ^{13}C and ^{31}P NMR spectra were recorded on Bruker AMX 250 and AMX400 spectrometers. ^1H and ^{13}C chemical shifts are reported in ppm downfield from TMS and referenced to the residual solvent (7.24 ppm chloroform-*d*, 7.15 ppm benzene d_6, 3.58 THF-d_8, 3.30 ppm methanol-d_4) and (77.0 ppm chloroform, 128.0 ppm benzene, 67.4 ppm THF, 49 ppm methanol), respectively. ^{31}P chemical shifts are in ppm downfield from H_3PO_4 and referenced to external 85% phosphoric acid sample. FT- IR spectra recorded on Nicolet PROTEGE 460 spectrometer. UV-VIS spectra were recorded on Hewlett Packard 8450A diode array spectrometer.

Preparation of the ligand system

a) **3,5-bis(hydroxymethyl)phenol** : A Schlenk flask was charged with a solution of 5-hydroxyisophthalic acid (12.74 gr, 70 mmol) in THF (50 ml). The solution was cooled to 0°c and BH_3.THF (210 ml, 210 mmol) was added dropwise. The mixture was allowed to warm to room temperature and was stirred overnight affording a white

precipitate. The crude precipitate was filtered off and was dissolved in 3N NaOH solution (85 ml) then stirred for 15 min. The solution was neutralized with glacial acetic acid to PH=6.7, then saturated with NaCl and extracted with ethylacetate. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuum to give 3,5-bis(hydroxymethy)lphenol as a viscous oil (7 gr, 45.5 mmol, 65% yield). ^{1}H NMR (CD_3OD, 250.2 MHz) 6.79 (s, 1H), 6.69 (s, 2H), 4.52 (s, 4H). ^{13}C NMR (CD_3OD, 62.5 MHz) 158.16, 143.86, 120.77, 113.47, 64.61.

b) **3,5-bis(bromomethy)phenol**: A Schlenk flask was charged with a solution of 3,5-bis(hydroxymethyl)phenol (6.7 gr, 43.5 mmol) in sulfolane (50 ml) and cooled to 10°c. A solution of PBr_3 (8 ml, 84.2 mmol) in sulfolane was added dropwise over a period of 1 hr. The mixture was stirred at room temperature for 2 days, then poured over ice water, saturated with NaCl, and extracted with ether (3x500 ml). The organic layer was washed with brine, dried over over Na_2SO_4, filtered and evaporated under vacuum. The crude product was charged on a silica column and eluted with hexane:ether 3:1 mixture to give 3,5-bis(bromomethy)phenol (4.5 gr, 17 mmol, 40 % yield). ^{1}H NMR ($CDCl_3$, 250.2 MHz) 6.95 (t, 1H, $J_{H\text{-}H}$= 1.6 Hz), 6.78 (d, 2H, $J_{H\text{-}H}$= 1.6 Hz), 5.44 (s, 1H) 4.38 (s, 4H). ^{13}C NMR ($CDCl_3$, 62.5 MHz) 155.91, 139.85, 121.93, 116.10, 32.56. c) **3,5-bis(di-t-butylphoshinomethyl)phenol (1)** : A Schlenk flask was charged with a solution of 3,5-di(bromomethy)phenol (4.05 gr, 15.3 mmol) in dry acetone (50 ml). A solution of di-t-butylphosphine (5.01 gr, 0.34 mmol) in dry acetone (50 ml) was added under argon and the mixture was refluxed for 4 hr, during

which a white powder precipitated. The reaction mixture was cooled to room temperature, the solvent was decanted and the remaining solid was washed with pentane. The solid was dissolved in degassed water and a solution of sodium acetate (25 gr) in water (75 ml) was added. The mixture was stirred at room temperature for 30 min., then extracted with methylene chloride. The organic layer was dried under high vacuum to give a white solid which after washing with pentane and filtration gave **1** (4.5 gr, 11 mmol, 72% yield). ^{1}H NMR ($CDCl_3$, 250.2 MHz) 6.80 (s, 1H), 6.66 (s, 2H), 5.93 (Br.s 1H), 2.73 (d, 4H, $J_{P\text{-}H}$=3.4 Hz), 1.08 (d, 36 H, $J_{P\text{-}H}$=10.9 Hz). ^{13}C NMR ($CDCl_3$, 62.5 MHz) 155.64 (s), 142.84 (d, $J_{P\text{-}C}$=12 Hz), 123.12 (d, $J_{P\text{-}C}$=7.1 Hz), 113.78 (d, $J_{P\text{-}C}$=9.5 Hz), 31.72 (d, $J_{P\text{-}C}$=21.1 Hz), 29.71 (d, $J_{P\text{-}C}$=12.8 Hz), 28.26 (d, $J_{P\text{-}C}$=22.6 Hz), ^{31}P {^{1}H} ($CDCl_3$, 101.3 MHz) 34.54 (s).

Preparation of **2a**: In a Schlenk flask were placed $Ru(O_2CCF_3)_2CO(PPh_3)_2$*$CH_3OH$ (190 mg, 0.24 mmol), **1** (110 mg, 0.27 mmol) and 2-methoxyethanol (5 ml) and the mixture was stirred at 100°C overnight. The red solution was evaporated to dryness and the residue was washed with pentane (3x5 ml). The remaining solid was crystallized from methylene chloride at -30°C to afford a yellow powder (130 mg, 0.20 mmol, 83% yield). IR (Film) 3284, 1919, 1678 cm^{-1}. ^{1}H NMR ($CDCl_3$, 250.2 MHz) 8.89 (br. s. 1H), 6.76 (s, 2H), 3.15 (m, 2H), 3.08 (m, 2H), 1.23 (t, 18H, $J_{P\text{-}H}$=6.4 Hz), 1.10 (t, 18H, $J_{P\text{-}H}$=6.4 Hz). ^{13}C NMR ($CDCl_3$, 62.5 MHz) 208.40 (t, $J_{P\text{-}C}$= 12.0 Hz), 159.98 (m), 154.06 (s), 152.83 (s), 150.60 (t, $J_{P\text{-}C}$= 6.4 Hz), 117.63 (m), 110.41

(t, J_{P-C}= 7.3 Hz), 37.42 (t, J_{P-C}= 7.1 Hz), 36.60 (t, J_{P-C}= 7.1 Hz), 34.00 (t, J_{P-C}= 11.0 Hz), 30.10 (s), 29.72 (s). ^{31}P {^{1}H} ($CDCl_3$, 101.3 MHz) 72.50 (s).

Preparation of **2b**: In a pressure bottle were placed $Ru(DMSO)_4Cl_2$ (146 mg, 0.3 mmol), **1** (122 mg, 0.3 mmol), triethylamine (83.5 µl, 0.6 mmol) and either THF or 2-methoxyethanol (5 ml). The mixture was stirred at 100°c over night. The red solution was evaporated to dryness and the residue was dissolved in benzene and filtered through a cotton-wool pad. Evaporation of the benzene yielded **2b** (165 mg, 0.26 mmol, 87% yield). ^{1}H NMR ($CDCl_3$, 250.2 MHz) 11.68 (br. s. 1H), 6.75 (s, 2H), 3.68 (m, 2H), 3.45 (m, 2H), 3.00 (q, 6H, J_{H-H}= 7.3 Hz) 1.41 (t, 18H, J_{P-H}=5.9 Hz), 1.30 (t, 9H, J_{H-H}=7.3 Hz), 1.15 (t, 18H, J_{P-H}=5.9 Hz). ^{13}C NMR ($CDCl_3$, 62.5 MHz) 154.66 (s), 152.60 (s), 152.33 (t, J_{P-C}= 7.0 Hz), 110.70 (t, J_{P-C}= 7.7 Hz), 45.79 (s) 37.12 (t, J_{P-C}= 7.2 Hz), 36.54 (t, J_{P-C}= 7.8 Hz), 34.36 (t, J_{P-C}= 11.2 Hz), 29.92 (s), 29.46 (s), 8.52 (s). ^{31}P {^{1}H} ($CDCl_3$, 101.3 MHz) 70.82 (s). ES-MS (CH_3OH): m/z=579.1 (M^{+1}-NEt_3+MeOH)

Preparation of **3a** and **3b**: CO was bubbled for 10 min. through a solution of **2a** or **2b** in either benzene, THF or MeOH in a Schlenk flask. Evaporation of the solvent gave the respective product in quantitative yield. Crystals suitable for X-ray structure analysis were obtained by slow diffusion of pentane into a methylene chloride solution of **3a**.

3a: IR (Film) 3309, 2025, 1962, 1674 cm^{-1}. ^1H NMR ($CDCl_3$, 250.2 MHz) 11.52 (br. s. 1H), 6.63 (s, 2H), 3.53 (dt, 2H, J_{P-H}= 15.4 Hz, J_{H-H}= 3.6 Hz), 3.28 (dt, 2H, J_{P-H}= 15.4 Hz, J_{H-H}= 3.6 Hz), 1.30 (t, 18H, J_{P-H}=6.4 Hz), 1.16 (t, 18H, J_{P-H}=6.4 Hz). ^{13}C NMR ($CDCl_3$, 100.6 MHz) 202.75 (t, J_{P-C}= 11.8 Hz) 198.01 (t, J_{P-C}= 6.6 Hz), 160.11 (m), 156.58 (s), 154.90 (s), 146.74(t, J_{P-C}= 6.4 Hz), 118.02 (m), 110.02 (t, J_{P-C}= 7.2 Hz), 38.90 (t, J_{P-C}= 6.5 Hz), 37.58 (t, J_{P-C}= 10.5 Hz), 37.11 (t, J_{P-C}= 7.2 Hz), 31.58 (s), 31.05 (s). ^{31}P {^1H} ($CDCl_3$, 101.3 MHz) 91.22 (s).

