(^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (1)

Crystallographic data. The X-ray diffraction data were measured at 150 K on a Bruker SMART APEX II CCD area detector system equipped with a graphite monochromator and a Mo Kα fine-focus sealed tube operated at 1.5 kW power (50 kV, 30 mA). A yellow rectangular prism of (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (1) of approximate dimensions 0.30 × 0.28 × 0.09 mm^3 was glued to a glass fiber using Paratone N oil. The detector was placed at a distance of 5.127 cm from the crystal during the data collection.

A series of narrow frames of data were collected with a scan width of 0.5° in ω or ϕ and an exposure time of 10 s per frame. The frames were integrated with the Bruker SAINT Software package[1] using a narrow-frame integration algorithm. The integration of the data using a monoclinic unit cell yielded a total of 108049 reflections in the θ range of 1.57 to 33.73° of which 28051 were independent with $I \geq 2\sigma(I)$ (R_{int} = 0.0481). The data were corrected for absorption effects by the multi-scan method (SADABS). Crystallographic data collection parameters and refinement data are collected below in Table 1. The structure was solved by the direct methods using the Bruker SHELXTL (V. 6.14) Software Package.[1] All non-hydrogen atoms were located in successive Fourier maps and refined anisotropically. The asymmetric unit consists of two crystallographically unique but chemically identical (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (1) complex molecules. All non-hydrogen atoms of the molecule are located on general positions and well ordered. The hydride hydrogen atoms were also located in the Fourier maps and refined isotropically. The rest of the hydrogen atoms were placed in calculated positions and refined isotropically. The final refinement parameters are R_1 = 0.0388 and wR_2 = 0.0702 for data with $F > 4\sigma(F)$ giving the data to parameter ratio of 27. The refinement data for all data are R_1 = 0.0602 and wR_2 = 0.0767.

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Reference

1. APEX2 Software Suite V. 2.2, Bruker AXS Inc.: Madison, WI, 2008.

Table 1a. Crystallographic Data for (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**).

compound (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**)			color
chemical formula	$C_{51}H_{43}F_{48}P_8Ru_4$	fw	2219.89
T, K	150(2)	λ, Å	0.71073
space group	$P2_1/c$	*a*, Å	10.4355(1)
b, Å	18.1346(2)	*c*, Å	37.1996(4)
β, °	92.392(1)	*V*, Å^3	7033.65(13)
Z	4	D_{calc}, Mg m^{-3}	2.096
μ, mm^{-1}	1.190	goodness of fit	1.034
$R1[I > 2\sigma(I)]$[a]	0.0388	$wR2[I > 2\sigma(I)]$[b]	0.0702

[a] $R1 = \sum||F_o| - |F_c||/\sum|F_o|$; [b] $_wR2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2]\}^{1/2}$

Table 1b. Crystal data and structure refinement for (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**)

Identification code	bcg08	
Empirical formula	C51 H43 F48 P8 Ru4	
Formula weight	2219.89	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.4355(1) Å	□= 90°.
	b = 18.1346(2) Å	□= 92.392(1)°.
	c = 37.1996(4) Å	□ = 90°.
Volume	7033.65(13) Å^3	
Z	4	
Density (calculated)	2.096 Mg/m^3	
Absorption coefficient	1.190 mm^{-1}	
F(000)	4308	
Crystal size	0.30 × 0.28 × 0.09 mm^3	
Theta range for data collection	1.57 to 33.73°.	
Index ranges	-16<=h<=16, -28<=k<=24, -57<=l<=51	
Reflections collected	108049	
Independent reflections	28051 [R(int) = 0.0481]	
Completeness to theta = 33.73°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8964 and 0.7144	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28051 / 3 / 1024	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0702	
R indices (all data)	R1 = 0.0602, wR2 = 0.0767	
Largest diff. peak and hole	0.897 and -0.639 e.Å^{-3}	

