Supporting material

Title: Preparation and Characterization of 4-Azoniaheptatrienyl, 4-Azaheptatrienyl, Ruthenapyrrolinone and Pyrrolinyl Complexes of Ruthenium

Authors: María L. Buil, Miguel A. Esteruelas, Ana M. López and Enrique Oñate.

Complex $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)C{=}O\}(P^iPr_3)$ (**3**):

Complex $Ru(\eta^5\text{-}C_5H_5)\{C{=}CHCPh_2(CH{=}CH_2)NCH_2CH{=}CH_2\}(CO)(P^iPr_3)$ (**4**):

Complex $[Ru(\eta^5\text{-}C_5H_5)\{C{=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)CPh_2CH_2\}(CO)(P^iPr_3)]BF_4$ (**5**):

Complex $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}NCH{=}CHCH_3\}(CO)(P^iPr_3)$ (**9**):

Table to be deposited

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for complex Ru(η^5-C_5H_5){C(CH=CPh$_2$)=N(CH$_2$CH=CH$_2$)CH(CH=CH$_2$)C=O}(P^{i}Pr$_3$) (**3**):

Atom	X/*a*	Y/*b*	Z/*c*	U_{eq}[a]
Ru	0.71451(6)	0.30860(4)	0.54063(3)	0.02439(17)
P	0.92263(19)	0.23860(13)	0.56406(9)	0.0253(5)
O	0.5249(5)	0.1710(3)	0.5733(2)	0.0300(13)
N	0.6811(5)	0.2139(3)	0.4208(3)	0.0220(15)
C1	0.7261(6)	0.2880(4)	0.4497(3)	0.0196(17)
C2	0.7717(7)	0.3532(5)	0.4027(3)	0.0243(18)
C3	0.7040(7)	0.3915(5)	0.3526(3)	0.0231(18)
C4	0.7653(7)	0.4631(5)	0.3157(3)	0.0287(19)
C5	0.9124(8)	0.4687(5)	0.3078(3)	0.033(2)
C6	0.9696(9)	0.5314(6)	0.2704(4)	0.043(2)
C7	0.8866(10)	0.5913(5)	0.2423(4)	0.049(3)
C8	0.7413(10)	0.5897(5)	0.2507(4)	0.045(2)
C9	0.6844(8)	0.5249(5)	0.2869(4)	0.036(2)
C10	0.5602(7)	0.3664(5)	0.3299(3)	0.0230(17)
C11	0.4508(7)	0.3617(5)	0.3713(4)	0.0297(19)
C12	0.3173(8)	0.3414(4)	0.3482(3)	0.0299(19)
C13	0.2948(7)	0.3256(5)	0.2836(3)	0.031(2)
C14	0.4027(7)	0.3290(4)	0.2398(3)	0.0289(19)
C15	0.5358(7)	0.3515(5)	0.2641(4)	0.031(2)
C16	0.6064(8)	0.1578(5)	0.4662(4)	0.030(2)
C17	0.4624(8)	0.1368(6)	0.4387(4)	0.033(2)
C18	0.4172(10)	0.0619(6)	0.4253(4)	0.043(2)
C19	0.6946(8)	0.1854(6)	0.3534(3)	0.0303(18)
C20	0.7581(8)	0.0997(6)	0.3492(4)	0.034(2)
C21	0.7016(10)	0.0333(6)	0.3213(5)	0.048(3)
C22	0.6037(7)	0.2017(5)	0.5333(3)	0.0233(17)
C23	1.0658(6)	0.3158(5)	0.5837(3)	0.0244(17)
C24	1.0905(7)	0.3821(5)	0.5305(3)	0.031(2)
C25	1.2053(7)	0.2775(4)	0.6073(3)	0.033(2)
C26	0.9912(7)	0.1614(4)	0.5034(3)	0.0262(18)
C27	1.0534(7)	0.2029(5)	0.4437(3)	0.038(2)
C28	1.0956(7)	0.0943(5)	0.5289(4)	0.036(2)
C29	0.9229(7)	0.1732(4)	0.6384(3)	0.0290(19)
C30	0.8892(7)	0.2230(4)	0.7002(3)	0.033(2)
C31	0.8203(7)	0.0994(5)	0.6317(3)	0.0306(19)
C32	0.7530(7)	0.4465(5)	0.5765(4)	0.031(2)
C33	0.7224(7)	0.3968(5)	0.6310(4)	0.033(2)
C34	0.5870(7)	0.3636(5)	0.6237(3)	0.0288(19)
C35	0.5338(8)	0.3931(5)	0.5625(3)	0.030(2)
C36	0.6394(7)	0.4445(5)	0.5338(3)	0.0264(19)

[a] Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *Uij* tensor.

Table to be deposited

Table S2. Anisotropic displacement coefficients U_{ij} (Å^2) for the non-hydrogen atoms for the complex Ru(η^5-C_5H_5){C(CH=CPh$_2$)=N(CH$_2$CH=CH$_2$)CH(CH=CH$_2$)C=O}(P^{i}Pr$_3$) (**3**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	0.0137(3)	0.0315(3)	0.0281(3)	-0.0004(4)	0.0023(2)	0.0005(4)
P	0.0165(11)	0.0333(13)	0.0261(11)	0.0000(10)	0.0011(9)	-0.0012(9)
O	0.023(3)	0.034(4)	0.034(3)	0.004(2)	0.007(2)	-0.001(2)
N	0.008(3)	0.030(4)	0.027(3)	-0.001(3)	0.000(3)	0.005(3)
C1	0.003(3)	0.025(4)	0.031(3)	0.006(3)	0.003(3)	0.002(3)
C2	0.010(4)	0.039(5)	0.023(4)	-0.015(4)	0.000(3)	-0.001(4)
C3	0.012(4)	0.038(5)	0.019(4)	-0.001(4)	0.002(3)	-0.006(4)
C4	0.020(4)	0.037(5)	0.029(5)	-0.007(4)	0.003(4)	-0.002(4)
C5	0.028(5)	0.046(5)	0.024(4)	-0.005(4)	0.005(4)	-0.009(4)
C6	0.037(5)	0.056(6)	0.035(5)	-0.003(5)	0.010(4)	-0.020(5)
C7	0.081(8)	0.035(6)	0.031(5)	-0.003(4)	0.010(5)	-0.030(5)
C8	0.060(7)	0.037(6)	0.040(5)	0.001(4)	0.007(5)	-0.004(5)
C9	0.035(5)	0.035(5)	0.037(5)	-0.003(4)	-0.001(4)	0.001(4)
C10	0.018(4)	0.031(5)	0.020(4)	0.002(3)	-0.003(3)	0.001(3)
C11	0.022(4)	0.043(5)	0.024(4)	0.005(4)	0.000(4)	-0.003(4)
C12	0.023(4)	0.036(5)	0.032(5)	0.010(4)	0.008(4)	0.001(4)
C13	0.020(4)	0.035(6)	0.037(5)	0.005(4)	-0.004(4)	0.005(4)
C14	0.027(4)	0.033(5)	0.027(4)	-0.006(4)	-0.005(3)	-0.002(4)
C15	0.012(4)	0.040(5)	0.042(5)	0.002(4)	0.007(4)	0.001(4)
C16	0.013(4)	0.036(5)	0.041(5)	-0.003(4)	0.004(4)	0.001(4)
C17	0.015(4)	0.040(6)	0.045(5)	0.010(5)	0.000(4)	-0.004(4)
C18	0.038(6)	0.049(7)	0.043(6)	-0.009(5)	0.012(5)	-0.012(5)
C19	0.029(4)	0.034(5)	0.028(4)	-0.001(5)	-0.003(3)	0.005(5)
C20	0.031(5)	0.041(6)	0.029(5)	-0.009(4)	0.006(4)	0.001(5)
C21	0.049(6)	0.042(7)	0.052(6)	0.000(6)	0.003(5)	0.009(5)
C22	0.016(4)	0.023(5)	0.031(4)	-0.002(4)	-0.003(3)	0.001(4)
C23	0.016(4)	0.029(4)	0.028(4)	-0.001(4)	-0.001(3)	-0.009(4)
C24	0.028(5)	0.033(5)	0.032(5)	0.000(4)	0.000(4)	-0.003(4)
C25	0.014(4)	0.039(5)	0.047(5)	0.001(4)	-0.002(4)	-0.006(4)
C26	0.025(4)	0.031(5)	0.022(4)	-0.002(3)	0.004(3)	-0.002(4)
C27	0.013(4)	0.062(6)	0.039(5)	-0.005(5)	-0.001(3)	-0.001(4)
C28	0.028(5)	0.038(5)	0.043(5)	-0.002(4)	0.005(4)	0.002(4)
C29	0.021(4)	0.033(5)	0.033(4)	-0.002(4)	0.003(3)	0.001(4)
C30	0.030(4)	0.035(5)	0.033(4)	0.010(4)	-0.003(4)	-0.009(4)
C31	0.029(5)	0.038(5)	0.025(4)	-0.002(4)	0.006(4)	-0.001(4)
C32	0.016(4)	0.035(5)	0.043(5)	-0.002(4)	-0.001(4)	-0.002(4)
C33	0.016(4)	0.047(6)	0.036(5)	0.000(4)	-0.006(4)	0.008(4)
C34	0.020(4)	0.046(5)	0.021(4)	-0.002(4)	0.007(3)	0.002(4)
C35	0.025(5)	0.032(5)	0.035(5)	-0.009(4)	0.010(4)	-0.001(4)
C36	0.021(4)	0.033(5)	0.024(4)	0.004(4)	-0.003(4)	0.002(4)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2 (h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12})$.

Table to be deposited

Table S3. Hydrogen atom coordinates* and isotropic displacement coefficient ($Å^2$) for the compound $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)C{=}O\}(P^iPr_3)$ (**3**).

Atom	X/*a*	Y/*b*	Z/*c*	*U*
H2[a]	0.861(6)	0.374(4)	0.419(3)	0.029
H5	0.9723	0.4281	0.3289	0.039
H6	1.0681	0.5329	0.2642	0.051
H7	0.9271	0.6349	0.2165	0.058
H8	0.6829	0.6327	0.2318	0.054
H9	0.5856	0.5232	0.2921	0.043
H11	0.4661	0.3725	0.4168	0.036
H12	0.2416	0.3385	0.3777	0.036
H13	0.2027	0.3118	0.2680	0.037
H14	0.3871	0.3166	0.1945	0.035
H15	0.6112	0.3565	0.2346	0.038
H16[a]	0.647(7)	0.110(4)	0.471(3)	0.036
H17[a]	0.408(6)	0.190(5)	0.427(3)	0.040
H18A[a]	0.332(8)	0.054(5)	0.401(3)	0.052
H18B[a]	0.454(8)	0.009(5)	0.424(4)	0.052
H19A[a]	0.599(7)	0.179(4)	0.328(3)	0.036
H19B[a]	0.746(7)	0.229(4)	0.330(3)	0.036
H20[a]	0.839(7)	0.103(5)	0.367(3)	0.040
H21A[a]	0.731(8)	-0.016(5)	0.326(4)	0.058
H21B[a]	0.611(8)	0.052(5)	0.284(3)	0.058
H23	1.0316	0.3491	0.6221	0.029
H24A	1.1406	0.4311	0.5497	0.046
H24B	1.0000	0.4010	0.5119	0.046
H24C	1.1469	0.3570	0.4958	0.046
H25A	1.2539	0.2531	0.5698	0.050
H25B	1.1877	0.2327	0.6396	0.050
H25C	1.2638	0.3221	0.6276	0.050
H26	0.9075	0.1289	0.4867	0.031
H27A	1.1408	0.2321	0.4566	0.057
H27B	0.9865	0.2443	0.4251	0.057
H27C	1.0732	0.1592	0.4108	0.057
H28A	1.1238	0.0577	0.4924	0.054
H28B	1.0513	0.0594	0.5626	0.054
H28C	1.1787	0.1226	0.5480	0.054
H29	1.0192	0.1486	0.6446	0.035
H30A	0.7953	0.2482	0.6954	0.049
H30B	0.9588	0.2684	0.7069	0.049
H30C	0.8917	0.1846	0.7382	0.049
H31A	0.8343	0.0601	0.6687	0.046
H31B	0.8365	0.0691	0.5904	0.046
H31C	0.7239	0.1213	0.6315	0.046
H32	0.8381	0.4766	0.5700	0.038
H33	0.7842	0.3869	0.6675	0.040
H34	0.5399	0.3283	0.6540	0.035
H35	0.4438	0.3808	0.5437	0.036
H36	0.6324	0.4724	0.4924	0.032

* The hydrogen atoms were included in observed or calculated positions and refined riding on their respective carbon atoms. [a] These hydrogen were refined as free isotropic atoms.