3b: IR (Film) 3229, 2014, 1942 cm^{-1}. ^1H NMR ($CDCl_3$, 250.2 MHz) 11.53 (br. s. 1H), 6.63 (s, 2H), 3.70 (dt, 2H, J_{P-H}= 15.3 Hz, J_{H-H}= 2.0 Hz), 3.21 (dt, 2H, J_{P-H}= 15.3 Hz, J_{H-H}= 2.0 Hz), 1.37 (t, 18H, J_{P-H}=6.3 Hz), 1.28 (t, 18H, J_{P-H}=6.3 Hz). ^{13}C NMR ($CDCl_3$, 100.6 MHz) 202.02 (t, J_{P-C}= 11.9 Hz) 197.55 (t, J_{P-C}= 6.7 Hz), 157.17 (s), 154.70 (s), 148.46(t, J_{P-C}= 7.0 Hz), 110.14 (t, J_{P-C}= 7.5 Hz), 38.96 (t, J_{P-C}= 6.5 Hz), 37.47 (t, J_{P-C}= 10.9 Hz), 37.27 (t, J_{P-C}= 7.4 Hz), 31.47 (s), 30.88 (s). ^{31}P {^1H} ($CDCl_3$, 101.3 MHz) 89.08 (s).

Preparation of **4**: method a: A solution of 1M KOH in ethanol (100 µl, 0.1 mmol) was added to a solution of **3b** (63 mg, 0.1 mmol) in benzene (10 ml). The mixture was stirred overnight at room temperature and filtered through celite. Evaporation of the solvent yielded **4** as an orange powder (28 mg, 0.05 mmol, 50% yield). Similar results were obtained using **3a** under the same conditions.

Method b: In a Schlenk flask were placed a solution of **3b** (30 mg, 0.05 mmol) in MeOH (4 ml). A solution of proton sponge (10.7 mg, 0.05 mmol) in MeOH (3 ml)

was added and the mixture was stirred under gentle reflux for 4 days. The MeOH was removed under vacuum and the residue was washed with pentane (5ml), then extracted with benzene and filtered through a cotton wool pad until the extractions were colorless. Evaporation of the benzene gave **4** (27 mg, 0.048 mmol, 95% yield). Similar results were obtained using Dabco and/or **3a**.

4a: IR (Film) 1983, 1926, 1659, 1590, 1577, 1030 cm^{-1}. UV-VIS(benzene). λ_{max}= 450 nm (35400). ^1H NMR (THF-d^8, 250.2 MHz) 6.38 (s, 2H), 3.18 (br.s., 4H), 1.38 (t, 18H, J_{P-H}=6.2 Hz), 1.26 (t, 18H, J_{P-H}=6.2 Hz). ^{13}C NMR (THF-d^8, 100.6 MHz) 303.08 (t, J_{P-C}= 5.7 Hz), 205.69 (t, J_{P-C}= 6.3 Hz) 204.74 (t, J_{P-C}= 8.3 Hz), 187.45 (s), 148.68 (t, J_{P-C}= 6.4 Hz), 111.55 (t, J_{P-C}= 8.9 Hz), 40.34 (t, J_{P-C}= 11.4 Hz), 36.70 (m), 30.52 (s), 29.85 (s). ^{31}P {^1H} (THF-d^8, 101.3 MHz) 103.41 (s). Anal. Calcd for $C_{26}H_{42}O_3P_2Ru$: C, 55.20; H, 7.49. Found: C, 55.21; H, 7.17.

4b: UV-VIS(methanol). λ_{max}= 432 nm (22700). ^1H NMR (CD_3OD, 250.2 MHz) 6.30 (s, 2H), 3.08 (br.s., 4H,), 1.23 (t, 18H, J_{P-H}=6.3 Hz), 1.10 (t, 18H, J_{P-H}=6.3 Hz). ^{13}C NMR (CD_3OD, 100.6 MHz) 205.95 (t, J_{P-C}= 6.4 Hz) 205.22 (t, J_{P-C}= 8.5 Hz), 160.64 (s), 151.45 (t, J_{P-C}= 6.4 Hz), 149.58(t, J_{P-C}= 8.7 Hz), 112.35 (t, J_{P-C}= 6.8 Hz), 40.58 (t, J_{P-C}= 11.7 Hz), 36.97 (m), 30.59 (s), 29.94 (s). ^{31}P {^1H} (CD_3OD, 101.3 MHz) 103.03 (s).

Table 1. Crystal data and structure refinement for **3a**.

Identification code	**3a**
Empirical formula	C28 H43 F3 O5 P2 Ru
Formula weight	679.63
Temperature	120(2) K
Wavelength	0.71070 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 8.8160(2) Å alpha = 90 deg.
	b = 18.9770(5) Å beta = 99.1510(13) deg.
	c = 18.6010(3) Å gamma = 90 deg.
Volume	3072.36(12) $Å^3$
Z, Calculated density	4, 1.469 Mg/m^3
Absorption coefficient	0.667 mm^{-1}
F(000)	1408
Crystal size	0.1 x 0.1 x 0.05 mm
Theta range for data collection	2.15 to 24.11 deg.
Limiting indices	0<=h<=10, 0<=k<=21, -21<=l<=21
Reflections collected / unique	4858 / 4858 [R(int) = 0.0000]
Completeness to theta = 24.11	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4858 / 0 / 368
Goodness-of-fit on F2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0778
R indices (all data)	R1 = 0.0395, wR2 = 0.0812
Largest diff. peak and hole	1.106 and -0.868 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	17(1)	1050(1)	7054(1)	13(1)
P(2)	1709(1)	1615(1)	6070(1)	17(1)
C(21)	2229(4)	838(2)	5494(2)	19(1)
C(22)	-924(4)	2269(2)	5455(2)	34(1)
C(23)	-3610(4)	1958(2)	6280(2)	25(1)
C(24)	-1787(4)	2253(2)	4667(2)	35(1)
C(25)	-979(6)	3021(2)	5765(2)	56(1)
C(26)	758(5)	2095(3)	5429(3)	72(2)
C(27)	-4430(4)	1354(2)	6606(2)	27(1)
C(28)	-4708(4)	2224(2)	5609(2)	33(1)
C(29)	-3344(5)	2570(2)	6834(2)	38(1)
P(3)	1042(1)	115(1)	7884(1)	16(1)
C(31)	-761(4)	-362(2)	7911(2)	22(1)
C(32)	2351(4)	-531(2)	7519(2)	31(1)
C(33)	1851(4)	292(2)	8878(2)	21(1)
C(34)	1465(5)	-901(2)	6833(2)	40(1)
C(35)	2899(6)	-1136(2)	8047(2)	51(1)
C(36)	3770(4)	-146(3)	7329(2)	46(1)
C(37)	1002(4)	917(2)	9139(2)	27(1)
C(38)	3554(4)	498(2)	8961(2)	32(1)
C(39)	1628(4)	-334(2)	9378(2)	33(1)
O(1)	-4585(3)	-1404(1)	5975(1)	32(1)
C(11)	-1523(3)	220(2)	6697(2)	15(1)
C(12)	-2373(3)	212(2)	5988(2)	17(1)
C(13)	-3354(4)	-343(2)	5756(2)	21(1)
C(14)	-3535(4)	-893(2)	6221(2)	20(1)
C(15)	-2710(4)	-897(2)	6925(2)	21(1)
C(16)	-1702(3)	-348(2)	7155(2)	18(1)
O(2)	-1475(2)	1285(1)	7832(1)	18(1)
O(3)	-600(3)	2345(1)	8266(1)	26(1)
C(41)	-1439(4)	1825(2)	8230(2)	22(1)
C(42)	-2636(4)	1815(3)	8747(2)	39(1)
F(1)	-3302(4)	1192(2)	8775(2)	121(2)
F(2)	-2004(3)	1884(2)	9434(1)	66(1)
F(3)	-3656(4)	2284(3)	8598(2)	149(2)
C(5)	1140(4)	756(2)	6358(2)	23(1)
O(5)	1797(3)	560(2)	5912(1)	40(1)
C(6)	1494(4)	1798(2)	7405(2)	22(1)
O(6)	2459(3)	2191(1)	7583(2)	36(1)

Table 3. Bond lengths [A] and angles [deg] for **5a**.