Table 1c. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2784(1)	2931(1)	4345(1)	14(1)
P(1)	963(1)	2278(1)	4326(1)	19(1)
P(2)	4791(1)	3126(1)	4590(1)	18(1)
P(3)	1983(1)	4086(1)	4227(1)	19(1)
C(1)	3532(2)	1850(1)	4341(1)	18(1)
Ru(2)	3696(1)	1939(1)	3772(1)	17(1)
P(4)	4467(1)	2369(1)	3265(1)	20(1)
C(2)	2733(2)	1285(1)	4179(1)	20(1)
C(3)	3237(2)	781(1)	3925(1)	26(1)
C(4)	4534(2)	800(1)	3849(1)	29(1)
C(5)	5377(2)	1292(1)	4041(1)	28(1)
C(6)	4901(2)	1788(1)	4291(1)	22(1)
C(7)	5773(2)	2318(1)	4490(1)	29(1)
C(8)	6095(2)	3847(2)	4541(1)	28(1)
F(8A)	7220(1)	3621(1)	4691(1)	40(1)
F(8B)	5815(2)	4489(1)	4693(1)	39(1)
F(8C)	6279(2)	3962(1)	4196(1)	38(1)
C(9)	4840(2)	3122(2)	5096(1)	33(1)
F(9A)	6030(2)	3112(1)	5246(1)	56(1)
F(9B)	4254(2)	3709(1)	5229(1)	46(1)
F(9C)	4248(2)	2523(1)	5216(1)	47(1)
C(10)	1322(2)	1305(1)	4238(1)	26(1)
C(11)	-498(2)	2394(1)	4012(1)	27(1)
F(11A)	-1207(2)	2971(1)	4097(1)	42(1)
F(11B)	-1286(2)	1811(1)	3999(1)	48(1)
F(11C)	-126(2)	2505(1)	3678(1)	43(1)
C(12)	69(2)	2178(2)	4754(1)	32(1)
F(12A)	-917(2)	1712(1)	4725(1)	61(1)
F(12B)	-396(2)	2813(1)	4871(1)	45(1)
F(12C)	864(2)	1922(1)	5013(1)	45(1)

C(13)	2196(2)	3665(1)	3330(1)	24(1)
C(14)	3083(2)	3623(1)	3061(1)	26(1)
C(15)	3602(3)	4274(2)	2931(1)	34(1)
C(16)	3244(3)	4950(2)	3070(1)	38(1)
C(17)	2406(3)	4980(1)	3350(1)	32(1)
C(18)	1890(2)	4334(1)	3488(1)	25(1)
C(19)	1067(2)	4352(1)	3809(1)	26(1)
C(20)	3081(3)	4912(1)	4266(1)	30(1)
F(20A)	4130(2)	4802(1)	4083(1)	36(1)
F(20B)	2554(2)	5546(1)	4146(1)	44(1)
F(20C)	3447(2)	5027(1)	4611(1)	42(1)
C(21)	810(3)	4439(2)	4565(1)	35(1)
F(21A)	-314(2)	4105(1)	4507(1)	53(1)
F(21B)	576(2)	5163(1)	4535(1)	62(1)
F(21C)	1206(2)	4320(1)	4901(1)	51(1)
C(22)	3503(2)	2881(1)	2923(1)	27(1)
C(23)	5184(3)	1639(2)	2971(1)	33(1)
F(23A)	6160(2)	1295(1)	3142(1)	54(1)
F(23B)	4298(2)	1135(1)	2890(1)	49(1)
F(23C)	5616(2)	1890(1)	2660(1)	46(1)
C(24)	5926(2)	2980(2)	3313(1)	31(1)
F(24A)	6329(2)	3251(1)	3003(1)	45(1)
F(24B)	6912(2)	2628(1)	3472(1)	61(1)
F(24C)	5661(2)	3558(1)	3517(1)	44(1)
Ru(3)	9617(1)	3302(1)	1468(1)	14(1)
P(5)	11488(1)	3948(1)	1498(1)	20(1)
P(6)	7889(1)	2940(1)	1139(1)	18(1)
P(7)	8740(1)	3439(1)	2020(1)	19(1)
Ru(4)	10860(1)	1899(1)	1247(1)	17(1)
P(8)	11790(1)	1128(1)	1643(1)	19(1)
C(25)	10480(2)	2940(1)	995(1)	18(1)
C(26)	9810(2)	2393(1)	784(1)	21(1)
C(27)	10462(2)	1766(1)	652(1)	27(1)
C(28)	11787(3)	1688(2)	715(1)	30(1)
C(29)	12493(2)	2264(1)	890(1)	27(1)
C(30)	11870(2)	2894(1)	1012(1)	23(1)