Table to be deposited

Table S4. Full experimental details for the X-Ray analysis of $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)C{=}O\}(P^iPr_3)$ (**3**).

Crystal data:

Formula	$C_{36}H_{46}NOPRu$
Molecular weight	640.78
Crystal habit	irregular block
color	orange
Size(mm)	0.12 x 0.04 x 0.02
Symmetry	monoclinic, $P2_1/c$
Unit cell dimensions	9.521(4), 15.691(6), 20.348(8) Å
	90, 91.315(7), 90 °
Packing: V (Å^3), Z	3039(2), 4
D_{calc}(g cm^{-3}), F (000)	1.401, 1344

Experimental data:

Radiation and technique	Bruker smart-APEX Mo-K_α (λ = 0.71073 Å)
Monochromator	Graphite oriented
Range	($4 < 2\theta < 50°$)
Number of reflections:	
measured	29818 (h: -11, 11; k: -18, -18; l: -24, 24)
unique	5472 (R_{int} = 0.2034)
Absorption correction	sadabs*
Max. and min. trans. fact.	0.970, 0.457
μ (mm^{-1})	0.598
Temperature (K)	100.0(2)

Table to be deposited

Table S4. Full experimental details for the X-Ray analysis of $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)C{=}O\}(P^iPr_3)$ (**3**).

Solution and refinement:	SHELX97 dos/win95/nt version
Solution mode	Patterson
Refinement	Full-matrix least-squares on F'^2s.
	All reflections.
Hydrogen atoms	see table **S3**.
No. parameters/restrains	397/ 6
Weighting scheme	$w^{-1}=[\sigma^2(F_o^2)+(0.0384P)^2+0.0P]$
	where $P=((\text{Max } F_o^2,0)+2F_c^2)/3$
ΔF final (max)	1.361 e/Å^3 (close to Ru atom)
ΔF final (min)	-1.268 e/Å^3
Max/Mean shift/esd	0.001, 0.000
$\omega R2(F^2, \text{ all data})^a$	0.1185
$R1(F, F_o > 4.0\ \sigma F)^b$	0.0585
Goodness-of-Fit[c]	0.780
Data-to-Parameter Ratio	13.8:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol C (1992). Anomalous dispersion is implemented by the program.

[a] $wR2(F^2) = \{\Sigma[w(F_o^2\text{-}F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ [b] $R1(F) = \Sigma||F_o|\text{-}|F_c||/\Sigma|F_o|$. [c] $S = \{\Sigma[w(F_o^2\text{-}F_c^2)^2]/(n\text{-}p)\}1/2$, where n is the number of observed reflections, and p is the number of parameters refined.

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* Shelxtl 6.1., Bruker-Siemens Analytical X-ray Instruments, Inc: Madison, WI.

Table to be deposited

Table S5. Bond Lenghts (Å) and angles (deg) for the Ru(η^5-C_5H_5){C(CH=CPh$_2$)=N(CH$_2$CH=CH$_2$)CH(CH=CH$_2$)C=O}(P^{i}Pr$_3$) (**3**).

Ru C1 1.884(6)	C25 H25A 0.9800
Ru C22 1.984(7)	C25 H25B 0.9800
Ru C35 2.224(7)	C25 H25C 0.9800
Ru C36 2.252(7)	C26 C27 1.511(9)
Ru C34 2.274(6)	C26 C28 1.531(9)
Ru C33 2.301(7)	C26 H26 1.0000
Ru P 2.306(2)	C27 H27A 0.9800
Ru C32 2.310(7)	C27 H27B 0.9800
P C29 1.829(7)	C27 H27C 0.9800
P C26 1.858(7)	C28 H28A 0.9800
P C23 1.861(7)	C28 H28B 0.9800
O C22 1.219(7)	C28 H28C 0.9800
N C1 1.367(8)	C29 C31 1.519(9)
N C19 1.451(8)	C29 C30 1.522(9)
N C16 1.472(9)	C29 H29 1.0000
C1 C2 1.473(9)	C30 H30A 0.9800
C2 C3 1.336(9)	C30 H30B 0.9800
C2 H2 0.96(6)	C30 H30C 0.9800
C3 C4 1.480(9)	C31 H31A 0.9800
C3 C10 1.487(9)	C31 H31B 0.9800
C4 C9 1.362(10)	C31 H31C 0.9800
C4 C5 1.416(9)	C32 C36 1.373(9)
C5 C6 1.365(10)	C32 C33 1.391(9)
C5 H5 0.9500	C32 H32 0.9500
C6 C7 1.347(11)	C33 C34 1.395(9)
C6 H6 0.9500	C33 H33 0.9500
C7 C8 1.398(11)	C34 C35 1.412(9)
C7 H7 0.9500	C34 H34 0.9500
C8 C9 1.374(10)	C35 C36 1.424(9)
C8 H8 0.9500	C35 H35 0.9500
C9 H9 0.9500	C36 H36 0.9500
C10 C11 1.356(8)	
C10 C15 1.373(9)	C1 Ru C22 79.9(3)
C11 C12 1.382(9)	C1 Ru C35 111.2(3)
C11 H11 0.9500	C22 Ru C35 96.1(3)
C12 C13 1.350(9)	C1 Ru C36 97.3(3)
C12 H12 0.9500	C22 Ru C36 128.9(3)
C13 C14 1.377(8)	C35 Ru C36 37.1(2)
C13 H13 0.9500	C1 Ru C34 147.1(3)
C14 C15 1.395(9)	C22 Ru C34 94.9(3)
C14 H14 0.9500	C35 Ru C34 36.6(2)
C15 H15 0.9500	C36 Ru C34 60.8(3)
C16 C17 1.506(10)	C1 Ru C33 152.4(3)
C16 C22 1.530(10)	C22 Ru C33 125.1(3)
C16 H16 0.85(6)	C35 Ru C33 59.6(3)
C17 C18 1.278(11)	C36 Ru C33 59.0(3)
C17 H17 1.01(7)	C34 Ru C33 35.5(2)
C18 H18A 0.95(7)	C1 Ru P 92.96(18)
C18 H18B 0.90(7)	C22 Ru P 93.8(2)
C19 C20 1.477(11)	C35 Ru P 155.1(2)
C19 H19A 1.04(6)	C36 Ru P 137.22(19)
C19 H19B 0.96(6)	C34 Ru P 119.87(19)
C20 C21 1.297(12)	C33 Ru P 96.27(18)
C20 H20 0.84(6)	C1 Ru C32 117.3(3)
C21 H21A 0.83(8)	C22 Ru C32 153.5(3)
C21 H21B 1.17(7)	C35 Ru C32 59.8(3)
C23 C24 1.523(9)	C36 Ru C32 35.0(2)
C23 C25 1.524(8)	C34 Ru C32 59.5(3)
C23 H23 1.0000	C33 Ru C32 35.1(2)
C24 H24A 0.9800	P Ru C32 104.56(19)
C24 H24B 0.9800	C29 P C26 100.9(3)
C24 H24C 0.9800	C29 P C23 101.6(3)

C26 P C23 107.5(3)
C29 P Ru 115.0(2)
C26 P Ru 119.1(2)
C23 P Ru 110.9(2)
C1 N C19 129.5(6)
C1 N C16 113.0(6)
C19 N C16 117.6(6)
N C1 C2 113.9(6)
N C1 Ru 122.9(5)
C2 C1 Ru 122.9(5)
C3 C2 C1 131.6(7)
C3 C2 H2 122(4)
C1 C2 H2 106(4)
C2 C3 C4 122.7(7)
C2 C3 C10 122.9(7)
C4 C3 C10 114.5(6)
C9 C4 C5 117.3(7)
C9 C4 C3 122.2(7)
C5 C4 C3 120.5(7)
C6 C5 C4 121.0(8)
C6 C5 H5 119.5
C4 C5 H5 119.5
C7 C6 C5 120.2(8)
C7 C6 H6 119.9
C5 C6 H6 119.9
C6 C7 C8 120.5(8)
C6 C7 H7 119.7
C8 C7 H7 119.7
C9 C8 C7 118.8(8)
C9 C8 H8 120.6
C7 C8 H8 120.6
C4 C9 C8 122.1(8)
C4 C9 H9 118.9
C8 C9 H9 118.9
C11 C10 C15 118.7(7)
C11 C10 C3 122.4(6)
C15 C10 C3 118.8(6)
C10 C11 C12 121.0(7)
C10 C11 H11 119.5
C12 C11 H11 119.5
C13 C12 C11 119.8(7)
C13 C12 H12 120.1
C11 C12 H12 120.1
C12 C13 C14 121.2(7)
C12 C13 H13 119.4
C14 C13 H13 119.4
C13 C14 C15 117.7(7)
C13 C14 H14 121.1
C15 C14 H14 121.1
C10 C15 C14 121.4(7)
C10 C15 H15 119.3
C14 C15 H15 119.3
N C16 C17 110.2(6)
N C16 C22 108.0(6)
C17 C16 C22 113.4(6)
N C16 H16 112(5)
C17 C16 H16 105(5)
C22 C16 H16 108(5)
C18 C17 C16 125.4(8)
C18 C17 H17 123(4)
C16 C17 H17 112(4)
C17 C18 H18A 121(5)
C17 C18 H18B 136(5)
H18A C18 H18B 101(7)
N C19 C20 112.4(6)
N C19 H19A 114(3)
C20 C19 H19A 104(4)
N C19 H19B 107(4)
C20 C19 H19B 113(4)
H19A C19 H19B 105(5)
C21 C20 C19 126.2(8)
C21 C20 H20 127(5)
C19 C20 H20 107(5)
C20 C21 H21A 124(6)
C20 C21 H21B 112(4)
H21A C21 H21B 123(7)
O C22 C16 116.1(6)
O C22 Ru 128.2(5)
C16 C22 Ru 115.4(5)
C24 C23 C25 110.2(5)
C24 C23 P 114.6(5)
C25 C23 P 116.0(5)
C24 C23 H23 104.9
C25 C23 H23 104.9
P C23 H23 104.9
C23 C24 H24A 109.5
C23 C24 H24B 109.5
H24A C24 H24B 109.5
C23 C24 H24C 109.5
H24A C24 H24C 109.5
H24B C24 H24C 109.5
C23 C25 H25A 109.5
C23 C25 H25B 109.5
H25A C25 H25B 109.5
C23 C25 H25C 109.5
H25A C25 H25C 109.5
H25B C25 H25C 109.5
C27 C26 C28 107.8(6)
C27 C26 P 113.8(5)
C28 C26 P 117.3(5)
C27 C26 H26 105.7
C28 C26 H26 105.7
P C26 H26 105.7
C26 C27 H27A 109.5
C26 C27 H27B 109.5
H27A C27 H27B 109.5
C26 C27 H27C 109.5
H27A C27 H27C 109.5
H27B C27 H27C 109.5
C26 C28 H28A 109.5
C26 C28 H28B 109.5
H28A C28 H28B 109.5
C26 C28 H28C 109.5
H28A C28 H28C 109.5
H28B C28 H28C 109.5
C31 C29 C30 108.6(6)
C31 C29 P 111.4(5)
C30 C29 P 113.5(5)
C31 C29 H29 107.7
C30 C29 H29 107.7
P C29 H29 107.7
C29 C30 H30A 109.5
C29 C30 H30B 109.5
H30A C30 H30B 109.5
C29 C30 H30C 109.5
H30A C30 H30C 109.5
H30B C30 H30C 109.5
C29 C31 H31A 109.5
C29 C31 H31B 109.5
H31A C31 H31B 109.5
C29 C31 H31C 109.5
H31A C31 H31C 109.5
H31B C31 H31C 109.5
C36 C32 C33 108.4(7)
C36 C32 Ru 70.2(4)
C33 C32 Ru 72.1(4)

C36 C32 H32 125.8
C33 C32 H32 125.8
Ru C32 H32 123.5
C32 C33 C34 109.6(7)
C32 C33 Ru 72.8(4)
C34 C33 Ru 71.2(4)
C32 C33 H33 125.2
C34 C33 H33 125.2
Ru C33 H33 122.4
C33 C34 C35 106.5(7)
C33 C34 Ru 73.3(4)
C35 C34 Ru 69.8(4)
C33 C34 H34 126.8
C35 C34 H34 126.8
Ru C34 H34 121.9
C34 C35 C36 107.7(7)
C34 C35 Ru 73.6(4)
C36 C35 Ru 72.5(4)
C34 C35 H35 126.1
C36 C35 H35 126.1
Ru C35 H35 119.6
C32 C36 C35 107.9(7)
C32 C36 Ru 74.8(4)
C35 C36 Ru 70.4(4)
C32 C36 H36 126.1
C35 C36 H36 126.1
Ru C36 H36 120.5

Table to be deposited

Table S6. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for Complex Ru(η^5-C_5H_5){C=CHCPh$_2$(CH=CH$_2$)NCH$_2$CH=CH$_2$}(CO)(P^{i}Pr$_3$) (**4**).