Ru(1)-C(5)	1.837(3)
Ru(1)-C(6)	1.967(4)
Ru(1)-C(11)	2.117(3)
Ru(1)-O(2)	2.152(2)
Ru(1)-P(3)	2.4296(8)
Ru(1)-P(2)	2.4352(8)
P(2)-C(21)	1.837(3)
P(2)-C(22)	1.891(4)
P(2)-C(23)	1.896(3)
C(21)-C(12)	1.519(4)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(26)	1.528(6)
C(22)-C(24)	1.541(5)
C(22)-C(25)	1.543(6)
C(23)-C(27)	1.530(5)
C(23)-C(28)	1.538(4)
C(23)-C(29)	1.544(5)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
P(3)-C(31)	1.838(3)
P(3)-C(32)	1.884(4)
P(3)-C(33)	1.903(3)
C(31)-C(16)	1.516(4)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(32)-C(36)	1.537(6)
C(32)-C(35)	1.538(5)
C(32)-C(34)	1.554(5)
C(33)-C(37)	1.523(5)
C(33)-C(38)	1.535(5)

C(33)-C(39)	1.539(5)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-H(37A)	0.9600
C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
O(1)-C(14)	1.370(4)
O(1)-H(1)	0.73(4)
C(11)-C(16)	1.398(4)
C(11)-C(12)	1.410(4)
C(12)-C(13)	1.387(5)
C(13)-C(14)	1.380(5)
C(13)-H(13)	0.9300
C(14)-C(15)	1.392(4)
C(15)-C(16)	1.392(5)
C(15)-H(15)	0.9300
O(2)-C(41)	1.262(4)
O(3)-C(41)	1.229(4)
C(41)-C(42)	1.536(5)
C(42)-F(3)	1.264(5)
C(42)-F(2)	1.316(4)
C(42)-F(1)	1.325(6)
C(5)-O(5)	1.147(4)
C(6)-O(6)	1.140(4)
C(5)-Ru(1)-C(6)	92.91(14)
C(5)-Ru(1)-C(11)	86.78(13)
C(6)-Ru(1)-C(11)	178.09(12)
C(5)-Ru(1)-O(2)	173.03(12)
C(6)-Ru(1)-O(2)	94.02(11)
C(11)-Ru(1)-O(2)	86.26(10)
C(5)-Ru(1)-P(3)	92.25(10)
C(6)-Ru(1)-P(3)	99.01(9)
C(11)-Ru(1)-P(3)	79.12(8)
O(2)-Ru(1)-P(3)	85.92(6)
C(5)-Ru(1)-P(2)	86.90(10)
C(6)-Ru(1)-P(2)	103.49(9)

C(11)-Ru(1)-P(2)	78.39(8)
O(2)-Ru(1)-P(2)	92.21(6)
P(3)-Ru(1)-P(2)	157.50(3)
C(21)-P(2)-C(22)	104.84(16)
C(21)-P(2)-C(23)	104.44(15)
C(22)-P(2)-C(23)	108.64(17)
C(21)-P(2)-Ru(1)	98.79(10)
C(22)-P(2)-Ru(1)	119.88(11)
C(23)-P(2)-Ru(1)	117.59(11)
C(12)-C(21)-P(2)	108.2(2)
C(12)-C(21)-H(21A)	110.0
P(2)-C(21)-H(21A)	110.1
C(12)-C(21)-H(21B)	110.0
P(2)-C(21)-H(21B)	110.1
H(21A)-C(21)-H(21B)	108.4
C(26)-C(22)-C(24)	107.5(3)
C(26)-C(22)-C(25)	107.5(4)
C(24)-C(22)-C(25)	109.5(3)
C(26)-C(22)-P(2)	109.1(3)
C(24)-C(22)-P(2)	112.9(2)
C(25)-C(22)-P(2)	110.2(3)
C(27)-C(23)-C(28)	106.9(3)
C(27)-C(23)-C(29)	109.3(3)
C(28)-C(23)-C(29)	107.7(3)
C(27)-C(23)-P(2)	108.2(2)
C(28)-C(23)-P(2)	114.1(2)
C(29)-C(23)-P(2)	110.5(2)
C(22)-C(24)-H(24A)	109.4
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.4
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.6
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.4
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(22)-C(26)-H(26A)	109.4
C(22)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	109.5
C(22)-C(26)-H(26C)	109.4
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	109.5
C(23)-C(27)-H(27C)	109.5

H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(23)-C(29)-H(29A)	109.4
C(23)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(23)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-P(3)-C(32)	105.72(17)
C(31)-P(3)-C(33)	104.60(14)
C(32)-P(3)-C(33)	107.94(15)
C(31)-P(3)-Ru(1)	98.16(11)
C(32)-P(3)-Ru(1)	115.70(12)
C(33)-P(3)-Ru(1)	122.24(11)
C(16)-C(31)-P(3)	108.3(2)
C(16)-C(31)-H(31A)	110.1
P(3)-C(31)-H(31A)	110.1
C(16)-C(31)-H(31B)	110.0
P(3)-C(31)-H(31B)	110.0
H(31A)-C(31)-H(31B)	108.4
C(36)-C(32)-C(35)	108.5(3)
C(36)-C(32)-C(34)	110.2(3)
C(35)-C(32)-C(34)	104.7(3)
C(36)-C(32)-P(3)	110.0(3)
C(35)-C(32)-P(3)	113.8(3)
C(34)-C(32)-P(3)	109.5(2)
C(37)-C(33)-C(38)	106.9(3)
C(37)-C(33)-C(39)	107.0(3)
C(38)-C(33)-C(39)	110.6(3)
C(37)-C(33)-P(3)	108.6(2)
C(38)-C(33)-P(3)	110.6(2)
C(39)-C(33)-P(3)	112.8(2)
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.4
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5

H(35B)-C(35)-H(35C)	109.5
C(32)-C(36)-H(36A)	109.5
C(32)-C(36)-H(36B)	109.4
H(36A)-C(36)-H(36B)	109.5
C(32)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(33)-C(37)-H(37A)	109.5
C(33)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(33)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(33)-C(38)-H(38A)	109.4
C(33)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(33)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(33)-C(39)-H(39A)	109.5
C(33)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(33)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(14)-O(1)-H(1)	111(3)
C(16)-C(11)-C(12)	117.8(3)
C(16)-C(11)-Ru(1)	120.8(2)
C(12)-C(11)-Ru(1)	121.4(2)
C(13)-C(12)-C(11)	120.7(3)
C(13)-C(12)-C(21)	120.9(3)
C(11)-C(12)-C(21)	118.3(3)
C(14)-C(13)-C(12)	120.5(3)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.7
O(1)-C(14)-C(13)	117.7(3)
O(1)-C(14)-C(15)	122.3(3)
C(13)-C(14)-C(15)	119.9(3)
C(16)-C(15)-C(14)	119.8(3)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(15)-C(16)-C(11)	121.2(3)
C(15)-C(16)-C(31)	120.0(3)
C(11)-C(16)-C(31)	118.8(3)
C(41)-O(2)-Ru(1)	127.0(2)
O(3)-C(41)-O(2)	130.0(3)
O(3)-C(41)-C(42)	116.3(3)
O(2)-C(41)-C(42)	113.7(3)
F(3)-C(42)-F(2)	108.7(4)

F(3)-C(42)-F(1)	109.5(4)
F(2)-C(42)-F(1)	100.0(4)
F(3)-C(42)-C(41)	112.9(4)
F(2)-C(42)-C(41)	112.3(3)
F(1)-C(42)-C(41)	112.8(3)
O(5)-C(5)-Ru(1)	177.6(3)
O(6)-C(6)-Ru(1)	173.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5a**.

The anisotropic displacement factor exponent takes the form:

$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Ru(1)	12(1)	13(1)	14(1)	1(1)	2(1)	-1(1)
P(2)	17(1)	14(1)	19(1)	4(1)	-2(1)	-3(1)
C(21)	24(2)	18(2)	15(2)	2(1)	1(1)	0(1)
C(22)	31(2)	34(2)	32(2)	18(2)	-8(2)	-13(2)
C(23)	21(2)	25(2)	26(2)	-4(2)	-6(1)	8(2)
C(24)	45(2)	32(2)	24(2)	13(2)	-2(2)	-13(2)
C(25)	84(3)	33(2)	39(2)	17(2)	-30(2)	-37(2)
C(26)	30(2)	117(5)	67(3)	69(3)	6(2)	-14(3)
C(27)	17(2)	32(2)	31(2)	-9(2)	4(1)	1(2)
C(28)	27(2)	34(2)	34(2)	-2(2)	-11(2)	10(2)
C(29)	45(2)	28(2)	33(2)	-9(2)	-11(2)	12(2)
P(3)	18(1)	15(1)	15(1)	0(1)	-2(1)	1(1)
C(31)	27(2)	17(2)	18(2)	1(1)	-2(1)	-4(1)
C(32)	34(2)	31(2)	25(2)	-5(2)	-4(2)	17(2)
C(33)	23(2)	21(2)	17(2)	-1(1)	-4(1)	-1(1)
C(34)	46(2)	37(2)	34(2)	-14(2)	-4(2)	23(2)
C(35)	69(3)	30(2)	45(2)	-11(2)	-18(2)	30(2)
C(36)	25(2)	73(3)	39(2)	-11(2)	6(2)	23(2)
C(37)	30(2)	32(2)	16(2)	-5(1)	-3(1)	-1(2)
C(38)	24(2)	38(2)	31(2)	-5(2)	-7(2)	-1(2)
C(39)	44(2)	32(2)	21(2)	6(2)	-5(2)	-5(2)
O(1)	41(2)	18(1)	29(1)	6(1)	-16(1)	-12(1)
C(11)	16(2)	14(2)	14(2)	-2(1)	4(1)	0(1)
C(12)	20(2)	14(2)	16(2)	0(1)	3(1)	3(1)
C(13)	26(2)	18(2)	15(2)	-1(1)	-5(1)	0(1)
C(14)	23(2)	12(2)	24(2)	-3(1)	-4(1)	-4(1)
C(15)	26(2)	16(2)	21(2)	5(1)	-2(1)	-3(1)
C(16)	20(2)	15(2)	17(2)	-2(1)	0(1)	0(1)
O(2)	15(1)	20(1)	19(1)	-4(1)	2(1)	-1(1)
O(3)	25(1)	21(1)	29(1)	-9(1)	-1(1)	4(1)
C(41)	15(2)	30(2)	20(2)	-4(2)	-1(1)	4(2)
C(42)	21(2)	64(3)	34(2)	-26(2)	6(2)	-9(2)
F(1)	107(3)	160(4)	120(3)	-81(3)	95(3)	-87(3)
F(2)	55(2)	115(3)	32(1)	-13(1)	15(1)	14(2)
F(3)	103(3)	273(6)	89(2)	86(3)	70(2)	148(4)
C(5)	20(2)	29(2)	19(2)	5(2)	2(1)	1(2)
O(5)	36(2)	63(2)	26(1)	-2(1)	16(1)	9(1)
C(6)	19(2)	18(2)	28(2)	4(1)	6(1)	4(2)
O(6)	23(1)	27(2)	57(2)	-4(1)	4(1)	-11(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3a**.