C(31)	12603(2)	3510(1)	1196(1)	29(1)
C(32)	12737(2)	4228(2)	1860(1)	32(1)
F(32A)	13826(1)	4470(1)	1717(1)	43(1)
F(32B)	12354(2)	4746(1)	2078(1)	51(1)
F(32C)	13077(2)	3634(1)	2053(1)	46(1)
C(33)	11287(3)	4901(1)	1297(1)	37(1)
F(33A)	10579(2)	5330(1)	1497(1)	58(1)
F(33B)	10692(2)	4855(1)	974(1)	53(1)
F(33C)	12396(2)	5249(1)	1249(1)	62(1)
C(34)	8380(2)	2444(1)	738(1)	24(1)
C(35)	6530(2)	2338(1)	1287(1)	24(1)
F(35A)	5834(2)	2026(1)	1019(1)	39(1)
F(35B)	6989(1)	1787(1)	1492(1)	35(1)
F(35C)	5726(2)	2722(1)	1484(1)	40(1)
C(36)	6837(3)	3679(1)	923(1)	32(1)
F(36A)	7553(2)	4124(1)	730(1)	48(1)
F(36B)	5921(2)	3405(1)	699(1)	55(1)
F(36C)	6251(2)	4092(1)	1162(1)	44(1)
C(37)	9368(2)	1614(1)	2164(1)	21(1)
C(38)	8903(2)	2126(1)	2406(1)	24(1)
C(39)	9378(3)	2122(1)	2761(1)	32(1)
C(40)	10353(3)	1631(2)	2864(1)	36(1)
C(41)	10869(3)	1161(1)	2616(1)	31(1)
C(42)	10371(2)	1141(1)	2263(1)	23(1)
C(43)	10927(2)	632(1)	1990(1)	24(1)
C(44)	13208(3)	1475(2)	1921(1)	33(1)
F(44A)	14158(2)	1673(1)	1717(1)	66(1)
F(44B)	13699(2)	992(1)	2157(1)	58(1)
F(44C)	12879(2)	2063(1)	2110(1)	59(1)
C(45)	12647(3)	316(2)	1441(1)	36(1)
F(45A)	13523(2)	531(1)	1217(1)	59(1)
F(45B)	13246(2)	-113(1)	1682(1)	75(1)
F(45C)	11810(2)	-92(1)	1253(1)	64(1)
C(46)	7947(2)	2697(1)	2274(1)	25(1)
C(47)	9791(2)	3835(1)	2398(1)	28(1)
F(47A)	9293(2)	3810(1)	2724(1)	39(1)

F(47B)	10904(1)	3473(1)	2422(1)	35(1)
F(47C)	10044(2)	4546(1)	2332(1)	39(1)
C(48)	7425(2)	4155(1)	2051(1)	30(1)
F(48A)	7181(2)	4362(1)	2387(1)	44(1)
F(48B)	6332(2)	3877(1)	1910(1)	49(1)
F(48C)	7666(2)	4771(1)	1871(1)	41(1)
C(49)	4330(7)	-4(6)	4984(2)	179(5)
C(50)	3405(11)	280(9)	5216(3)	234(7)
C(51)	2083(10)	122(5)	5157(2)	171(4)

Table 1d. Bond lengths [Å] and angles [°] for (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**).