Atom	X/*a*	Y/*b*	Z/*c*	U_{eq}[a]
Ru	0.90660(4)	0.73161(3)	0.67357(2)	0.01920(8)
P	0.70554(11)	0.67067(10)	0.73837(7)	0.0220(2)
O	0.7105(3)	0.5843(2)	0.49013(17)	0.0351(7)
N	0.8299(3)	0.9741(3)	0.64748(19)	0.0234(8)
C1	0.8893(4)	0.9182(3)	0.7048(2)	0.0201(9)
C2	0.9429(4)	1.0133(4)	0.7884(2)	0.0205(9)
C3	0.9161(4)	1.1414(3)	0.7957(2)	0.0184(8)
C4	1.0464(4)	1.2663(4)	0.8492(2)	0.0203(9)
C5	1.1882(4)	1.2622(4)	0.8630(2)	0.0227(9)
C6	1.3080(4)	1.3768(4)	0.9035(2)	0.0270(10)
C7	1.2870(4)	1.4971(4)	0.9317(2)	0.0276(10)
C8	1.1461(4)	1.5035(4)	0.9209(2)	0.0277(10)
C9	1.0269(4)	1.3884(3)	0.8803(2)	0.0226(9)
C10	0.7797(4)	1.1433(3)	0.8370(2)	0.0204(9)
C11	0.6457(4)	1.1340(3)	0.7907(3)	0.0282(10)
C12	0.5252(4)	1.1310(4)	0.8313(3)	0.0312(10)
C13	0.5342(4)	1.1343(3)	0.9195(3)	0.0286(10)
C14	0.6644(4)	1.1423(3)	0.9669(3)	0.0303(10)
C15	0.7856(4)	1.1480(3)	0.9270(2)	0.0247(9)
C16	0.8861(4)	1.1197(4)	0.6926(3)	0.0220(9)
C17	1.0194(4)	1.1802(4)	0.6611(3)	0.0284(10)
C18	1.0303(5)	1.2723(4)	0.6270(3)	0.0353(11)
C19	0.8028(5)	0.9226(4)	0.5500(3)	0.0316(11)
C20	0.6921(5)	0.9571(5)	0.5049(3)	0.0474(14)
C21	0.6892(6)	0.9912(6)	0.4361(4)	0.0716(19)
C22	0.7395(4)	0.6859(4)	0.8586(2)	0.0249(9)
C23	0.8232(4)	0.5983(4)	0.8775(2)	0.0365(11)
C24	0.8154(4)	0.8282(3)	0.9248(2)	0.0283(10)
C25	0.5891(4)	0.4958(3)	0.6741(3)	0.0263(9)
C26	0.4699(4)	0.4372(4)	0.7202(3)	0.0424(12)
C27	0.6728(4)	0.4011(3)	0.6397(3)	0.0340(11)
C28	0.5830(4)	0.7689(3)	0.7383(2)	0.0214(9)
C29	0.4709(4)	0.7638(4)	0.8013(2)	0.0328(10)
C30	0.5027(4)	0.7431(4)	0.6439(2)	0.0307(10)
C31	1.0609(4)	0.6157(4)	0.6339(3)	0.0264(9)
C32	1.0527(4)	0.6335(4)	0.7242(2)	0.0255(9)
C33	1.1074(4)	0.7712(4)	0.7772(3)	0.0290(10)
C34	1.1509(4)	0.8341(4)	0.7169(3)	0.0307(10)
C35	1.1227(4)	0.7402(4)	0.6289(3)	0.0306(10)
C36	0.7838(4)	0.6480(4)	0.5639(2)	0.0236(9)

[a] Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *Uij* tensor.

Table to be deposited

Table S7. Anisotropic displacement coefficients U_{ij} (Å^2) for the non-hydrogen atoms for the complex Ru(η^5-C_5H_5){C=CHCPh$_2$(CH=CH$_2$)NCH$_2$CH=CH$_2$}(CO)(P^{i}Pr$_3$) (**4**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	0.01655(17)	0.01764(17)	0.02319(17)	0.00761(14)	0.00554(13)	0.00486(13)
P	0.0197(6)	0.0223(6)	0.0267(6)	0.0120(5)	0.0060(5)	0.0072(5)
O	0.0351(18)	0.0283(17)	0.0320(17)	0.0081(14)	0.0016(14)	0.0010(14)
N	0.032(2)	0.0221(19)	0.0170(17)	0.0063(15)	0.0052(15)	0.0119(16)
C1	0.015(2)	0.024(2)	0.023(2)	0.0119(18)	0.0071(17)	0.0044(17)
C2	0.020(2)	0.023(2)	0.023(2)	0.0118(19)	0.0046(18)	0.0096(18)
C3	0.019(2)	0.021(2)	0.017(2)	0.0080(17)	0.0057(17)	0.0083(18)
C4	0.023(2)	0.021(2)	0.019(2)	0.0110(18)	0.0067(17)	0.0050(19)
C5	0.026(2)	0.020(2)	0.022(2)	0.0068(18)	0.0050(18)	0.0093(19)
C6	0.024(2)	0.028(2)	0.032(2)	0.014(2)	0.0118(19)	0.007(2)
C7	0.026(2)	0.021(2)	0.028(2)	0.0061(19)	0.0033(19)	-0.0003(19)
C8	0.031(3)	0.026(2)	0.030(2)	0.014(2)	0.010(2)	0.011(2)
C9	0.024(2)	0.020(2)	0.025(2)	0.0088(18)	0.0049(18)	0.0098(19)
C10	0.022(2)	0.013(2)	0.027(2)	0.0060(17)	0.0084(18)	0.0066(17)
C11	0.029(3)	0.028(2)	0.026(2)	0.0091(19)	0.0078(19)	0.009(2)
C12	0.021(2)	0.036(3)	0.036(3)	0.011(2)	0.009(2)	0.012(2)
C13	0.021(2)	0.025(2)	0.035(3)	0.003(2)	0.015(2)	0.0061(19)
C14	0.035(3)	0.025(2)	0.022(2)	0.0018(19)	0.005(2)	0.006(2)
C15	0.024(2)	0.022(2)	0.027(2)	0.0092(19)	0.0068(19)	0.0062(19)
C16	0.024(2)	0.024(2)	0.023(2)	0.0122(19)	0.0078(18)	0.0093(19)
C17	0.032(3)	0.029(3)	0.028(2)	0.013(2)	0.010(2)	0.011(2)
C18	0.042(3)	0.032(3)	0.037(3)	0.017(2)	0.017(2)	0.013(2)
C19	0.043(3)	0.020(2)	0.025(2)	0.011(2)	0.003(2)	0.000(2)
C20	0.058(4)	0.062(4)	0.027(3)	0.013(3)	0.003(2)	0.032(3)
C21	0.068(5)	0.106(5)	0.077(4)	0.069(4)	0.021(4)	0.040(4)
C22	0.025(2)	0.029(2)	0.028(2)	0.0132(19)	0.0105(18)	0.0143(19)
C23	0.048(3)	0.043(3)	0.035(2)	0.024(2)	0.013(2)	0.026(2)
C24	0.028(2)	0.037(3)	0.026(2)	0.015(2)	0.0110(19)	0.013(2)
C25	0.019(2)	0.024(2)	0.037(2)	0.015(2)	0.0075(19)	0.0049(19)
C26	0.032(3)	0.031(3)	0.061(3)	0.017(2)	0.018(2)	0.001(2)
C27	0.036(3)	0.022(2)	0.045(3)	0.012(2)	0.012(2)	0.010(2)
C28	0.020(2)	0.019(2)	0.029(2)	0.0116(18)	0.0080(18)	0.0089(18)
C29	0.024(2)	0.042(3)	0.043(3)	0.023(2)	0.014(2)	0.017(2)
C30	0.023(2)	0.031(2)	0.040(3)	0.017(2)	0.005(2)	0.009(2)
C31	0.023(2)	0.023(2)	0.033(2)	0.007(2)	0.0070(19)	0.0100(19)
C32	0.022(2)	0.028(2)	0.034(2)	0.014(2)	0.0101(19)	0.0137(19)
C33	0.024(2)	0.036(3)	0.030(2)	0.009(2)	0.0051(19)	0.018(2)
C34	0.016(2)	0.023(2)	0.048(3)	0.008(2)	0.002(2)	0.0059(19)
C35	0.024(2)	0.035(3)	0.045(3)	0.023(2)	0.017(2)	0.015(2)
C36	0.031(3)	0.021(2)	0.020(2)	0.0080(18)	0.0086(19)	0.0084(19)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2 (h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12})$

Table to be deposited

Table S8. Hydrogen atom coordinates* and isotropic displacement coefficient ($Å^2$) for the compound $Ru(\eta^5\text{-}C_5H_5)\{C{=}CHCPh_2(CH{=}CH_2)NCH_2CH{=}CH_2\}(CO)(P^iPr_3)$ (**4**).

Atom	X/*a*	Y/*b*	Z/*c*	*U*
H2[a]	0.977(3)	1.007(3)	0.839(2)	0.025
H5	1.2032	1.1793	0.8443	0.027
H6	1.4045	1.3724	0.9118	0.032
H7	1.3692	1.5759	0.9585	0.033
H8	1.1314	1.5865	0.9412	0.033
H9	0.9304	1.3930	0.8737	0.027
H11	0.6364	1.1297	0.7294	0.034
H12	0.4356	1.1265	0.7982	0.037
H13	0.4511	1.1311	0.9471	0.034
H14	0.6715	1.1440	1.0276	0.036
H15	0.8754	1.1552	0.9614	0.030
H16[a]	0.814(3)	1.157(3)	0.676(2)	0.026
H17[a]	1.099(4)	1.147(3)	0.669(2)	0.034
H18A[a]	0.949(4)	1.311(3)	0.616(2)	0.042
H18B[a]	1.112(4)	1.318(3)	0.611(2)	0.042
H19A[a]	0.781(4)	0.824(3)	0.525(2)	0.038
H19B[a]	0.894(4)	0.962(3)	0.532(2)	0.038
H20[a]	0.599(4)	0.959(4)	0.534(2)	0.057
H21A[a]	0.604(5)	1.007(4)	0.409(3)	0.086
H21B[a]	0.784(5)	1.008(4)	0.413(3)	0.086
H22	0.6408	0.6556	0.8735	0.030
H23A	0.9225	0.6266	0.8661	0.055
H23B	0.7712	0.5064	0.8373	0.055
H23C	0.8293	0.6059	0.9413	0.055
H24A	0.8191	0.8319	0.9877	0.043
H24B	0.7602	0.8836	0.9136	0.043
H24C	0.9156	0.8606	0.9155	0.043
H25	0.5338	0.4963	0.6176	0.032
H26A	0.4058	0.3501	0.6776	0.064
H26B	0.4116	0.4954	0.7380	0.064
H26C	0.5164	0.4287	0.7746	0.064
H27A	0.7247	0.3908	0.6916	0.051
H27B	0.7440	0.4362	0.6066	0.051
H27C	0.6035	0.3151	0.5986	0.051
H28	0.6493	0.8628	0.7617	0.026
H29A	0.4298	0.8348	0.8070	0.049
H29B	0.5202	0.7750	0.8617	0.049
H29C	0.3915	0.6785	0.7751	0.049
H30A	0.4234	0.6578	0.6214	0.046
H30B	0.5717	0.7418	0.6025	0.046
H30C	0.4612	0.8130	0.6466	0.046
H31	1.0301	0.5334	0.5841	0.032
H32	1.0166	0.5652	0.7467	0.031
H33	1.1131	0.8121	0.8408	0.035
H34	1.1931	0.9267	0.7333	0.037
H35	1.1418	0.7574	0.5756	0.037

* The hydrogen atoms were included in observed or calculated positions and refined riding on their respective carbon atoms. [a] These hydrogen were refined as free isotropic atoms.