	x	y	z	U(eq)
H(21A)	-3196	919	5176	23
H(21B)	-1444	747	5195	23
H(24A)	-2840	2385	4662	52
H(24B)	-1745	1785	4473	52
H(24C)	-1315	2577	4374	52
H(25A)	-405	3334	5505	85
H(25B)	-540	3020	6272	85
H(25C)	-2027	3177	5712	85
H(26A)	1198	2458	5167	108
H(26B)	821	1651	5187	108
H(26C)	1312	2066	5916	108
H(27A)	-5360	1527	6749	40
H(27B)	-3771	1168	7023	40
H(27C)	-4671	989	6248	40
H(28A)	-4844	1863	5243	50
H(28B)	-4281	2637	5420	50
H(28C)	-5684	2338	5746	50
H(29A)	-4133	2564	7135	56
H(29B)	-3375	3010	6577	56
H(29C)	-2358	2515	7133	56
H(31A)	-543	-846	8064	26
H(31B)	-1328	-141	8256	26
H(34A)	2155	-1201	6623	60
H(34B)	1048	-552	6483	60
H(34C)	646	-1179	6968	60
H(35A)	3476	-1469	7811	76
H(35B)	2025	-1367	8190	76
H(35C)	3538	-950	8471	76
H(36A)	4547	-122	7753	68
H(36B)	3487	322	7164	68
H(36C)	4162	-399	6950	68
H(37A)	1397	1011	9641	40
H(37B)	-74	811	9089	40
H(37C)	1148	1324	8851	40
H(38A)	3680	866	8621	49
H(38B)	4149	95	8866	49
H(38C)	3896	662	9448	49
H(39A)	2024	-212	9874	50
H(39B)	2169	-737	9237	50
H(39C)	554	-442	9336	50
H(1)	-4490(50)	-1710(20)	6210(20)	30(13)
H(13)	-3893	-345	5284	25
H(15)	-2832	-1266	7240	26

Table 1. Crystal data and structure refinement for **4b**.

Identification code	**4b**
Empirical formula	C29 H42 N O3 P2 Ru
Formula weight	615.65
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Orthorombic, pbca
Unit cell dimensions	a = 14.1190(2) Å, alpha = 90 deg. b = 12.0480(2) Å ,beta = 90 deg. c = 36.3270(4) Å, gamma = 90 deg.
Volume	6179.43(15) $Å^3$
Z, Calculated density	8, 1.323 Mg/m^3
Absorption coefficient	0.639 mm^{-1}
F(000)	2568
Crystal size	0.2 x 0.05 x 0.02 mm
Theta range for data collection	2.67 to 20.39 deg.
Limiting indices	0<=h<=13, 0<=k<=11, 0<=l<=35
Reflections collected / unique	3000 / 3000 [R(int) = 0.0000]
Completeness to theta = 20.39	98.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3000 / 0 / 365
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.1282
R indices (all data)	R1 = 0.0529, wR2 = 0.1302
Extinction coefficient	0.0013(3)
Largest diff. peak and hole	1.303 and -0.902 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	9817(1)	1609(1)	8555(1)	24(1)
P(2)	9640(1)	-1(1)	8915(1)	22(1)
P(3)	10601(1)	3105(1)	8277(1)	21(1)
O(1)	13217(4)	2419(4)	9658(1)	55(2)
C(11)	10948(4)	1857(5)	8931(2)	23(2)
C(13)	12166(5)	3043(6)	9196(2)	32(2)
C(12)	11428(4)	2868(5)	8951(2)	26(2)
C(14)	12478(5)	2208(6)	9422(2)	39(2)
C(15)	12030(5)	1178(6)	9409(2)	36(2)
C(16)	11266(4)	1015(5)	9165(2)	26(2)
C(21)	10815(5)	-120(5)	9134(2)	31(2)
C(22)	9496(5)	-1381(6)	8675(2)	35(2)
C(23)	8783(5)	99(6)	9315(2)	41(2)
C(24)	10121(6)	-1349(7)	8322(2)	49(2)
C(25)	8462(6)	-1532(6)	8554(2)	48(2)
C(26)	9824(7)	-2371(6)	8905(2)	59(3)
C(27)	8656(7)	-990(7)	9534(2)	64(3)
C(28)	9198(6)	945(7)	9585(2)	53(2)
C(29)	7819(5)	495(7)	9176(2)	57(2)
C(31)	11144(5)	3774(5)	8682(2)	28(2)
C(32)	11633(5)	2733(6)	7971(2)	44(2)
C(33)	9891(5)	4268(6)	8054(2)	36(2)
C(34)	10416(6)	5378(6)	8043(2)	46(2)
C(35)	9612(6)	3919(6)	7667(2)	58(2)
C(36)	8992(5)	4441(7)	8275(2)	58(2)
C(37)	12366(5)	2107(7)	8207(2)	54(2)
C(38)	11294(7)	1930(7)	7665(2)	64(3)
C(39)	12129(7)	3721(7)	7794(3)	71(3)
O(2)	8371(4)	1108(4)	7951(2)	55(2)
C(2)	8895(5)	1295(6)	8180(2)	34(2)
C(3)	9073(5)	2590(6)	8860(2)	38(2)
O(3)	8704(4)	3204(5)	9058(2)	71(2)
N(1)	10591(5)	5708(5)	9872(2)	50(2)
C(101)	9763(10)	6375(13)	10038(5)	41(4)
C(102)	11008(11)	4512(13)	9842(5)	51(4)
C(103)	10227(13)	5096(14)	9550(4)	48(4)
C(104)	10485(14)	5807(16)	10293(5)	68(5)
C(105)	9692(14)	5740(20)	9694(6)	75(6)
C(106)	11023(11)	5061(16)	10126(4)	51(5)

Table 3. Bond lengths [Å] and angles [deg] for **4b**.

Ru(1)-C(2)	1.923(8)
Ru(1)-C(3)	1.930(8)
Ru(1)-C(11)	2.121(6)
Ru(1)-P(3)	2.3437(17)
Ru(1)-P(2)	2.3532(17)
P(2)-C(21)	1.846(6)
P(2)-C(22)	1.889(7)
P(2)-C(23)	1.894(7)
P(3)-C(31)	1.842(6)
P(3)-C(32)	1.888(7)
P(3)-C(33)	1.903(7)
O(1)-C(14)	1.373(8)
C(11)-C(12)	1.396(9)
C(11)-C(16)	1.397(9)
C(13)-C(14)	1.372(9)
C(13)-C(12)	1.386(9)
C(13)-H(13)	0.9300
C(12)-C(31)	1.519(9)
C(14)-C(15)	1.393(10)
C(15)-C(16)	1.410(9)
C(15)-H(15)	0.9300
C(16)-C(21)	1.513(9)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(26)	1.528(10)
C(22)-C(25)	1.536(11)
C(22)-C(24)	1.558(11)
C(23)-C(29)	1.528(11)
C(23)-C(28)	1.531(10)
C(23)-C(27)	1.545(10)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600

C(29)-H(29C)	0.9600
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(32)-C(39)	1.523(11)
C(32)-C(37)	1.540(11)
C(32)-C(38)	1.549(11)
C(33)-C(36)	1.517(10)
C(33)-C(35)	1.518(10)
C(33)-C(34)	1.530(10)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-H(37A)	0.9600
C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
O(2)-C(2)	1.136(8)
C(3)-O(3)	1.157(8)
N(1)-C(106)	1.353(16)
N(1)-C(105)	1.43(2)
N(1)-C(103)	1.473(17)
N(1)-C(101)	1.542(16)
N(1)-C(104)	1.543(19)
N(1)-C(102)	1.561(17)
C(101)-C(105)	1.47(3)
C(101)-C(104)	1.54(3)
C(101)-C(102)#1	1.59(2)
C(102)-C(106)	1.23(2)
C(102)-C(101)#1	1.59(2)
C(102)-C(103)	1.68(2)
C(102)-C(105)#1	1.98(2)
C(103)-C(105)	1.20(2)
C(103)-C(104)#1	1.59(2)
C(104)-C(106)	1.33(2)
C(104)-C(103)#1	1.59(2)
C(104)-C(105)#1	1.88(3)
C(105)-C(106)#1	1.54(2)
C(105)-C(104)#1	1.88(3)