Ru(1)-C(1)	2.110(2)
Ru(1)-P(1)	2.2383(6)
Ru(1)-P(2)	2.2756(6)
Ru(1)-P(3)	2.2917(6)
Ru(1)-Ru(2)	2.9773(2)
Ru(1)-H(1)	1.45(3)
Ru(1)-H(1B)	1.96(3)
P(1)-C(10)	1.835(2)
P(1)-C(12)	1.887(3)
P(1)-C(11)	1.893(3)
P(2)-C(7)	1.834(2)
P(2)-C(9)	1.882(3)
P(2)-C(8)	1.902(2)
P(3)-C(19)	1.856(3)
P(3)-C(20)	1.888(3)
P(3)-C(21)	1.901(3)
C(1)-C(2)	1.438(3)
C(1)-C(6)	1.453(3)
C(1)-Ru(2)	2.139(2)
Ru(2)-C(2)	2.198(2)
Ru(2)-P(4)	2.2210(6)
Ru(2)-C(3)	2.233(2)
Ru(2)-C(4)	2.257(2)
Ru(2)-C(6)	2.277(2)
Ru(2)-C(5)	2.305(2)
Ru(2)-H(1B)	1.71(3)
Ru(2)-H(2)	1.59(3)
P(4)-C(22)	1.840(3)
P(4)-C(24)	1.885(3)
P(4)-C(23)	1.891(3)
C(2)-C(3)	1.429(3)
C(2)-C(10)	1.499(3)
C(3)-C(4)	1.395(4)
C(3)-H(3A)	1.0000

C(4)-C(5)	1.425(4)
C(4)-H(4A)	1.0000
C(5)-C(6)	1.398(3)
C(5)-H(5A)	1.0000
C(6)-C(7)	1.499(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-F(8C)	1.321(3)
C(8)-F(8B)	1.333(3)
C(8)-F(8A)	1.343(3)
C(9)-F(9B)	1.333(3)
C(9)-F(9C)	1.334(3)
C(9)-F(9A)	1.340(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-F(11A)	1.327(3)
C(11)-F(11C)	1.333(3)
C(11)-F(11B)	1.339(3)
C(12)-F(12C)	1.329(3)
C(12)-F(12B)	1.331(3)
C(12)-F(12A)	1.332(3)
C(13)-C(18)	1.390(3)
C(13)-C(14)	1.395(3)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.393(4)
C(14)-C(22)	1.511(3)
C(15)-C(16)	1.388(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.387(4)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.394(3)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.501(4)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-F(20A)	1.330(3)

C(20)-F(20C)	1.338(3)
C(20)-F(20B)	1.343(3)
C(21)-F(21C)	1.319(3)
C(21)-F(21A)	1.329(3)
C(21)-F(21B)	1.339(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-F(23B)	1.326(3)
C(23)-F(23A)	1.332(3)
C(23)-F(23C)	1.341(3)
C(24)-F(24B)	1.327(3)
C(24)-F(24C)	1.330(3)
C(24)-F(24A)	1.338(3)
Ru(3)-C(25)	2.115(2)
Ru(3)-P(6)	2.2332(6)
Ru(3)-P(5)	2.2773(6)
Ru(3)-P(7)	2.2971(6)
Ru(3)-Ru(4)	2.9870(2)
Ru(3)-H(3)	1.48(3)
Ru(3)-H(3B)	1.96(3)
P(5)-C(31)	1.832(3)
P(5)-C(33)	1.890(3)
P(5)-C(32)	1.903(3)
P(6)-C(34)	1.833(2)
P(6)-C(36)	1.890(3)
P(6)-C(35)	1.890(2)
P(7)-C(46)	1.858(2)
P(7)-C(47)	1.889(3)
P(7)-C(48)	1.897(2)
Ru(4)-C(25)	2.138(2)
Ru(4)-C(26)	2.195(2)
Ru(4)-P(8)	2.2239(6)
Ru(4)-C(27)	2.246(2)
Ru(4)-C(28)	2.269(2)
Ru(4)-C(30)	2.283(2)
Ru(4)-C(29)	2.301(2)