Table to be deposited

Table S9. Full experimental details for the X-Ray analysis of $Ru(\eta^5\text{-}C_5H_5)\{C{=}CHCPh_2(CH{=}CH_2)NCH_2CH{=}CH_2\}(CO)(P^iPr_3)$ (**4**).

Crystal data:

Formula	$C_{36}H_{46}NOPRu$
Molecular weight	640.78
Crystal habit	plate
color	yellow
Size(mm)	0.14 x 0.14 x 0.13
Symmetry	triclinic, P-1
Unit cell dimensions	9.6984(12), 11.3808(15), 15.840(2) Å
	108.998(2), 95.494(2), 106.465(2) °
Packing: V (Å^3), Z	1550.9(3), 2
D_{calc}(g cm^{-3}), F (000)	1.372, 672

Experimental data:

	Bruker smart-APEX
Radiation and technique	Mo-K_α (λ = 0.71073 Å)
Monochromator	Graphite oriented
Range	($4 < 2\theta < 57°$)
Number of reflections:	
measured	18914 (h: -12, 12; k: -15, 14; l: -21, 20)
unique	7194 (R_{int} = 0.0694)
Absorption correction	sadabs*
Max. and min. trans. fact.	0.956, 0.793
μ (mm^{-1})	0.586
Temperature (K)	100.0(2)

Table to be deposited

Table S9. Full experimental details for the X-Ray analysis of $Ru(\eta^5\text{-}C_5H_5)\{C{=}CHCPh_2(CH{=}CH_2)NCH_2CH{=}CH_2\}(CO)(P^iPr_3)$ (**4**).

Solution and refinement:	SHELX97 dos/win95/nt version
Solution mode	Patterson
Refinement	Full-matrix least-squares on F'^2s.
	All reflections.
Hydrogen atoms	see table **S8**.
No. parameters/restrains	397/0
Weighting scheme	$w^{-1}=[\sigma^2(F_o^2)+(0.0056P)^2+0.0P]$
	where $P=((\text{Max } F_o^2,0)+2F_c^2)/3$
ΔF final (max)	0.576 e/Å^3 (close to Ru atom)
ΔF final (min)	-0.564 e/Å^3
Max/Mean shift/esd	0.00'5, 0.000
$\omega R2(F^2, \text{ all data})^a$	0.0655
$R1(F, F_o > 4.0\ \sigma F)^b$	0.0474
Goodness-of-Fit[c]	0.759
Data-to-Parameter Ratio	18.1:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol C (1992). Anomalous dispersion is implemented by the program.

[a] $wR2(F^2) = \{\Sigma[w(F_o^2\text{-}F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ [b] $R1(F) = \Sigma||F_o|\text{-}|F_c||/\Sigma|F_o|$. [c] $S = \{\Sigma[w(F_o^2\text{-}F_c^2)^2]/(n\text{-}p)\}^{1/2}$, where n is the number of observed reflections, and p is the number of parameters refined.

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* Shelxtl 6.1., Bruker-Siemens Analytical X-ray Instruments, Inc: Madison, WI.

Table to be deposited

Table S10. Bond Lenghts (Å) and angles (deg) for the complex $Ru(\eta^5\text{-}C_5H_5)\{C{=}CHCPh_2(CH{=}CH_2)NCH_2CH{=}CH_2\}(CO)(P^iPr_3)$ (**4**).

Ru C36 1.796(4)	C23 H23C 0.9800
Ru C1 2.077(4)	C24 H24A 0.9800
Ru C34 2.246(4)	C24 H24B 0.9800
Ru C33 2.258(4)	C24 H24C 0.9800
Ru C35 2.261(4)	C25 C27 1.522(4)
Ru C31 2.266(3)	C25 C26 1.535(4)
Ru C32 2.272(3)	C25 H25 1.0000
Ru P 2.3274(11)	C26 H26A 0.9800
P C22 1.843(3)	C26 H26B 0.9800
P C28 1.848(3)	C26 H26C 0.9800
P C25 1.860(4)	C27 H27A 0.9800
O C36 1.180(4)	C27 H27B 0.9800
N C19 1.429(4)	C27 H27C 0.9800
N C1 1.430(4)	C28 C30 1.514(4)
N C16 1.482(4)	C28 C29 1.546(4)
C1 C2 1.346(4)	C28 H28 1.0000
C2 C3 1.522(5)	C29 H29A 0.9800
C2 H2 0.87(3)	C29 H29B 0.9800
C3 C4 1.526(5)	C29 H29C 0.9800
C3 C10 1.533(4)	C30 H30A 0.9800
C3 C16 1.555(5)	C30 H30B 0.9800
C4 C5 1.388(4)	C30 H30C 0.9800
C4 C9 1.389(4)	C31 C32 1.392(4)
C5 C6 1.384(4)	C31 C35 1.405(5)
C5 H5 0.9500	C31 H31 0.9500
C6 C7 1.376(5)	C32 C33 1.425(5)
C6 H6 0.9500	C32 H32 0.9500
C7 C8 1.386(5)	C33 C34 1.398(5)
C7 H7 0.9500	C33 H33 0.9500
C8 C9 1.384(5)	C34 C35 1.397(5)
C8 H8 0.9500	C34 H34 0.9500
C9 H9 0.9500	C35 H35 0.9500
C10 C11 1.389(5)	
C10 C15 1.404(4)	C36 Ru C1 99.65(15)
C11 C12 1.384(4)	C36 Ru C34 132.91(16)
C11 H11 0.9500	C1 Ru C34 86.49(14)
C12 C13 1.379(5)	C36 Ru C33 154.09(15)
C12 H12 0.9500	C1 Ru C33 102.07(14)
C13 C14 1.369(5)	C34 Ru C33 36.16(12)
C13 H13 0.9500	C36 Ru C35 99.33(16)
C14 C15 1.383(5)	C1 Ru C35 107.18(13)
C14 H14 0.9500	C34 Ru C35 36.11(12)
C15 H15 0.9500	C33 Ru C35 60.74(14)
C16 C17 1.496(5)	C36 Ru C31 93.39(15)
C16 H16 0.97(3)	C1 Ru C31 143.03(13)
C17 C18 1.312(5)	C34 Ru C31 60.03(13)
C17 H17 0.97(3)	C33 Ru C31 60.71(13)
C18 H18A 1.03(3)	C35 Ru C31 36.16(12)
C18 H18B 0.92(3)	C36 Ru C32 120.46(15)
C19 C20 1.446(6)	C1 Ru C32 138.74(13)
C19 H19A 1.01(3)	C34 Ru C32 59.95(13)
C19 H19B 0.98(3)	C33 Ru C32 36.68(11)
C20 C21 1.271(6)	C35 Ru C32 60.00(13)
C20 H20 1.06(4)	C31 Ru C32 35.72(11)
C21 H21A 0.98(4)	C36 Ru P 87.84(12)
C21 H21B 1.01(4)	C1 Ru P 89.83(10)
C22 C24 1.528(4)	C34 Ru P 139.12(11)
C22 C23 1.532(4)	C33 Ru P 106.09(10)
C22 H22 1.0000	C35 Ru P 159.95(10)
C23 H23A 0.9800	C31 Ru P 125.32(10)
C23 H23B 0.9800	C32 Ru P 100.22(10)

C22 P C28 102.24(16)
C22 P C25 104.97(17)
C28 P C25 105.86(17)
C22 P Ru 118.51(13)
C28 P Ru 112.82(12)
C25 P Ru 111.28(12)
C19 N C1 124.9(3)
C19 N C16 116.2(3)
C1 N C16 109.1(3)
C2 C1 N 107.1(3)
C2 C1 Ru 122.7(3)
N C1 Ru 130.1(2)
C1 C2 C3 113.6(3)
C1 C2 H2 129(2)
C3 C2 H2 117(2)
C2 C3 C4 114.9(3)
C2 C3 C10 107.9(3)
C4 C3 C10 111.1(3)
C2 C3 C16 99.2(3)
C4 C3 C16 111.0(3)
C10 C3 C16 112.3(3)
C5 C4 C9 118.3(3)
C5 C4 C3 121.0(3)
C9 C4 C3 120.6(3)
C6 C5 C4 121.1(4)
C6 C5 H5 119.5
C4 C5 H5 119.5
C7 C6 C5 119.8(4)
C7 C6 H6 120.1
C5 C6 H6 120.1
C6 C7 C8 120.1(4)
C6 C7 H7 119.9
C8 C7 H7 119.9
C9 C8 C7 119.7(4)
C9 C8 H8 120.2
C7 C8 H8 120.2
C8 C9 C4 121.0(4)
C8 C9 H9 119.5
C4 C9 H9 119.5
C11 C10 C15 116.2(4)
C11 C10 C3 125.0(3)
C15 C10 C3 118.7(3)
C12 C11 C10 121.9(4)
C12 C11 H11 119.1
C10 C11 H11 119.1
C13 C12 C11 120.5(4)
C13 C12 H12 119.8
C11 C12 H12 119.8
C14 C13 C12 119.2(4)
C14 C13 H13 120.4
C12 C13 H13 120.4
C13 C14 C15 120.3(4)
C13 C14 H14 119.8
C15 C14 H14 119.8
C14 C15 C10 121.9(4)
C14 C15 H15 119.0
C10 C15 H15 119.0
N C16 C17 111.7(3)
N C16 C3 103.0(3)
C17 C16 C3 113.6(3)
N C16 H16 110.6(19)
C17 C16 H16 105.0(19)
C3 C16 H16 113.1(19)
C18 C17 C16 123.6(4)
C18 C17 H17 122(2)
C16 C17 H17 114(2)
C17 C18 H18A 126(2)
C17 C18 H18B 128(2)
H18A C18 H18B 107(3)
N C19 C20 115.5(4)
N C19 H19A 111.0(19)
C20 C19 H19A 110.7(19)
N C19 H19B 107(2)
C20 C19 H19B 105(2)
H19A C19 H19B 107(3)
C21 C20 C19 130.7(5)
C21 C20 H20 113(2)
C19 C20 H20 116(2)
C20 C21 H21A 123(3)
C20 C21 H21B 116(3)
H21A C21 H21B 121(4)
C24 C22 C23 109.7(3)
C24 C22 P 113.0(2)
C23 C22 P 114.3(3)
C24 C22 H22 106.4
C23 C22 H22 106.4
P C22 H22 106.4
C22 C23 H23A 109.5
C22 C23 H23B 109.5
H23A C23 H23B 109.5
C22 C23 H23C 109.5
H23A C23 H23C 109.5
H23B C23 H23C 109.5
C22 C24 H24A 109.5
C22 C24 H24B 109.5
H24A C24 H24B 109.5
C22 C24 H24C 109.5
H24A C24 H24C 109.5
H24B C24 H24C 109.5
C27 C25 C26 109.9(3)
C27 C25 P 115.2(3)
C26 C25 P 115.8(3)
C27 C25 H25 104.9
C26 C25 H25 104.9
P C25 H25 104.9
C25 C26 H26A 109.5
C25 C26 H26B 109.5
H26A C26 H26B 109.5
C25 C26 H26C 109.5
H26A C26 H26C 109.5
H26B C26 H26C 109.5
C25 C27 H27A 109.5
C25 C27 H27B 109.5
H27A C27 H27B 109.5
C25 C27 H27C 109.5
H27A C27 H27C 109.5
H27B C27 H27C 109.5
C30 C28 C29 108.6(3)
C30 C28 P 113.6(2)
C29 C28 P 117.1(2)
C30 C28 H28 105.5
C29 C28 H28 105.5
P C28 H28 105.5
C28 C29 H29A 109.5
C28 C29 H29B 109.5
H29A C29 H29B 109.5
C28 C29 H29C 109.5
H29A C29 H29C 109.5
H29B C29 H29C 109.5
C28 C30 H30A 109.5
C28 C30 H30B 109.5
H30A C30 H30B 109.5
C28 C30 H30C 109.5
H30A C30 H30C 109.5
H30B C30 H30C 109.5
C32 C31 C35 108.3(3)

C32 C31 Ru 72.4(2)
C35 C31 Ru 71.7(2)
C32 C31 H31 125.9
C35 C31 H31 125.9
Ru C31 H31 121.8
C31 C32 C33 108.5(3)
C31 C32 Ru 71.9(2)
C33 C32 Ru 71.1(2)
C31 C32 H32 125.7
C33 C32 H32 125.7
Ru C32 H32 122.8
C34 C33 C32 106.2(3)
C34 C33 Ru 71.4(2)
C32 C33 Ru 72.2(2)
C34 C33 H33 126.9
C32 C33 H33 126.9
Ru C33 H33 121.3
C35 C34 C33 109.7(4)
C35 C34 Ru 72.6(2)
C33 C34 Ru 72.4(2)
C35 C34 H34 125.2
C33 C34 H34 125.2
Ru C34 H34 121.5
C34 C35 C31 107.3(4)
C34 C35 Ru 71.3(2)
C31 C35 Ru 72.1(2)
C34 C35 H35 126.3
C31 C35 H35 126.3
Ru C35 H35 121.9
O C36 Ru 173.4(3)

Table to be deposited

Table S11. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for complex [Ru(η^5-C_5H_5){C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^{i}Pr$_3$)]BF_4 (**5**).