C(105)-C(102)#1	1.98(2)
C(106)-C(105)#1	1.54(2)
C(2)-Ru(1)-C(3)	99.1(3)
C(2)-Ru(1)-C(11)	173.4(3)
C(3)-Ru(1)-C(11)	87.4(3)
C(2)-Ru(1)-P(3)	99.6(2)
C(3)-Ru(1)-P(3)	91.9(2)
C(11)-Ru(1)-P(3)	79.22(17)
C(2)-Ru(1)-P(2)	99.2(2)
C(3)-Ru(1)-P(2)	97.3(2)
C(11)-Ru(1)-P(2)	80.69(17)
P(3)-Ru(1)-P(2)	157.46(6)
C(21)-P(2)-C(22)	103.2(3)
C(21)-P(2)-C(23)	104.4(3)
C(22)-P(2)-C(23)	110.0(3)
C(21)-P(2)-Ru(1)	102.0(2)
C(22)-P(2)-Ru(1)	118.7(2)
C(23)-P(2)-Ru(1)	116.2(2)
C(31)-P(3)-C(32)	104.7(3)
C(31)-P(3)-C(33)	103.7(3)
C(32)-P(3)-C(33)	109.2(3)
C(31)-P(3)-Ru(1)	100.9(2)
C(32)-P(3)-Ru(1)	115.8(2)
C(33)-P(3)-Ru(1)	120.1(2)
C(12)-C(11)-C(16)	116.4(6)
C(12)-C(11)-Ru(1)	121.5(4)
C(16)-C(11)-Ru(1)	122.1(4)
C(14)-C(13)-C(12)	120.9(6)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(13)-C(12)-C(11)	122.1(6)
C(13)-C(12)-C(31)	120.1(6)
C(11)-C(12)-C(31)	117.7(5)
C(13)-C(14)-O(1)	118.7(6)
C(13)-C(14)-C(15)	119.1(6)
O(1)-C(14)-C(15)	122.2(6)
C(14)-C(15)-C(16)	119.6(6)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(11)-C(16)-C(15)	121.8(6)
C(11)-C(16)-C(21)	118.4(5)
C(15)-C(16)-C(21)	119.6(6)
C(16)-C(21)-P(2)	109.9(4)
C(16)-C(21)-H(21A)	109.7
P(2)-C(21)-H(21A)	109.7
C(16)-C(21)-H(21B)	109.7
P(2)-C(21)-H(21B)	109.7
H(21A)-C(21)-H(21B)	108.2
C(26)-C(22)-C(25)	110.7(6)

C(26)-C(22)-C(24)	107.3(6)
C(25)-C(22)-C(24)	107.8(6)
C(26)-C(22)-P(2)	113.7(5)
C(25)-C(22)-P(2)	109.8(5)
C(24)-C(22)-P(2)	107.3(5)
C(29)-C(23)-C(28)	110.2(6)
C(29)-C(23)-C(27)	109.4(6)
C(28)-C(23)-C(27)	106.3(6)
C(29)-C(23)-P(2)	109.6(5)
C(28)-C(23)-P(2)	106.8(5)
C(27)-C(23)-P(2)	114.5(5)
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(22)-C(26)-H(26A)	109.5
C(22)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(22)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(23)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(23)-C(29)-H(29A)	109.5
C(23)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(23)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(12)-C(31)-P(3)	108.0(4)
C(12)-C(31)-H(31A)	110.1

P(3)-C(31)-H(31A)	110.1
C(12)-C(31)-H(31B)	110.1
P(3)-C(31)-H(31B)	110.1
H(31A)-C(31)-H(31B)	108.4
C(39)-C(32)-C(37)	107.9(7)
C(39)-C(32)-C(38)	109.1(7)
C(37)-C(32)-C(38)	107.5(7)
C(39)-C(32)-P(3)	114.7(5)
C(37)-C(32)-P(3)	107.9(5)
C(38)-C(32)-P(3)	109.4(5)
C(36)-C(33)-C(35)	108.0(7)
C(36)-C(33)-C(34)	107.4(6)
C(35)-C(33)-C(34)	110.1(6)
C(36)-C(33)-P(3)	108.4(5)
C(35)-C(33)-P(3)	109.1(5)
C(34)-C(33)-P(3)	113.6(5)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(32)-C(37)-H(37A)	109.5
C(32)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(32)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(32)-C(38)-H(38A)	109.5
C(32)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(32)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(32)-C(39)-H(39A)	109.5
C(32)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5

C(32)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
O(2)-C(2)-Ru(1)	178.1(6)
O(3)-C(3)-Ru(1)	173.8(7)
C(106)-N(1)-C(105)	136.8(11)
C(106)-N(1)-C(103)	114.2(11)
C(105)-N(1)-C(103)	49.1(11)
C(106)-N(1)-C(101)	112.1(10)
C(105)-N(1)-C(101)	59.1(12)
C(103)-N(1)-C(101)	107.9(11)
C(106)-N(1)-C(104)	54.0(11)
C(105)-N(1)-C(104)	111.2(13)
C(103)-N(1)-C(104)	142.3(10)
C(101)-N(1)-C(104)	59.9(10)
C(106)-N(1)-C(102)	49.1(10)
C(105)-N(1)-C(102)	109.4(13)
C(103)-N(1)-C(102)	67.4(10)
C(101)-N(1)-C(102)	142.7(9)
C(104)-N(1)-C(102)	100.2(11)
C(105)-C(101)-C(104)	109.1(14)
C(105)-C(101)-N(1)	56.5(10)
C(104)-C(101)-N(1)	60.1(9)
C(105)-C(101)-C(102)#1	80.6(12)
C(104)-C(101)-C(102)#1	89.4(12)
N(1)-C(101)-C(102)#1	106.0(11)
C(106)-C(102)-N(1)	56.6(10)
C(106)-C(102)-C(101)#1	98.3(14)
N(1)-C(102)-C(101)#1	110.1(11)
C(106)-C(102)-C(103)	108.4(14)
N(1)-C(102)-C(103)	53.8(8)
C(101)#1-C(102)-C(103)	90.3(12)
C(106)-C(102)-C(105)#1	51.3(13)
N(1)-C(102)-C(105)#1	84.0(10)
C(101)#1-C(102)-C(105)#1	47.1(10)
C(103)-C(102)-C(105)#1	105.9(11)
C(105)-C(103)-N(1)	63.4(13)
C(105)-C(103)-C(104)#1	83.7(16)
N(1)-C(103)-C(104)#1	106.3(11)
C(105)-C(103)-C(102)	114.1(15)
N(1)-C(103)-C(102)	58.8(8)
C(104)#1-C(103)-C(102)	84.4(12)
C(106)-C(104)-C(101)	113.9(15)
C(106)-C(104)-N(1)	55.7(10)
C(101)-C(104)-N(1)	60.0(10)
C(106)-C(104)-C(103)#1	93.6(15)
C(101)-C(104)-C(103)#1	95.8(13)
N(1)-C(104)-C(103)#1	111.3(12)
C(106)-C(104)-C(105)#1	54.2(12)

C(101)-C(104)-C(105)#1	111.6(13)
N(1)-C(104)-C(105)#1	87.7(11)
C(103)#1-C(104)-C(105)#1	39.4(9)
C(103)-C(105)-N(1)	67.6(13)
C(103)-C(105)-C(101)	131.5(19)
N(1)-C(105)-C(101)	64.4(12)
C(103)-C(105)-C(106)#1	100.9(19)
N(1)-C(105)-C(106)#1	111.8(13)
C(101)-C(105)-C(106)#1	90.5(14)
C(103)-C(105)-C(104)#1	56.8(14)
N(1)-C(105)-C(104)#1	94.4(13)
C(101)-C(105)-C(104)#1	120.2(14)
C(106)#1-C(105)-C(104)#1	44.1(10)
C(103)-C(105)-C(102)#1	125.7(16)
N(1)-C(105)-C(102)#1	93.1(12)
C(101)-C(105)-C(102)#1	52.3(10)
C(106)#1-C(105)-C(102)#1	38.3(9)
C(104)#1-C(105)-C(102)#1	76.1(10)
C(102)-C(106)-C(104)	137.9(18)
C(102)-C(106)-N(1)	74.3(12)
C(104)-C(106)-N(1)	70.3(12)
C(102)-C(106)-C(105)#1	90.4(17)
C(104)-C(106)-C(105)#1	81.7(15)
N(1)-C(106)-C(105)#1	110.8(12)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4b**.
The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Ru(1)	20(1)	26(1)	27(1)	9(1)	-7(1)	-8(1)
P(2)	27(1)	20(1)	19(1)	1(1)	-1(1)	-2(1)
P(3)	22(1)	17(1)	24(1)	-1(1)	1(1)	-2(1)
O(1)	54(3)	43(3)	69(4)	-12(3)	-46(3)	2(3)
C(11)	22(4)	21(4)	25(4)	-2(3)	-1(3)	-1(3)
C(13)	30(4)	22(4)	44(4)	-9(4)	-9(4)	-1(3)
C(12)	21(4)	25(4)	31(4)	-7(3)	-6(3)	3(3)
C(14)	37(4)	34(5)	46(4)	-12(4)	-21(4)	7(4)
C(15)	43(4)	30(5)	34(4)	-2(3)	-16(4)	14(4)
C(16)	27(4)	22(4)	28(4)	-8(3)	0(3)	2(3)
C(21)	37(4)	29(4)	28(4)	4(3)	-12(3)	4(3)
C(22)	46(5)	21(4)	38(4)	0(3)	-10(4)	-6(3)
C(23)	59(5)	36(4)	29(4)	-2(4)	16(4)	-14(4)
C(24)	67(6)	43(5)	38(5)	-15(4)	-1(4)	7(4)
C(25)	62(6)	31(5)	51(5)	-1(4)	-12(4)	-14(4)
C(26)	99(7)	23(5)	56(5)	3(4)	-27(5)	-2(4)
C(27)	92(7)	63(6)	38(5)	11(4)	19(5)	-23(5)
C(28)	66(6)	59(5)	33(4)	-17(4)	13(4)	-3(5)
C(29)	37(5)	71(6)	62(5)	-10(5)	29(4)	-13(4)
C(31)	28(4)	23(4)	32(4)	-4(3)	0(3)	-3(3)
C(32)	47(5)	39(5)	46(5)	-9(4)	20(4)	-10(4)
C(33)	41(4)	23(4)	43(4)	9(3)	-10(4)	-2(3)
C(34)	63(5)	23(4)	51(5)	8(4)	-14(4)	-7(4)
C(35)	86(6)	33(5)	56(5)	12(4)	-36(5)	-17(4)
C(36)	36(5)	48(5)	90(6)	21(5)	-6(5)	22(4)
C(37)	31(4)	57(5)	74(6)	-10(5)	18(4)	14(4)
C(38)	81(7)	62(6)	47(5)	-22(5)	26(5)	0(5)
C(39)	72(6)	61(6)	82(7)	2(5)	51(5)	-16(5)
O(2)	57(4)	56(4)	53(3)	15(3)	-38(3)	-19(3)
C(2)	28(4)	36(4)	39(4)	17(4)	-10(4)	-6(3)
C(3)	34(4)	33(4)	46(4)	9(4)	9(4)	7(4)
O(3)	76(4)	63(4)	74(4)	17(3)	21(4)	28(4)
N(1)	49(5)	40(4)	60(5)	-8(4)	28(4)	-8(3)
C(101)	31(9)	33(9)	58(11)	-4(8)	12(8)	-2(7)
C(102)	58(11)	39(10)	56(11)	-12(9)	36(9)	-7(8)
C(103)	79(13)	40(10)	25(9)	-4(8)	5(9)	7(10)
C(104)	76(13)	66(13)	62(13)	-31(11)	9(11)	-21(12)
C(105)	56(14)	81(16)	89(16)	50(15)	5(12)	-1(12)
C(106)	42(10)	76(13)	35(10)	-2(11)	-7(8)	22(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **4b**.

	x	y	z	U(eq)
H(13)	12454	3736	9207	39
H(15)	12234	603	9559	43
H(21A)	10748	-442	9378	37
H(21B)	11216	-604	8989	37
H(24A)	10766	-1199	8389	74
H(24B)	9896	-775	8161	74
H(24C)	10086	-2052	8198	74
H(25A)	8412	-2174	8398	72
H(25B)	8259	-887	8420	72
H(25C)	8068	-1629	8767	72
H(26A)	9415	-2456	9114	89
H(26B)	10461	-2246	8988	89
H(26C)	9804	-3032	8758	89
H(27A)	8282	-848	9750	96
H(27B)	9265	-1270	9605	96
H(27C)	8340	-1528	9382	96
H(28A)	9292	1640	9461	79
H(28B)	9794	678	9676	79
H(28C)	8769	1047	9787	79
H(29A)	7403	610	9381	85
H(29B)	7553	-56	9015	85
H(29C)	7895	1179	9043	85
H(31A)	11696	4197	8608	33
H(31B)	10695	4276	8797	33
H(34A)	10002	5942	7948	69
H(34B)	10962	5314	7887	69
H(34C)	10612	5577	8287	69
H(35A)	9312	3204	7676	87
H(35B)	10167	3879	7515	87
H(35C)	9180	4454	7566	87
H(36A)	9153	4633	8524	87
H(36B)	8626	3770	8274	87
H(36C)	8628	5030	8167	87
H(37A)	12863	1831	8051	81
H(37B)	12063	1498	8329	81
H(37C)	12630	2604	8386	81
H(38A)	10881	2319	7499	95
H(38B)	10959	1321	7774	95
H(38C)	11832	1654	7532	95
H(39A)	12251	4275	7978	107
H(39B)	11732	4029	7606	107
H(39C)	12717	3482	7688	107

Computed-Structures.xyz

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26
C1 Model System, B3LYP/LANL2DZ, E =  -719.536385551
Ru     1.098513    0.001107   -0.018591
P      0.732879    2.355620    0.324513
P      0.713871   -2.344442   -0.395365
O     -5.182077    0.001874   -0.020153
C     -0.944310    0.004268   -0.005616
C     -3.126120   -1.233800    0.064755
H     -3.697685   -2.157440    0.136305
C     -1.750674   -1.233580    0.081985
C     -3.906383    0.002564   -0.013188
C     -3.126400    1.239314   -0.082387
H     -3.698670    2.162144   -0.159693
C     -1.750444    1.242175   -0.087318
C     -1.044508    2.579199   -0.257100
H     -1.552196    3.389773    0.274861
H     -0.992844    2.852813   -1.319237
H      0.757257    2.856734    1.664066
H     -0.943178   -2.811773    1.324849
C      2.516197    0.187865   -1.304878
C      2.328370   -0.217443    1.424053
O      3.001698   -0.381579    2.385359
H      1.487658   -3.383782    0.211816
H      0.677851   -2.825812   -1.741945
H      1.482498    3.384725   -0.328888
O      3.312938    0.339267   -2.168152
C     -1.038150   -2.565549    0.258928
H     -1.562440   -3.390351   -0.233181
26
C2 Model System, B3LYP/LANL2DZ, E =  -719.536362524
Ru     0.000000    0.000000    1.098339
C      1.381959   -0.004227    2.425197
C     -1.381959    0.004227    2.425197
O      2.309801    0.017184    3.161652
O     -2.309801   -0.017184    3.161652
P      0.000000    2.377321    0.719629
P      0.000000   -2.377321    0.719629
H     -1.254018    3.065165    0.697965
H      1.254018   -3.065165    0.697965
H     -0.770343   -3.307608    1.486981
H      0.770343    3.307608    1.486981
C     -0.662577   -2.497894   -1.038974
C      0.662577    2.497894   -1.038974
H      0.297077    3.388584   -1.559013
H     -0.297077   -3.388584   -1.559013
H      1.754388    2.578361   -0.953451
H     -1.754388   -2.578361   -0.953451
C      0.000000    0.000000   -0.944744
C     -0.279951   -1.209018   -1.750643
C      0.279951    1.209018   -1.750643
C     -0.268862   -1.209569   -3.126284
C      0.268862    1.209569   -3.126284
C      0.000000    0.000000   -3.906316
H     -0.488704   -2.109198   -3.698322
H      0.488704    2.109198   -3.698322
O      0.000000    0.000000   -5.181967
26
Cs Model System, B3LYP/LANL2DZ, E =  -719.537526670
Ru     0.073481   -1.095625    0.000000
```

C	0.000000	0.943492	0.000000
C	-0.771839	3.788649	0.000000
C	-0.103150	1.738856	1.238807
C	-0.103150	1.738856	-1.238807
C	-0.502285	3.056287	-1.240139
C	-0.502285	3.056287	1.240139
C	0.267930	1.081986	2.558233
C	0.267930	1.081986	-2.558233
H	-0.620396	3.616910	-2.165346
H	-0.620396	3.616910	2.165346
O	-1.176278	4.999092	0.000000
C	1.820214	-1.801050	0.000000
C	-0.782152	-2.847674	0.000000
H	0.701252	-1.423390	3.341207
H	0.701252	-1.423390	-3.341207
H	1.349936	1.160604	2.728071
P	-0.121352	-0.753437	2.381163
H	-0.243692	1.529053	3.415468
H	1.349936	1.160604	-2.728071
H	-0.243692	1.529053	-3.415468
P	-0.121352	-0.753437	-2.381163
H	-1.399579	-0.922340	-3.003214
H	-1.399579	-0.922340	3.003214
O	-1.369409	-3.875036	0.000000
O	2.956321	-2.141193	0.000000

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C1 Real system, ONIOM(B3LYP/LANL2DZ:HF/LANL1MB), E = -1336.796203161223

O	-0.152185	-1.008162	-3.252378
C	-0.085503	-0.901652	-2.069026
C	0.032544	-2.416599	0.245389
O	0.049878	-3.547033	0.609444
H	2.570814	1.403754	-1.854415
H	3.404014	2.080899	-0.456758
C	2.512464	1.526888	-0.766214
H	-2.367537	1.574739	1.881290
H	-3.296746	2.125642	0.498527
C	-2.389596	1.584858	0.785427
C	-1.138203	2.287115	0.283883
H	-2.003739	4.243401	0.563756
C	-1.126145	3.667850	0.277015
C	0.065287	4.439235	-0.066755
C	1.238157	2.270074	-0.394212
H	2.154129	4.209727	-0.623701
C	1.253877	3.649393	-0.380869
C	0.036113	1.483210	-0.077107
O	0.073188	5.718721	-0.075621
P	2.410528	-0.196480	-0.017050
P	-2.400871	-0.209404	0.206918
Ru	0.000645	-0.545621	-0.251014
C	3.722765	-1.290800	-1.118543
C	3.114679	0.021629	1.899497
C	-3.640840	-0.181525	-1.406728
C	-3.262917	-1.187107	1.774922
H	4.943938	0.456031	2.951258
H	5.191261	-0.622291	1.592118
H	4.929279	1.102484	1.318888
C	4.644946	0.250510	1.926698
H	3.088171	-1.125870	3.727874
H	1.670405	-1.382990	2.718080
H	3.206426	-2.132370	2.289644
C	2.744657	-1.244319	2.703690