Atom	X/*a*	Y/*b*	Z/*c*	U_{eq}[a]
Ru	0.365494(17)	0.65157(3)	0.80954(2)	0.02374(10)
P	0.34632(5)	0.80146(9)	0.75167(7)	0.0235(3)
F1	0.64369(12)	0.6813(2)	1.05859(17)	0.0743(12)
F2	0.56265(13)	0.7185(2)	0.94570(18)	0.0560(9)
F3	0.62109(11)	0.61094(17)	0.94448(15)	0.0395(8)
F4	0.57240(12)	0.57914(19)	1.00178(16)	0.0480(9)
O1	0.24669(13)	0.6494(3)	0.76427(18)	0.0459(9)
N1	0.38388(14)	0.6724(2)	0.9733(2)	0.0215(10)
B1	0.6004(2)	0.6478(5)	0.9877(4)	0.0329(14)
C1	0.39654(18)	0.6960(3)	0.9212(2)	0.0202(11)
C2	0.4504(2)	0.7527(4)	0.9693(3)	0.0262(13)
C3	0.45618(19)	0.7841(3)	1.0478(3)	0.0226(12)
C4	0.5166(2)	0.7894(3)	1.1197(3)	0.0256(12)
C5	0.5624(2)	0.7576(3)	1.1210(3)	0.0318(13)
C6	0.6156(2)	0.7617(3)	1.1891(3)	0.0409(15)
C7	0.6240(2)	0.7989(4)	1.2576(3)	0.0438(16)
C8	0.5789(2)	0.8341(5)	1.2569(3)	0.063(2)
C9	0.5264(2)	0.8299(4)	1.1887(3)	0.0569(18)
C10	0.42589(19)	0.8775(3)	1.0333(2)	0.0204(12)
C11	0.37341(19)	0.8891(3)	1.0208(2)	0.0290(13)
C12	0.3490(2)	0.9772(3)	1.0074(3)	0.0304(13)
C13	0.3749(2)	1.0549(3)	1.0024(3)	0.0328(13)
C14	0.4267(2)	1.0450(3)	1.0125(3)	0.0309(13)
C15	0.45134(19)	0.9581(3)	1.0276(2)	0.0279(13)
C16	0.42492(19)	0.7012(3)	1.0572(3)	0.0213(11)
C17	0.4594(2)	0.6177(4)	1.1018(3)	0.0321(14)
C18	0.4559(2)	0.5742(4)	1.1563(3)	0.0372(15)
C19	0.3405(2)	0.6056(3)	0.9610(3)	0.0255(13)
C20	0.2961(2)	0.6513(4)	0.9666(3)	0.0331(12)
C21	0.2844(2)	0.6281(4)	1.0195(4)	0.0535(19)
C22	0.3601(2)	0.5196(3)	0.7430(3)	0.0361(14)
C23	0.3925(2)	0.5838(3)	0.7343(3)	0.0323(13)
C24	0.4407(2)	0.6022(3)	0.8099(3)	0.0328(13)
C25	0.4373(2)	0.5495(3)	0.8654(3)	0.0357(14)
C26	0.3872(2)	0.4989(3)	0.8247(3)	0.0349(14)
C27	0.29259(18)	0.6517(4)	0.7825(2)	0.0291(11)
C28	0.33628(18)	0.8916(3)	0.8101(3)	0.0248(12)
C29	0.2801(2)	0.8840(4)	0.8025(3)	0.0524(18)
C30	0.3441(2)	0.9947(3)	0.7957(3)	0.0514(17)
C31	0.27977(19)	0.8031(3)	0.6531(3)	0.0304(13)
C32	0.26823(19)	0.7129(3)	0.6030(2)	0.0372(14)
C33	0.26948(19)	0.8908(3)	0.6016(3)	0.0403(14)
C34	0.39753(17)	0.8569(3)	0.7351(2)	0.0254(11)
C35	0.45388(18)	0.8753(3)	0.8123(2)	0.0348(14)
C36	0.40791(19)	0.8040(3)	0.6775(3)	0.0352(14)

[a] Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *Uij* tensor.

Table to be deposited

Table S12. Anisotropic displacement coefficients U_{ij} (Å^2) for the non-hydrogen atoms for the complex [Ru(η^5-C_5H_5){C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^{i}Pr$_3$)]BF_4 (**5**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	0.0261(2)	0.0244(2)	0.0216(2)	-0.0011(2)	0.01345(17)	0.0004(3)
P	0.0227(8)	0.0242(8)	0.0234(8)	-0.0007(6)	0.0122(7)	-0.0003(6)
F1	0.035(2)	0.121(3)	0.066(2)	-0.050(2)	0.0268(19)	-0.013(2)
F2	0.067(3)	0.053(2)	0.071(2)	0.0256(18)	0.052(2)	0.0266(19)
F3	0.050(2)	0.0343(19)	0.0446(19)	0.0024(14)	0.0322(17)	0.0055(15)
F4	0.072(2)	0.040(2)	0.055(2)	0.0032(16)	0.049(2)	-0.0079(18)
O1	0.027(2)	0.055(2)	0.049(2)	0.013(2)	0.0159(19)	-0.002(2)
N1	0.023(2)	0.024(3)	0.020(2)	-0.0024(18)	0.014(2)	-0.0024(19)
B1	0.030(4)	0.031(4)	0.042(4)	-0.003(4)	0.023(3)	0.001(4)
C1	0.019(3)	0.017(3)	0.028(3)	0.002(2)	0.015(2)	0.004(2)
C2	0.030(3)	0.034(4)	0.020(3)	0.004(2)	0.017(3)	0.006(3)
C3	0.020(3)	0.035(3)	0.017(3)	-0.007(2)	0.013(2)	-0.006(2)
C4	0.028(3)	0.027(3)	0.025(3)	0.003(2)	0.017(3)	-0.004(3)
C5	0.029(3)	0.025(3)	0.035(3)	-0.008(2)	0.014(3)	0.002(3)
C6	0.025(4)	0.030(4)	0.057(4)	-0.001(3)	0.016(3)	0.003(3)
C7	0.031(4)	0.056(4)	0.026(3)	0.012(3)	0.004(3)	-0.008(3)
C8	0.026(3)	0.140(6)	0.021(3)	-0.011(4)	0.011(3)	-0.017(4)
C9	0.033(3)	0.121(6)	0.027(3)	-0.016(4)	0.023(3)	-0.018(4)
C10	0.026(3)	0.024(3)	0.017(3)	-0.002(2)	0.015(2)	-0.003(2)
C11	0.026(3)	0.028(3)	0.027(3)	0.000(2)	0.010(3)	0.001(3)
C12	0.032(3)	0.026(3)	0.040(3)	-0.002(3)	0.024(3)	-0.001(3)
C13	0.043(4)	0.025(3)	0.034(3)	-0.005(2)	0.023(3)	0.003(3)
C14	0.042(4)	0.024(3)	0.030(3)	-0.005(2)	0.022(3)	-0.009(3)
C15	0.031(3)	0.031(3)	0.032(3)	-0.006(2)	0.024(3)	-0.001(3)
C16	0.022(3)	0.027(3)	0.015(3)	0.005(2)	0.011(2)	0.007(2)
C17	0.025(3)	0.042(4)	0.028(3)	-0.005(3)	0.013(3)	-0.003(3)
C18	0.041(4)	0.035(4)	0.033(3)	0.007(3)	0.018(3)	0.010(3)
C19	0.027(3)	0.024(3)	0.027(3)	-0.002(2)	0.016(3)	-0.005(3)
C20	0.031(3)	0.029(3)	0.043(3)	-0.002(3)	0.022(3)	-0.002(3)
C21	0.053(4)	0.047(5)	0.092(5)	-0.004(4)	0.059(4)	-0.008(3)
C22	0.051(4)	0.027(3)	0.028(3)	-0.003(3)	0.020(3)	-0.002(3)
C23	0.048(4)	0.028(3)	0.035(3)	0.007(3)	0.032(3)	0.010(3)
C24	0.037(4)	0.025(3)	0.046(4)	0.002(3)	0.028(3)	0.007(3)
C25	0.042(4)	0.035(4)	0.036(3)	0.005(3)	0.025(3)	0.020(3)
C26	0.057(4)	0.026(3)	0.034(3)	0.002(3)	0.033(3)	0.014(3)
C27	0.026(3)	0.026(3)	0.029(3)	0.007(3)	0.010(3)	-0.001(3)
C28	0.021(3)	0.029(3)	0.022(3)	0.000(2)	0.010(2)	0.005(2)
C29	0.042(4)	0.071(5)	0.053(4)	-0.029(3)	0.032(3)	-0.004(3)
C30	0.066(5)	0.027(3)	0.060(4)	-0.003(3)	0.033(4)	0.005(3)
C31	0.035(3)	0.024(3)	0.034(3)	0.003(3)	0.020(3)	0.002(3)
C32	0.040(4)	0.039(4)	0.025(3)	-0.002(3)	0.013(3)	-0.011(3)
C33	0.037(4)	0.040(4)	0.033(3)	0.005(3)	0.012(3)	-0.002(3)
C34	0.022(3)	0.019(3)	0.030(3)	0.003(2)	0.012(2)	-0.002(3)
C35	0.035(3)	0.032(4)	0.035(3)	0.005(2)	0.017(3)	-0.007(3)
C36	0.039(3)	0.036(3)	0.039(3)	0.006(3)	0.027(3)	-0.001(3)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2 (h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12})$.

Table to be deposited

Table S13. Hydrogen atom coordinates* and isotropic displacement coefficient ($Å^2$) for the compound $[Ru(\eta^5\text{-}C_5H_5)\{C{=}N(CH_2CH{=}CH_2)CH(CH{=}CH_2)CPh_2CH_2\}(CO)(P^iPr_3)]BF_4$ (**5**).

Atom	X/*a*	Y/*b*	Z/*c*	*U*
H2A[a]	0.4803(16)	0.712(3)	0.975(2)	0.031
H2B[a]	0.4481(17)	0.796(3)	0.936(2)	0.031
H5	0.5576	0.7321	1.0738	0.038
H6	0.6466	0.7383	1.1882	0.049
H7	0.6603	0.8004	1.3048	0.053
H8	0.5839	0.8616	1.3036	0.075
H9	0.4958	0.8557	1.1892	0.068
H11	0.3536	0.8355	1.0213	0.035
H12	0.3137	0.9834	1.0017	0.037
H13	0.3577	1.1150	0.9920	0.039
H14	0.4453	1.0985	1.0090	0.037
H15	0.4870	0.9527	1.0343	0.033
H16	0.3978(15)	0.726(2)	1.078(2)	0.026
H17	0.4828(17)	0.597(3)	1.087(2)	0.038
H18A[a]	0.4788(18)	0.521(3)	1.184(2)	0.045
H18B[a]	0.4243(17)	0.601(3)	1.168(2)	0.045
H19A[a]	0.3300(17)	0.581(3)	0.915(2)	0.031
H19B[a]	0.3558(16)	0.554(3)	1.001(2)	0.031
H20[a]	0.2779(17)	0.702(3)	0.931(2)	0.040
H21A[a]	0.2531(18)	0.657(3)	1.021(3)	0.064
H21B[a]	0.3099(19)	0.566(3)	1.061(2)	0.064
H22	0.3256	0.4938	0.7016	0.043
H23	0.3839	0.6111	0.6856	0.039
H24	0.4703	0.6436	0.8209	0.039
H25	0.4641	0.5480	0.9210	0.043
H26	0.3738	0.4576	0.8481	0.042
H28	0.3654	0.8786	0.8671	0.030
H29A	0.2505	0.9082	0.7506	0.079
H29B	0.2812	0.9210	0.8446	0.079
H29C	0.2725	0.8179	0.8074	0.079
H30A	0.3140	1.0132	0.7420	0.077
H30B	0.3803	1.0021	0.8010	0.077
H30C	0.3431	1.0347	0.8348	0.077
H31	0.2497	0.8046	0.6647	0.036
H32A	0.2306	0.7163	0.5547	0.056
H32B	0.2708	0.6577	0.6341	0.056
H32C	0.2960	0.7076	0.5884	0.056
H33A	0.2956	0.8908	0.5840	0.060
H33B	0.2753	0.9477	0.6329	0.060
H33C	0.2310	0.8899	0.5551	0.060
H34	0.3819	0.9198	0.7107	0.031
H35A	0.4714	0.8152	0.8376	0.052
H35B	0.4480	0.9127	0.8484	0.052
H35C	0.4784	0.9099	0.8005	0.052
H36A	0.4298	0.8437	0.6641	0.053
H36B	0.3720	0.7886	0.6290	0.053
H36C	0.4286	0.7458	0.7026	0.053

* The hydrogen atoms were included in observed or calculated positions and refined riding on their respective carbon atoms. [a] These hydrogens were refined as free isotropic atoms.

Table to be deposited

Table S14. Full experimental details for the X-Ray analysis of [Ru(η^5-C_5H_5){C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^iPr_3)]BF_4 (**5**).

Crystal data:

Formula	$C_{36}H_{47}BF_4NOPRu$
Molecular weight	728.60
Crystal habit	needle
color	colorless
Size(mm)	0.18 x 0.06 x 0.04
Symmetry	monoclinic, C2/c
Unit cell dimensions	28.434(3), 14.2093(15), 20.023(2) Å
	90, 90, 90 °
Packing: V (Å^3), Z	6800.1(12), 8
D_{calc}(g cm^{-3}), F (000)	1.423, 3024

Experimental data:

Radiation and technique	Bruker smart-APEX Mo-K_α (λ = 0.71073 Å)
Monochromator	Graphite oriented
Range	($4 < 2\theta < 57°$)
Number of reflections:	
measured	20473 (h: -36, 38; k: -18, 16; l: -16, 26)
unique	7902 (R_{int} = 0.1042)
Absorption correction	sadabs*
Max. and min. trans. fact.	0.962, 0.763
μ (mm^{-1})	0.560
Temperature (K)	100.0(2)

Table to be deposited

Table S14. Full experimental details for the X-Ray analysis of [Ru(η^5-C_5H_5){C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^iPr_3)]BF_4 (**5**).

Solution and refinement:	SHELX97 dos/win95/nt version
Solution mode	Patterson
Refinement	Full-matrix least-squares on F'^2s.
	All reflections.
Hydrogen atoms	see table **S13**.
No. parameters/restrains	445/0
Weighting scheme	$w^{-1}=[\sigma^2(F_o^2)+(0.0000P)^2+0.0P]$
	where $P=((\text{Max } F_o^2,0)+2F_c^2)/3$
ΔF final (max)	0.480 e/Å^3 (close to Ru atom)
ΔF final (min)	-0.820 e/Å^3
Max/Mean shift/esd	0.007, 0.000
$\omega R2(F^2, \text{ all data})^a$	0.0559
$R1(F, F_o > 4.0\ \sigma F)^b$	0.0464
Goodness-of-Fit[c]	0.620
Data-to-Parameter Ratio	17.8:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol C (1992). Anomalous dispersion is implemented by the program.

[a] $wR2(F^2) = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ [b] $R1(F) = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [c] $S = \{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}1/2$, where n is the number of observed reflections, and p is the number of parameters refined.

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* Shelxtl 6.1., Bruker-Siemens Analytical X-ray Instruments, Inc: Madison, WI.

Table to be deposited

Table S15. Bond Lenghts (Å) and angles (deg) for the complex [Ru(η^5-C_5H_5){C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^iPr_3)]BF_4 (**5**).

Ru C27 1.837(4)	C27 Ru C25 136.3(2)
Ru C1 2.010(4)	C1 Ru C25 85.17(17)
Ru C26 2.231(4)	C26 Ru C25 36.32(16)
Ru C23 2.245(4)	C23 Ru C25 60.55(17)
Ru C24 2.246(4)	C24 Ru C25 35.95(14)
Ru C25 2.247(5)	C27 Ru C22 97.0(2)
Ru C22 2.257(4)	C1 Ru C22 140.00(17)
Ru P 2.3434(13)	C26 Ru C22 36.64(15)
P C34 1.837(4)	C23 Ru C22 35.53(15)
P C31 1.852(5)	C24 Ru C22 60.19(18)
P C28 1.858(4)	C25 Ru C22 60.68(18)
F1 B1 1.365(6)	C27 Ru P 86.00(16)
F2 B1 1.375(6)	C1 Ru P 96.25(12)
F3 B1 1.387(5)	C26 Ru P 157.56(12)
F4 B1 1.381(6)	C23 Ru P 97.51(12)
O1 C27 1.149(4)	C24 Ru P 104.57(12)
N1 C1 1.317(4)	C25 Ru P 137.59(14)
N1 C19 1.468(5)	C22 Ru P 122.71(12)
N1 C16 1.492(5)	C34 P C31 104.8(2)
C1 C2 1.525(6)	C34 P C28 103.0(2)
C2 C3 1.557(6)	C31 P C28 104.2(2)
C3 C10 1.521(6)	C34 P Ru 118.97(16)
C3 C4 1.533(6)	C31 P Ru 111.58(15)
C3 C16 1.547(6)	C28 P Ru 112.90(14)
C4 C5 1.364(6)	C1 N1 C19 126.7(4)
C4 C9 1.379(5)	C1 N1 C16 116.0(4)
C5 C6 1.385(6)	C19 N1 C16 116.0(3)
C6 C7 1.366(6)	F1 B1 F2 110.3(5)
C7 C8 1.368(6)	F1 B1 F4 109.3(5)
C8 C9 1.373(6)	F2 B1 F4 107.2(4)
C10 C11 1.382(5)	F1 B1 F3 109.4(4)
C10 C15 1.394(5)	F2 B1 F3 110.4(4)
C11 C12 1.385(5)	F4 B1 F3 110.3(5)
C12 C13 1.363(6)	N1 C1 C2 104.3(4)
C13 C14 1.381(6)	N1 C1 Ru 131.1(3)
C14 C15 1.370(6)	C2 C1 Ru 123.6(3)
C16 C17 1.488(6)	C1 C2 C3 108.0(4)
C17 C18 1.305(6)	C10 C3 C4 111.6(4)
C19 C20 1.476(6)	C10 C3 C16 112.6(4)
C20 C21 1.313(6)	C4 C3 C16 110.4(4)
C22 C23 1.374(6)	C10 C3 C2 108.6(4)
C22 C26 1.411(6)	C4 C3 C2 114.4(4)
C23 C24 1.411(6)	C16 C3 C2 98.7(4)
C24 C25 1.387(6)	C5 C4 C9 116.5(5)
C25 C26 1.396(6)	C5 C4 C3 125.1(4)
C28 C29 1.524(5)	C9 C4 C3 118.4(4)
C28 C30 1.533(5)	C4 C5 C6 121.9(5)
C31 C33 1.542(5)	C7 C6 C5 120.5(5)
C31 C32 1.549(5)	C6 C7 C8 118.6(5)
C34 C35 1.530(5)	C7 C8 C9 120.1(5)
C34 C36 1.534(5)	C8 C9 C4 122.4(5)
	C11 C10 C15 116.4(5)
C27 Ru C1 94.19(18)	C11 C10 C3 125.7(4)
C27 Ru C26 103.1(2)	C15 C10 C3 117.8(4)
C1 Ru C26 103.38(17)	C10 C11 C12 121.5(5)
C27 Ru C23 123.0(2)	C13 C12 C11 120.7(5)
C1 Ru C23 141.04(18)	C12 C13 C14 119.0(5)
C26 Ru C23 60.27(16)	C15 C14 C13 120.0(5)
C27 Ru C24 157.1(2)	C14 C15 C10 122.2(5)
C1 Ru C24 104.53(17)	C17 C16 N1 108.5(4)
C26 Ru C24 60.19(17)	C17 C16 C3 116.4(4)
C23 Ru C24 36.61(15)	N1 C16 C3 102.9(3)

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C18 C17 C16 123.9(5)
N1 C19 C20 112.2(4)
C21 C20 C19 123.5(5)
C23 C22 C26 107.6(5)
C23 C22 Ru 71.8(3)
C26 C22 Ru 70.7(3)
C22 C23 C24 108.4(4)
C22 C23 Ru 72.7(3)
C24 C23 Ru 71.7(3)
C25 C24 C23 108.1(5)
C25 C24 Ru 72.1(3)
C23 C24 Ru 71.6(3)
C24 C25 C26 107.6(5)
C24 C25 Ru 72.0(3)
C26 C25 Ru 71.2(3)
C25 C26 C22 108.3(4)
C25 C26 Ru 72.5(3)
C22 C26 Ru 72.7(3)
O1 C27 Ru 178.0(5)
C29 C28 C30 107.5(4)
C29 C28 P 113.5(3)
C30 C28 P 116.9(3)
C33 C31 C32 109.8(4)
C33 C31 P 115.9(3)
C32 C31 P 114.6(3)
C35 C34 C36 108.7(3)
C35 C34 P 112.9(3)
C36 C34 P 114.8(3)
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Table to be deposited

Table S16. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for Complex Ru(η^5-C_5H_5){C(CH=CPh$_2$)=NCH=CHCH$_3$}(CO)(P^{i}Pr$_3$) (**9**).

Atom	X/*a*	Y/*b*	Z/*c*	U_{eq}[a]
Ru	0.55772(3)	0.52517(3)	0.74100(2)	0.01917(10)
P	0.77836(10)	0.50514(9)	0.67884(6)	0.0214(2)
O	0.4442(3)	0.6922(2)	0.59046(17)	0.0326(7)
N	0.6883(3)	0.6252(3)	0.86757(19)	0.0211(7)
C1	0.6183(4)	0.6511(3)	0.7978(2)	0.0213(8)
C2	0.7128(4)	0.7103(3)	0.9109(3)	0.0229(9)
C3	0.7667(4)	0.6875(4)	0.9884(2)	0.0243(9)
C4	0.7906(4)	0.7746(3)	1.0380(2)	0.0301(10)
C5	0.5741(4)	0.7703(3)	0.7597(2)	0.0219(9)
C6	0.4492(4)	0.8232(3)	0.7631(2)	0.0215(8)
C7	0.4262(4)	0.9404(3)	0.7138(2)	0.0246(9)
C8	0.4935(4)	0.9803(3)	0.6338(3)	0.0315(10)
C9	0.4772(5)	1.0919(4)	0.5902(3)	0.0369(11)
C10	0.3932(5)	1.1654(4)	0.6248(3)	0.0423(12)
C11	0.3230(4)	1.1282(4)	0.7043(3)	0.0369(11)
C12	0.3394(4)	1.0166(3)	0.7477(3)	0.0315(10)
C13	0.3321(4)	0.7672(3)	0.8182(2)	0.0220(9)
C14	0.1976(4)	0.7773(3)	0.7863(3)	0.0293(10)
C15	0.0894(4)	0.7235(3)	0.8370(3)	0.0329(10)
C16	0.1090(4)	0.6571(3)	0.9183(3)	0.0317(10)
C17	0.2409(4)	0.6470(4)	0.9508(3)	0.0307(10)
C18	0.3496(4)	0.7023(3)	0.9017(2)	0.0251(9)
C19	0.5511(4)	0.3674(3)	0.8499(2)	0.0233(9)
C20	0.5074(4)	0.3394(3)	0.7736(2)	0.0275(9)
C21	0.3876(4)	0.4020(3)	0.7495(2)	0.0259(9)
C22	0.3540(4)	0.4722(3)	0.8102(2)	0.0242(9)
C23	0.4572(4)	0.4480(3)	0.8718(2)	0.0262(9)
C24	0.4951(4)	0.6289(3)	0.6473(2)	0.0232(9)
C25	0.7874(4)	0.4552(3)	0.5768(2)	0.0245(9)
C26	0.7240(4)	0.5381(3)	0.5001(2)	0.0322(10)
C27	0.7182(4)	0.3417(3)	0.5889(3)	0.0314(10)
C28	0.8812(4)	0.3910(3)	0.7507(2)	0.0240(9)
C29	1.0029(4)	0.3324(3)	0.7101(3)	0.0313(10)
C30	0.9257(4)	0.4316(3)	0.8287(2)	0.0309(10)
C31	0.8848(4)	0.6313(3)	0.6595(3)	0.0274(9)
C32	1.0377(4)	0.6160(3)	0.6308(3)	0.0314(10)
C33	0.8219(4)	0.7357(3)	0.5977(3)	0.0326(10)
C34	1.0811(9)	0.9430(4)	0.4514(5)	0.076(2)
C35	0.9516(9)	0.9787(6)	0.4281(4)	0.072(2)
C36	0.8717(5)	1.0361(6)	0.4759(5)	0.076(2)
C37	0.0884(7)	0.9299(5)	0.1084(4)	0.0698(18)
C38	0.1751(7)	0.9011(4)	0.0457(4)	0.0709(19)
C39	0.3176(7)	0.9032(4)	0.0500(4)	0.0763(19)
C40	0.3684(7)	0.9338(5)	0.1186(5)	0.086(2)
C41	0.2860(8)	0.9612(5)	0.1829(4)	0.080(2)
C42	0.1411(8)	0.9610(5)	0.1786(4)	0.082(2)