```
H     2.673617    2.163195    1.998126
H     1.345352    1.134568    2.528153
H     2.757092    1.348667    3.555461
C     2.420654    1.251761    2.526907
H     3.764985   -2.139376   -3.101754
H     2.202689   -2.296990   -2.318701
H     2.706832   -0.741321   -2.979781
C     3.045342   -1.632857   -2.464491
H     4.656079   -3.238689   -1.038285
H     4.624565   -2.434352    0.521249
H     3.152081   -3.151672   -0.129439
C     4.057315   -2.610245   -0.384202
H     4.796587    0.418977   -1.962855
H     5.559585   -0.236684   -0.519590
H     5.666875   -1.103355   -2.040417
C     5.017006   -0.492790   -1.419260
H    -2.555477   -1.757660   -2.463757
H    -3.908525   -2.351415   -1.510782
H    -4.199943   -1.501514   -3.021690
C    -3.565085   -1.539987   -2.140607
H    -3.764933    0.964607   -3.231212
H    -3.218176    1.918255   -1.858958
H    -2.118590    0.793084   -2.643883
C    -3.144969    0.949483   -2.339160
H    -5.545654   -0.721199   -0.468765
H    -5.196423    1.008556   -0.416585
H    -5.691447    0.249613   -1.921000
C    -5.110134    0.107533   -1.013676
H    -4.861646   -0.950310    3.202865
H    -4.226694    0.583710    2.636089
H    -5.295755   -0.363945    1.608909
C    -4.490997   -0.421381    2.328901
H    -4.496928   -2.584040    0.628177
H    -2.843823   -3.140310    0.888146
H    -4.005971   -3.170162    2.208794
C    -3.677561   -2.610795    1.336715
H    -2.652310   -1.740744    3.769514
H    -1.357751   -1.884187    2.588000
H    -1.834592   -0.299168    3.174923
C    -2.200928   -1.279801    2.894727
74
C2 Real system, ONIOM(B3LYP/LANL2DZ:HF/LANL1MB), E = -1336.795348604219
O     0.000000    0.000000   -5.707944
H     0.133080    2.159025   -4.215018
H    -0.133080   -2.159025   -4.215018
C     0.000000    0.000000   -4.429726
C     0.061104    1.233650   -3.647726
C    -0.061104   -1.233650   -3.647726
C     0.070923    1.232559   -2.269109
C    -0.070923   -1.232559   -2.269109
C     0.000000    0.000000   -1.465364
H    -1.304943   -2.738028   -1.378272
H     1.304943    2.738028   -1.378272
H     0.151959   -3.393349   -2.114052
H    -0.151959    3.393349   -2.114052
C     0.238256    2.551869   -1.536723
C    -0.238256   -2.551869   -1.536723
P     0.552719   -2.358493    0.159157
P    -0.552719    2.358493    0.159157
O    -2.241873   -0.337705    2.654209
O     2.241873    0.337705    2.654209
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C     -1.330356   -0.206352    1.901168
C      1.330356    0.206352    1.901168
Ru     0.000000    0.000000    0.567482
C      0.325077    3.764668    1.332244
C     -0.325077   -3.764668    1.332244
C      2.525936   -2.800117   -0.151948
C     -2.525936    2.800117   -0.151948
H      2.279026   -3.867742   -2.045336
H      3.753400   -4.245144   -1.175042
H      2.228503   -4.927676   -0.639236
H     -3.753400    4.245144   -1.175042
H     -2.228503    4.927676   -0.639236
H     -2.279026    3.867742   -2.045336
H      2.221380    2.666168    1.217957
H      2.130084    4.044886    0.128366
H      2.350418    4.301214    1.850414
H     -2.130084   -4.044886    0.128366
H     -2.350418   -4.301214    1.850414
H     -2.221380   -2.666168    1.217957
H     -2.681697    1.370049   -1.797792
H     -3.160090    0.709393   -0.241206
H     -4.218401    1.841039   -1.075891
H      4.218401   -1.841039   -1.075891
H      2.681697   -1.370049   -1.797792
H      3.160090   -0.709393   -0.241206
H     -1.065895    3.478875    3.000491
H      0.373411    2.471992    3.093063
H      0.479276    4.188878    3.446900
H     -0.479276   -4.188878    3.446900
H      1.065895   -3.478875    3.000491
H     -0.373411   -2.471992    3.093063
H     -4.288807    3.145735    1.045268
H     -3.068465    2.191168    1.875467
H     -2.860410    3.933200    1.693835
H      2.860410   -3.933200    1.693835
H      4.288807   -3.145735    1.045268
H      3.068465   -2.191168    1.875467
H      0.024250    5.432177   -0.055397
H     -1.180276    5.357985    1.232858
H      0.448255    5.905473    1.582772
H      1.180276   -5.357985    1.232858
H     -0.448255   -5.905473    1.582772
H     -0.024250   -5.432177   -0.055397
C      0.000000    3.449233    2.811215
C      1.854518    3.679118    1.110572
C     -0.135473    5.203497    0.992744
C      0.135473   -5.203497    0.992744
C      0.000000   -3.449233    2.811215
C     -1.854518   -3.679118    1.110572
C      3.220500   -3.033434    1.209821
C      2.691601   -4.045001   -1.058961
C      3.181372   -1.594313   -0.863085
C     -3.181372    1.594313   -0.863085
C     -3.220500    3.033434    1.209821
C     -2.691601    4.045001   -1.058961
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Cs Real system, ONIOM(B3LYP/LANL2DZ:HF/LANL1MB), E = -1336.797351208354
O      1.824056    3.046414    0.000000
O     -2.700555    2.169638    0.000000
H      1.410887   -1.669790    3.408633
H      1.410887   -1.669790   -3.408633
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P	-0.032407	0.157135	2.424481
P	-0.032407	0.157135	-2.424481
H	2.344018	-0.401490	2.622841
H	2.344018	-0.401490	-2.622841
C	-1.651162	1.612868	0.000000
C	1.061325	2.131210	0.000000
O	2.435155	-5.095336	0.000000
H	2.138216	-3.626125	-2.163003
H	2.138216	-3.626125	2.163003
C	1.439751	-1.011789	2.537581
C	1.439751	-1.011789	-2.537581
C	1.912257	-3.102704	-1.237037
C	1.912257	-3.102704	1.237037
C	1.501657	-1.785531	1.233383
C	1.501657	-1.785531	-1.233383
C	2.095812	-3.862530	0.000000
C	1.131414	-1.077631	0.000000
Ru	0.000000	0.607852	0.000000
C	-1.599571	-0.956370	-3.139010
C	-1.599571	-0.956370	3.139010
C	0.375036	1.709467	3.674467
C	0.375036	1.709467	-3.674467
H	-2.102733	-2.269980	4.768940
H	-2.102733	-2.269980	-4.768940
H	-0.410119	-2.361700	4.323409
H	-0.410119	-2.361700	-4.323409
H	-1.005385	-0.993866	5.259833
H	-1.005385	-0.993866	-5.259833
H	-0.358718	3.214707	2.273368
H	-0.358718	3.214707	-2.273368
H	-1.591852	2.625576	3.383261
H	-1.591852	2.625576	-3.383261
H	-0.345959	3.729385	3.952660
H	-0.345959	3.729385	-3.952660
H	-3.057298	0.504346	2.430035
H	-3.057298	0.504346	-2.430035
H	-3.682290	-0.636610	3.613172
H	-3.682290	-0.636610	-3.613172
H	-2.652772	0.686343	4.137009
H	-2.652772	0.686343	-4.137009
H	-0.868385	1.168271	5.399774
H	-0.868385	1.168271	-5.399774
H	0.763613	0.496060	5.455983
H	0.763613	0.496060	-5.455983
H	0.496656	2.203558	5.770765
H	0.496656	2.203558	-5.770765
H	2.525798	1.365475	3.874312
H	2.525798	1.365475	-3.874312
H	2.093628	2.273957	2.429420
H	2.093628	2.273957	-2.429420
H	2.036230	3.045254	4.005852
H	2.036230	3.045254	-4.005852
H	-2.734176	-2.654941	2.452412
H	-2.734176	-2.654941	-2.452412
H	-2.264651	-1.563089	1.154620
H	-2.264651	-1.563089	-1.154620
H	-1.074735	-2.649170	1.858789
H	-1.074735	-2.649170	-1.858789
C	0.172374	1.358607	5.168668
C	0.172374	1.358607	-5.168668
C	-0.545525	2.891215	3.290509

C	-0.545525	2.891215	-3.290509
C	1.854764	2.116090	3.473036
C	1.854764	2.116090	-3.473036
C	-1.933608	-2.024547	2.074201
C	-1.933608	-2.024547	-2.074201
C	-2.821171	-0.031190	3.342901
C	-2.821171	-0.031190	-3.342901
C	-1.242739	-1.681675	4.460252
C	-1.242739	-1.681675	-4.460252
74			
C1	Real system, ONIOM(B3LYP/LANL2DZ+P:HF/LANL1MB), E = -1337.008970932447		
O	-0.160141	-1.069094	-3.235851
C	-0.090552	-0.944809	-2.085557
C	0.053991	-2.424251	0.219331
O	0.087164	-3.526646	0.565948
H	2.586600	1.409056	-1.819962
H	3.399934	2.070867	-0.396868
C	2.502834	1.525772	-0.726652
H	-2.322032	1.533646	1.884165
H	-3.288972	2.092697	0.525899
C	-2.363030	1.557109	0.783277
C	-1.132909	2.281295	0.280359
H	-2.017415	4.223253	0.555971
C	-1.131998	3.650202	0.268692
C	0.050459	4.434673	-0.076627
C	1.232279	2.275826	-0.383246
H	2.144735	4.210479	-0.618133
C	1.241367	3.643912	-0.377744
C	0.038708	1.483924	-0.078319
O	0.049685	5.674303	-0.092510
P	2.353872	-0.171007	-0.022334
P	-2.343471	-0.199491	0.207212
Ru	0.004444	-0.543376	-0.272304
C	3.685327	-1.249413	-1.101711
C	3.034089	0.010133	1.896936
C	-3.601944	-0.178440	-1.381497
C	-3.190864	-1.185717	1.764940
H	4.847240	0.424895	2.983841
H	5.114619	-0.637265	1.616874
H	4.862731	1.091440	1.360471
C	4.564830	0.232856	1.952120
H	2.990582	-1.160523	3.710725
H	1.576261	-1.393891	2.692238
H	3.107896	-2.149851	2.261206
C	2.651346	-1.263144	2.683564
H	2.604118	2.152850	2.028548
H	1.266974	1.124197	2.533540
H	2.673039	1.312461	3.572411
C	2.342765	1.234176	2.540412
H	3.778984	-2.062117	-3.098987
H	2.205345	-2.256911	-2.350618
H	2.697877	-0.682439	-2.974419
C	3.039949	-1.577346	-2.467292
H	4.614934	-3.200220	-1.036505
H	4.561271	-2.420312	0.534057
H	3.098239	-3.124981	-0.149507
C	4.007435	-2.580437	-0.382379
H	4.782106	0.461197	-1.916311
H	5.514930	-0.202923	-0.462107
H	5.648059	-1.063115	-1.983477
C	4.988145	-0.453524	-1.372259