[a] Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *Uij* tensor. [b] Disordered PF_6 anion. [c] Solvent water molecule.

Table to be deposited

Table S17. Anisotropic displacement coefficients U_{ij} (Å^2) for the non-hydrogen atoms for the complex Ru(η^5-C_5H_5){C(CH=CPh$_2$)=NCH=CHCH$_3$}(CO)(P^{i}Pr$_3$) (**9**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	0.01232(16)	0.02452(18)	0.02054(17)	-0.00335(13)	-0.00406(12)	-0.00339(12)
P	0.0159(5)	0.0263(6)	0.0221(5)	-0.0048(5)	-0.0032(4)	-0.0024(4)
O	0.0311(16)	0.0354(17)	0.0297(16)	-0.0009(14)	-0.0128(13)	-0.0015(13)
N	0.0137(16)	0.0270(19)	0.0226(17)	-0.0046(14)	-0.0028(13)	-0.0016(14)
C1	0.0155(19)	0.027(2)	0.021(2)	-0.0049(17)	0.0016(16)	-0.0015(16)
C2	0.0126(19)	0.028(2)	0.028(2)	-0.0044(19)	-0.0019(16)	-0.0022(17)
C3	0.015(2)	0.031(2)	0.025(2)	-0.0023(19)	-0.0022(17)	-0.0030(17)
C4	0.029(2)	0.032(2)	0.031(2)	-0.0069(19)	-0.0093(19)	-0.0049(19)
C5	0.023(2)	0.024(2)	0.020(2)	-0.0050(17)	-0.0044(17)	-0.0080(17)
C6	0.018(2)	0.026(2)	0.023(2)	-0.0083(17)	-0.0077(16)	-0.0011(17)
C7	0.021(2)	0.025(2)	0.029(2)	-0.0054(18)	-0.0144(18)	-0.0041(17)
C8	0.031(2)	0.034(3)	0.030(2)	-0.007(2)	-0.0140(19)	-0.001(2)
C9	0.043(3)	0.033(3)	0.035(3)	-0.004(2)	-0.014(2)	-0.006(2)
C10	0.037(3)	0.027(3)	0.061(3)	0.001(2)	-0.028(2)	-0.004(2)
C11	0.023(2)	0.029(3)	0.064(3)	-0.019(2)	-0.017(2)	0.0022(19)
C12	0.022(2)	0.030(2)	0.046(3)	-0.011(2)	-0.011(2)	-0.0017(18)
C13	0.0152(19)	0.026(2)	0.027(2)	-0.0099(18)	-0.0061(17)	-0.0004(16)
C14	0.018(2)	0.037(3)	0.035(2)	-0.009(2)	-0.0093(18)	-0.0004(18)
C15	0.016(2)	0.040(3)	0.048(3)	-0.019(2)	-0.008(2)	-0.0041(19)
C16	0.017(2)	0.041(3)	0.041(3)	-0.015(2)	0.0020(19)	-0.0081(19)
C17	0.024(2)	0.044(3)	0.026(2)	-0.011(2)	-0.0015(18)	-0.0009(19)
C18	0.016(2)	0.034(2)	0.028(2)	-0.0107(19)	-0.0019(17)	-0.0012(17)
C19	0.016(2)	0.027(2)	0.024(2)	-0.0007(18)	-0.0040(16)	-0.0048(17)
C20	0.023(2)	0.031(2)	0.027(2)	-0.0049(19)	-0.0012(18)	-0.0059(18)
C21	0.018(2)	0.032(2)	0.026(2)	-0.0018(18)	-0.0018(17)	-0.0090(18)
C22	0.017(2)	0.025(2)	0.030(2)	-0.0013(18)	-0.0025(17)	-0.0068(17)
C23	0.027(2)	0.031(2)	0.021(2)	-0.0059(18)	-0.0010(17)	-0.0104(18)
C24	0.016(2)	0.026(2)	0.029(2)	-0.0058(19)	-0.0014(17)	-0.0069(17)
C25	0.018(2)	0.029(2)	0.026(2)	-0.0060(18)	-0.0037(17)	0.0018(17)
C26	0.032(2)	0.040(3)	0.026(2)	-0.009(2)	-0.0049(19)	-0.001(2)
C27	0.029(2)	0.038(3)	0.031(2)	-0.015(2)	-0.0035(19)	-0.005(2)
C28	0.019(2)	0.029(2)	0.024(2)	-0.0031(18)	-0.0050(17)	0.0007(17)
C29	0.020(2)	0.042(3)	0.033(2)	-0.010(2)	-0.0039(18)	0.0036(19)
C30	0.019(2)	0.044(3)	0.029(2)	-0.007(2)	-0.0069(18)	0.0027(19)
C31	0.022(2)	0.033(2)	0.029(2)	-0.0102(19)	-0.0018(18)	-0.0030(18)
C32	0.018(2)	0.041(3)	0.036(2)	-0.011(2)	0.0046(18)	-0.0115(19)
C33	0.030(2)	0.029(2)	0.037(3)	-0.003(2)	0.006(2)	-0.0097(19)
C34	0.107(6)	0.038(3)	0.070(5)	0.002(3)	0.036(4)	0.007(4)
C35	0.102(6)	0.069(4)	0.047(4)	0.001(3)	-0.026(4)	-0.055(4)
C36	0.026(3)	0.080(5)	0.094(5)	0.043(4)	-0.009(4)	-0.008(3)
C37	0.079(5)	0.051(4)	0.079(5)	-0.001(3)	-0.034(4)	-0.025(3)
C38	0.093(5)	0.039(3)	0.085(5)	-0.006(3)	-0.057(4)	-0.013(3)
C39	0.088(5)	0.042(3)	0.103(5)	-0.016(3)	-0.044(4)	0.003(3)
C40	0.093(5)	0.037(4)	0.131(7)	-0.007(4)	-0.075(5)	0.008(3)
C41	0.119(6)	0.045(4)	0.077(5)	0.000(3)	-0.064(5)	-0.027(4)
C42	0.125(6)	0.059(4)	0.064(4)	-0.002(3)	-0.027(4)	-0.036(4)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2 (h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12})$

Table to be deposited

Table S18. Hydrogen atom coordinates* and isotropic displacement coefficient ($Å^2$) for the compound $Ru(\eta^5\text{-}C_5H_5)\{C(CH{=}CPh_2){=}NCH{=}CHCH_3\}(CO)(P^iPr_3)$ (**9**).

Atom	X/*a*	Y/*b*	Z/*c*	*U*
H2[a]	0.685(3)	0.790(3)	0.884(2)	0.020(10)
H3[a]	0.788(4)	0.604(3)	1.016(2)	0.029(11)
H4A	0.7605	0.8492	1.0048	0.045
H4B	0.8895	0.7745	1.0483	0.045
H4C	0.7375	0.7573	1.0935	0.045
H5[a]	0.638(4)	0.814(3)	0.722(2)	0.021(10)
H8	0.5519	0.9300	0.6086	0.038
H9	0.5247	1.1175	0.5358	0.044
H10	0.3826	1.2420	0.5947	0.051
H11	0.2643	1.1791	0.7286	0.044
H12	0.2906	0.9912	0.8017	0.038
H14	0.1816	0.8211	0.7299	0.035
H15	-0.0009	0.7325	0.8153	0.039
H16	0.0339	0.6189	0.9516	0.038
H17	0.2561	0.6020	1.0069	0.037
H18	0.4384	0.6960	0.9252	0.030
H19	0.6307	0.3364	0.8805	0.028
H20	0.5530	0.2868	0.7444	0.033
H21	0.3358	0.3993	0.7011	0.031
H22	0.2774	0.5245	0.8090	0.029
H23	0.4617	0.4811	0.9202	0.031
H25	0.8875	0.4428	0.5608	0.029
H26A	0.7236	0.5021	0.4509	0.048
H26B	0.7790	0.6057	0.4841	0.048
H26C	0.6287	0.5593	0.5163	0.048
H27A	0.6182	0.3524	0.5998	0.047
H27B	0.7569	0.2879	0.6382	0.047
H27C	0.7352	0.3125	0.5365	0.047
H28	0.8145	0.3304	0.7747	0.029
H29A	1.0711	0.3883	0.6832	0.047
H29B	0.9691	0.2970	0.6661	0.047
H29C	1.0465	0.2745	0.7550	0.047
H30A	0.9581	0.3667	0.8727	0.046
H30B	0.8468	0.4701	0.8529	0.046
H30C	1.0009	0.4842	0.8107	0.046
H31	0.8861	0.6523	0.7167	0.033
H32A	1.0434	0.5876	0.5777	0.047
H32B	1.0850	0.5618	0.6764	0.047
H32C	1.0822	0.6887	0.6200	0.047
H33A	0.8587	0.8043	0.6090	0.049
H33B	0.7209	0.7378	0.6070	0.049
H33C	0.8462	0.7316	0.5378	0.049
H34	1.1387	0.9034	0.4168	0.091
H35	0.9172	0.9628	0.3776	0.087
H36	0.7813	1.0623	0.4587	0.091
H37	-0.0090	0.9287	0.1040	0.084
H38	0.1375	0.8792	-0.0016	0.085
H39	0.3781	0.8837	0.0060	0.092
H40	0.4660	0.9361	0.1215	0.104
H41	0.3255	0.9805	0.2307	0.095
H42	0.0811	0.9815	0.2224	0.099

* The hydrogen atoms were included in observed or calculated positions and refined riding on their respective carbon atoms. [a] this Hydrogen was refined as free isotropic .

Table to be deposited

Table S19. Full experimental details for the X-Ray analysis of [Ru(η^5-C_5H_5){ κ^2-*C,C*-C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^iPr_3)]BF_4 (**5**).

Crystal data:

Formula	$C_{33}H_{42}NOPRu$ x 1.5 C_6H_6
Molecular weight	717.88
Crystal habit	irregular prism
color	colorless
Size(mm)	0.20 x 0.8 x 0.04
Symmetry	triclinic, P-1
Unit cell dimensions	9.674(2), 12.170(3), 15.904(3) Å
	76.879(3), 86.662(3), 87.046(3) °
Packing: V (Å^3), Z	1819.0(7), 2
D_{calc}(g cm^{-3}), F (000)	1.822, 1292

Experimental data:	Bruker smart-APEX
Radiation and technique	Mo-K_α (λ = 0.71073 Å)
Monochromator	Graphite oriented
Range	($4 < 2\theta < 57°$)
Number of reflections:	
measured	21506 (*h*: -12, 12; *k*: -16, 16; *l*: -21, 21)
unique	8342 (R_{int} = 0.0637)
Absorption correction	sadabs*
Max. and min. trans. fact.	0.962, 0.784
μ (mm^{-1})	0.508
Temperature (K)	100.0(2)

Table to be deposited

Table S19. Full experimental details for the X-Ray analysis of [Ru(η^5-C_5H_5){ κ^2-*C,C*-C=N($CH_2CH=CH_2$)CH($CH=CH_2$)CPh_2CH_2}(CO)(P^iPr_3)]BF_4 (**5**).

Solution and refinement:	SHELX97 dos/win95/nt version
Solution mode	Patterson
Refinement	Full-matrix least-squares on F'^2s.
	All reflections.
Hydrogen atoms	see table **S18**.
No. parameters/restrains	435/0
Weighting scheme	$w^{-1}=[\sigma^2(F_o^2)+(0.0364P)^2+0.0P]$
	where $P=((\text{Max } F_o^2,0)+2F_c^2)/3$
ΔF final (max)	1.427 e/Å^3
ΔF final (min)	-1.100 e/Å^3
Max/Mean shift/esd	0.002, 0.000
$\omega R2(F^2, \text{ all data})^a$	0.0991
$R1(F, F_o > 4.0\ \sigma F)^b$	0.0488
Goodness-of-Fit[c]	0.828
Data-to-Parameter Ratio	19.2:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol C (1992). Anomalous dispersion is implemented by the program.

[a] $wR2(F^2) = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ [b] $R1(F) = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [c] $S = \{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, where n is the number of observed reflections, and p is the number of parameters refined.

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* Shelxtl 6.1., Bruker-Siemens Analytical X-ray Instruments, Inc: Madison, WI.

Table to be deposited

Table S20. Bond Lenghts (Å) and angles (deg) for the complex Ru(η^5-C_5H_5){C(CH=CPh$_2$)=NCH=CHCH$_3$}(CO)(P^{i}Pr$_3$) (**9**).

Ru C24 1.831(4)	C26 H26A 0.9800
Ru C1 2.071(4)	C26 H26B 0.9800
Ru C22 2.251(4)	C26 H26C 0.9800
Ru C21 2.261(4)	C27 H27A 0.9800
Ru C23 2.265(4)	C27 H27B 0.9800
Ru C20 2.274(4)	C27 H27C 0.9800
Ru C19 2.276(4)	C28 C30 1.527(5)
Ru P 2.3245(11)	C28 C29 1.532(5)
P C31 1.850(4)	C28 H28 1.0000
P C25 1.854(4)	C29 H29A 0.9800
P C28 1.869(4)	C29 H29B 0.9800
O C24 1.162(4)	C29 H29C 0.9800
N C1 1.303(4)	C30 H30A 0.9800
N C2 1.404(5)	C30 H30B 0.9800
C1 C5 1.491(5)	C30 H30C 0.9800
C2 C3 1.331(5)	C31 C32 1.538(5)
C2 H2 1.00(3)	C31 C33 1.541(5)
C3 C4 1.492(5)	C31 H31 1.0000
C3 H3 1.02(4)	C32 H32A 0.9800
C4 H4A 0.9800	C32 H32B 0.9800
C4 H4B 0.9800	C32 H32C 0.9800
C4 H4C 0.9800	C33 H33A 0.9800
C5 C6 1.343(5)	C33 H33B 0.9800
C5 H5 0.93(3)	C33 H33C 0.9800
C6 C7 1.476(5)	C34 C36 1.347(8) 2_776
C6 C13 1.485(5)	C34 C35 1.349(8)
C7 C8 1.391(5)	C34 H34 0.9500
C7 C12 1.397(5)	C35 C36 1.335(8)
C8 C9 1.383(5)	C35 H35 0.9500
C8 H8 0.9500	C36 C34 1.347(8) 2_776
C9 C10 1.364(6)	C36 H36 0.9500
C9 H9 0.9500	C37 C38 1.360(8)
C10 C11 1.391(6)	C37 C42 1.389(7)
C10 H10 0.9500	C37 H37 0.9500
C11 C12 1.383(5)	C38 C39 1.386(8)
C11 H11 0.9500	C38 H38 0.9500
C12 H12 0.9500	C39 C40 1.355(8)
C13 C18 1.397(5)	C39 H39 0.9500
C13 C14 1.414(5)	C40 C41 1.352(9)
C14 C15 1.381(5)	C40 H40 0.9500
C14 H14 0.9500	C41 C42 1.407(8)
C15 C16 1.379(5)	C41 H41 0.9500
C15 H15 0.9500	C42 H42 0.9500
C16 C17 1.393(5)	
C16 H16 0.9500	C24 Ru C1 91.79(15)
C17 C18 1.381(5)	C24 Ru C22 99.81(15)
C17 H17 0.9500	C1 Ru C22 104.14(14)
C18 H18 0.9500	C24 Ru C21 96.57(15)
C19 C23 1.391(5)	C1 Ru C21 141.35(14)
C19 C20 1.425(5)	C22 Ru C21 37.25(13)
C19 H19 0.9500	C24 Ru C23 132.60(15)
C20 C21 1.378(5)	C1 Ru C23 86.14(14)
C20 H20 0.9500	C22 Ru C23 36.48(12)
C21 C22 1.441(5)	C21 Ru C23 60.75(14)
C21 H21 0.9500	C24 Ru C20 124.44(15)
C22 C23 1.414(5)	C1 Ru C20 141.40(14)
C22 H22 0.9500	C22 Ru C20 60.75(14)
C23 H23 0.9500	C21 Ru C20 35.38(13)
C25 C26 1.531(5)	C23 Ru C20 60.38(14)
C25 C27 1.533(5)	C24 Ru C19 156.42(14)
C25 H25 1.0000	C1 Ru C19 104.93(14)

C22 Ru C19 60.40(13)
C21 Ru C19 60.02(13)
C23 Ru C19 35.67(13)
C20 Ru C19 36.51(12)
C24 Ru P 94.47(12)
C1 Ru P 92.02(10)
C22 Ru P 157.95(10)
C21 Ru P 124.62(11)
C23 Ru P 132.91(10)
C20 Ru P 97.29(10)
C19 Ru P 101.30(10)
C31 P C25 106.82(17)
C31 P C28 105.21(17)
C25 P C28 101.60(17)
C31 P Ru 115.59(13)
C25 P Ru 116.01(12)
C28 P Ru 110.20(12)
C1 N C2 118.9(3)
N C1 C5 121.2(3)
N C1 Ru 120.1(3)
C5 C1 Ru 118.6(3)
C3 C2 N 122.2(4)
C3 C2 H2 119.3(19)
N C2 H2 118.5(19)
C2 C3 C4 124.1(4)
C2 C3 H3 117(2)
C4 C3 H3 119(2)
C3 C4 H4A 109.5
C3 C4 H4B 109.5
H4A C4 H4B 109.5
C3 C4 H4C 109.5
H4A C4 H4C 109.5
H4B C4 H4C 109.5
C6 C5 C1 129.8(4)
C6 C5 H5 113(2)
C1 C5 H5 117(2)
C5 C6 C7 120.4(4)
C5 C6 C13 121.3(3)
C7 C6 C13 118.2(3)
C8 C7 C12 117.6(4)
C8 C7 C6 121.7(4)
C12 C7 C6 120.7(4)
C9 C8 C7 121.2(4)
C9 C8 H8 119.4
C7 C8 H8 119.4
C10 C9 C8 120.4(4)
C10 C9 H9 119.8
C8 C9 H9 119.8
C9 C10 C11 120.0(4)
C9 C10 H10 120.0
C11 C10 H10 120.0
C12 C11 C10 119.5(4)
C12 C11 H11 120.2
C10 C11 H11 120.2
C11 C12 C7 121.3(4)
C11 C12 H12 119.3
C7 C12 H12 119.3
C18 C13 C14 117.5(4)
C18 C13 C6 122.3(3)
C14 C13 C6 120.2(3)
C15 C14 C13 120.1(4)
C15 C14 H14 120.0
C13 C14 H14 120.0
C16 C15 C14 121.7(4)
C16 C15 H15 119.1
C14 C15 H15 119.1
C15 C16 C17 118.8(4)
C15 C16 H16 120.6
C17 C16 H16 120.6
C18 C17 C16 120.2(4)
C18 C17 H17 119.9
C16 C17 H17 119.9
C17 C18 C13 121.6(4)
C17 C18 H18 119.2
C13 C18 H18 119.2
C23 C19 C20 108.3(3)
C23 C19 Ru 71.7(2)
C20 C19 Ru 71.7(2)
C23 C19 H19 125.9
C20 C19 H19 125.9
Ru C19 H19 122.4
C21 C20 C19 108.1(4)
C21 C20 Ru 71.8(2)
C19 C20 Ru 71.8(2)
C21 C20 H20 126.0
C19 C20 H20 126.0
Ru C20 H20 122.1
C20 C21 C22 108.5(3)
C20 C21 Ru 72.8(2)
C22 C21 Ru 71.0(2)
C20 C21 H21 125.8
C22 C21 H21 125.7
Ru C21 H21 122.1
C23 C22 C21 106.6(3)
C23 C22 Ru 72.3(2)
C21 C22 Ru 71.7(2)
C23 C22 H22 126.7
C21 C22 H22 126.7
Ru C22 H22 121.1
C19 C23 C22 108.6(3)
C19 C23 Ru 72.6(2)
C22 C23 Ru 71.2(2)
C19 C23 H23 125.7
C22 C23 H23 125.7
Ru C23 H23 122.1
O C24 Ru 174.2(3)
C26 C25 C27 108.4(3)
C26 C25 P 114.7(3)
C27 C25 P 111.2(3)
C26 C25 H25 107.4
C27 C25 H25 107.4
P C25 H25 107.4
C25 C26 H26A 109.5
C25 C26 H26B 109.5
H26A C26 H26B 109.5
C25 C26 H26C 109.5
H26A C26 H26C 109.5
H26B C26 H26C 109.5
C25 C27 H27A 109.5
C25 C27 H27B 109.5
H27A C27 H27B 109.5
C25 C27 H27C 109.5
H27A C27 H27C 109.5
H27B C27 H27C 109.5
C30 C28 C29 111.0(3)
C30 C28 P 110.4(3)
C29 C28 P 118.4(3)
C30 C28 H28 105.3
C29 C28 H28 105.3
P C28 H28 105.3
C28 C29 H29A 109.5
C28 C29 H29B 109.5
H29A C29 H29B 109.5
C28 C29 H29C 109.5
H29A C29 H29C 109.5
H29B C29 H29C 109.5

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C28 C30 H30A 109.5
C28 C30 H30B 109.5
H30A C30 H30B 109.5
C28 C30 H30C 109.5
H30A C30 H30C 109.5
H30B C30 H30C 109.5
C32 C31 C33 108.3(3)
C32 C31 P 116.8(3)
C33 C31 P 114.2(3)
C32 C31 H31 105.5
C33 C31 H31 105.5
P C31 H31 105.5
C31 C32 H32A 109.5
C31 C32 H32B 109.5
H32A C32 H32B 109.5
C31 C32 H32C 109.5
H32A C32 H32C 109.5
H32B C32 H32C 109.5
C31 C33 H33A 109.5
C31 C33 H33B 109.5
H33A C33 H33B 109.5
C31 C33 H33C 109.5
H33A C33 H33C 109.5
H33B C33 H33C 109.5
C36 C34 C35 119.6(6) 2_776
C36 C34 H34 120.2 2_776
C35 C34 H34 120.2
C36 C35 C34 120.2(6)
C36 C35 H35 119.9
C34 C35 H35 119.9
C35 C36 C34 120.3(5) . 2_776
C35 C36 H36 119.9
C34 C36 H36 119.9 2_776
C38 C37 C42 120.5(6)
C38 C37 H37 119.7
C42 C37 H37 119.7
C37 C38 C39 120.9(6)
C37 C38 H38 119.5
C39 C38 H38 119.5
C40 C39 C38 118.3(7)
C40 C39 H39 120.9
C38 C39 H39 120.9
C41 C40 C39 122.7(7)
C41 C40 H40 118.6
C39 C40 H40 118.6
C40 C41 C42 119.4(6)
C40 C41 H41 120.3
C42 C41 H41 120.3
C37 C42 C41 118.1(7)
C37 C42 H42 120.9
C41 C42 H42 120.9
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