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 H     -2.540898   -1.761366   -2.455382
 H     -3.885884   -2.346740   -1.487466
 H     -4.189025   -1.491590   -2.992140
 C     -3.544088   -1.536085   -2.118847
 H     -3.750466    0.964057   -3.207697
 H     -3.184025    1.919927   -1.845188
 H     -2.096413    0.793007   -2.642578
 C     -3.118520    0.950027   -2.324212
 H     -5.502416   -0.715484   -0.432220
 H     -5.147439    1.012693   -0.373947
 H     -5.654872    0.262808   -1.877898
 C     -5.067388    0.114339   -0.975703
 H     -4.778398   -0.971367    3.208965
 H     -4.154683    0.571493    2.656241
 H     -5.228927   -0.367108    1.627133
 C     -4.417245   -0.430627    2.338415
 H     -4.441010   -2.580979    0.633569
 H     -2.781701   -3.132759    0.857788
 H     -3.917667   -3.175112    2.200005
 C     -3.607996   -2.608605    1.325811
 H     -2.573688   -1.749622    3.755575
 H     -1.284389   -1.891715    2.569313
 H     -1.754361   -0.308200    3.164293
 C     -2.124823   -1.286330    2.880869
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 C2 Real system, ONIOM(B3LYP/LANL2DZ+P:HF/LANL1MB), E = -1337.008950525259
 O      0.000000    0.000000   -5.651211
 H      0.179383    2.156106   -4.191828
 H     -0.179383   -2.156106   -4.191828
 C      0.000000    0.000000   -4.412115
 C      0.086412    1.227234   -3.623298
 C     -0.086412   -1.227234   -3.623298
 C      0.095932    1.222945   -2.255596
 C     -0.095932   -1.222945   -2.255596
 C      0.000000    0.000000   -1.454439
 H     -1.356200   -2.674930   -1.324666
 H      1.356200    2.674930   -1.324666
 H      0.070264   -3.391624   -2.077330
 H     -0.070264    3.391624   -2.077330
 C      0.281844    2.522230   -1.505783
 C     -0.281844   -2.522230   -1.505783
 P      0.507447   -2.307709    0.145930
 P     -0.507447    2.307709    0.145930
 O     -2.205962   -0.267236    2.679238
 O      2.205962    0.267236    2.679238
 C     -1.322943   -0.166579    1.936562
 C      1.322943    0.166579    1.936562
 Ru     0.000000    0.000000    0.583144
 C      0.350210    3.713264    1.318837
 C     -0.350210   -3.713264    1.318837
 C      2.465772   -2.768924   -0.179125
 C     -2.465772    2.768924   -0.179125
 H      2.216927   -3.779283   -2.102953
 H      3.669519   -4.217769   -1.225483
 H      2.121439   -4.875961   -0.728012
 H     -3.669519    4.217769   -1.225483
 H     -2.121439    4.875961   -0.728012
 H     -2.216927    3.779283   -2.102953
 H      2.242812    2.602768    1.244289
 H      2.183938    3.982606    0.154977
 H      2.368508    4.236036    1.880913
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H    -2.183938   -3.982606    0.154977
H    -2.368508   -4.236036    1.880913
H    -2.242812   -2.602768    1.244289
H    -2.648403    1.305402   -1.793400
H    -3.145266    0.689969   -0.224691
H    -4.175914    1.825821   -1.086928
H     4.175914   -1.825821   -1.086928
H     2.648403   -1.305402   -1.793400
H     3.145266   -0.689969   -0.224691
H    -1.067874    3.459199    2.970747
H     0.361124    2.442146    3.096083
H     0.475856    4.161401    3.431111
H    -0.475856   -4.161401    3.431111
H     1.067874   -3.459199    2.970747
H    -0.361124   -2.442146    3.096083
H    -4.234652    3.162501    0.994175
H    -3.031477    2.219367    1.859800
H    -2.805701    3.953626    1.634542
H     2.805701   -3.953626    1.634542
H     4.234652   -3.162501    0.994175
H     3.031477   -2.219367    1.859800
H     0.095190    5.373000   -0.087333
H    -1.134415    5.324800    1.177595
H     0.493288    5.855080    1.554073
H     1.134415   -5.324800    1.177595
H    -0.493288   -5.855080    1.554073
H    -0.095190   -5.373000   -0.087333
C     0.000000    3.418779    2.796572
C     1.884146    3.617878    1.130415
C    -0.087418    5.154762    0.959270
C     0.087418   -5.154762    0.959270
C     0.000000   -3.418779    2.796572
C    -1.884146   -3.617878    1.130415
C     3.168944   -3.044895    1.170578
C     2.611802   -3.993933   -1.116756
C     3.145121   -1.561463   -0.865541
C    -3.145121    1.561463   -0.865541
C    -3.168944    3.044895    1.170578
C    -2.611802    3.993933   -1.116756
74
Cs Real system, ONIOM(B3LYP/LANL2DZ+P:HF/LANL1MB), E = -1337.010118505291
O     1.607559    3.175080    0.000000
O    -2.742342    2.045377    0.000000
H     1.434709   -1.626748    3.404362
H     1.434709   -1.626748   -3.404362
P    -0.002995    0.152977    2.370727
P    -0.002995    0.152977   -2.370727
H     2.342185   -0.364743    2.564981
H     2.342185   -0.364743   -2.564981
C    -1.696374    1.551972    0.000000
C     0.938311    2.227649    0.000000
O     2.350610   -5.065832    0.000000
H     2.097091   -3.622271   -2.163465
H     2.097091   -3.622271    2.163465
C     1.437971   -0.989269    2.510878
C     1.437971   -0.989269   -2.510878
C     1.874894   -3.095025   -1.232491
C     1.874894   -3.095025    1.232491
C     1.492577   -1.781501    1.225811
C     1.492577   -1.781501   -1.225811
C     2.043937   -3.865494    0.000000
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C	1.128593	-1.069692	0.000000
Ru	0.000000	0.615521	0.000000
C	-1.560682	-0.950260	-3.093770
C	-1.560682	-0.950260	3.093770
C	0.396336	1.686064	3.631178
C	0.396336	1.686064	-3.631178
H	-2.054460	-2.272156	4.720223
H	-2.054460	-2.272156	-4.720223
H	-0.389207	-2.431426	4.199614
H	-0.389207	-2.431426	-4.199614
H	-0.878933	-1.058717	5.188005
H	-0.878933	-1.058717	-5.188005
H	-0.387018	3.207381	2.273379
H	-0.387018	3.207381	-2.273379
H	-1.587162	2.585962	3.400243
H	-1.587162	2.585962	-3.400243
H	-0.340992	3.693094	3.959568
H	-0.340992	3.693094	-3.959568
H	-3.020170	0.548018	2.467587
H	-3.020170	0.548018	-2.467587
H	-3.631022	-0.630427	3.619396
H	-3.631022	-0.630427	-3.619396
H	-2.581918	0.663872	4.171535
H	-2.581918	0.663872	-4.171535
H	-0.798708	1.104595	5.379609
H	-0.798708	1.104595	-5.379609
H	0.843152	0.455753	5.387393
H	0.843152	0.455753	-5.387393
H	0.559709	2.154326	5.731116
H	0.559709	2.154326	-5.731116
H	2.556302	1.384208	3.803463
H	2.556302	1.384208	-3.803463
H	2.090389	2.284250	2.365314
H	2.090389	2.284250	-2.365314
H	2.036931	3.053642	3.942687
H	2.036931	3.053642	-3.942687
H	-2.732343	-2.625924	2.412355
H	-2.732343	-2.625924	-2.412355
H	-2.309225	-1.505903	1.123925
H	-2.309225	-1.505903	-1.123925
H	-1.098471	-2.614658	1.752436
H	-1.098471	-2.614658	-1.752436
C	0.232943	1.313109	5.125299
C	0.232943	1.313109	-5.125299
C	-0.546118	2.863609	3.288475
C	-0.546118	2.863609	-3.288475
C	1.865875	2.121856	3.411294
C	1.865875	2.121856	-3.411294
C	-1.943633	-1.990824	2.017646
C	-1.943633	-1.990824	-2.017646
C	-2.769949	-0.022569	3.355018
C	-2.769949	-0.022569	-3.355018
C	-1.182317	-1.716865	4.385960
C	-1.182317	-1.716865	-4.385960