Ru(4)-H(3B)	1.76(3)
Ru(4)-H(4)	1.57(3)
P(8)-C(43)	1.840(2)
P(8)-C(44)	1.880(3)
P(8)-C(45)	1.893(3)
C(25)-C(26)	1.429(3)
C(25)-C(30)	1.452(3)
C(26)-C(27)	1.422(3)
C(26)-C(34)	1.498(3)
C(27)-C(28)	1.399(4)
C(27)-H(27A)	1.0000
C(28)-C(29)	1.420(4)
C(28)-H(28A)	1.0000
C(29)-C(30)	1.400(3)
C(29)-H(29A)	1.0000
C(30)-C(31)	1.502(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-F(32B)	1.315(3)
C(32)-F(32C)	1.334(3)
C(32)-F(32A)	1.348(3)
C(33)-F(33A)	1.324(4)
C(33)-F(33B)	1.332(4)
C(33)-F(33C)	1.337(3)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-F(35B)	1.333(3)
C(35)-F(35C)	1.334(3)
C(35)-F(35A)	1.334(3)
C(36)-F(36C)	1.330(3)
C(36)-F(36A)	1.331(3)
C(36)-F(36B)	1.340(3)
C(37)-C(42)	1.392(3)
C(37)-C(38)	1.395(3)
C(37)-H(37A)	0.9500
C(38)-C(39)	1.393(4)

C(38)-C(46)	1.506(3)
C(39)-C(40)	1.393(4)
C(39)-H(39A)	0.9500
C(40)-C(41)	1.381(4)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.392(4)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.507(3)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-F(44A)	1.323(3)
C(44)-F(44B)	1.327(3)
C(44)-F(44C)	1.330(4)
C(45)-F(45A)	1.322(3)
C(45)-F(45C)	1.323(3)
C(45)-F(45B)	1.325(4)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-F(47B)	1.335(3)
C(47)-F(47A)	1.339(3)
C(47)-F(47C)	1.339(3)
C(48)-F(48C)	1.331(3)
C(48)-F(48B)	1.334(3)
C(48)-F(48A)	1.339(3)
C(49)-C(49)#1	1.399(14)
C(49)-C(50)	1.417(11)
C(49)-H(49A)	0.9900
C(49)-H(49C)	0.9900
C(50)-C(51)	1.418(11)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800

C(1)-Ru(1)-P(1)	79.71(6)

C(1)-Ru(1)-P(2)	79.21(6)
P(1)-Ru(1)-P(2)	149.39(2)
C(1)-Ru(1)-P(3)	168.53(6)
P(1)-Ru(1)-P(3)	100.09(2)
P(2)-Ru(1)-P(3)	104.93(2)
C(1)-Ru(1)-Ru(2)	45.91(6)
P(1)-Ru(1)-Ru(2)	87.329(16)
P(2)-Ru(1)-Ru(2)	93.689(15)
P(3)-Ru(1)-Ru(2)	122.680(17)
C(1)-Ru(1)-H(1)	105.8(11)
P(1)-Ru(1)-H(1)	84.1(12)
P(2)-Ru(1)-H(1)	80.6(12)
P(3)-Ru(1)-H(1)	85.6(11)
Ru(2)-Ru(1)-H(1)	151.6(11)
C(1)-Ru(1)-H(1B)	78.3(9)
P(1)-Ru(1)-H(1B)	100.3(9)
P(2)-Ru(1)-H(1B)	96.8(9)
P(3)-Ru(1)-H(1B)	90.5(9)
Ru(2)-Ru(1)-H(1B)	32.9(9)
H(1)-Ru(1)-H(1B)	174.5(15)
C(10)-P(1)-C(12)	99.77(12)
C(10)-P(1)-C(11)	99.38(12)
C(12)-P(1)-C(11)	96.70(12)
C(10)-P(1)-Ru(1)	109.60(8)
C(12)-P(1)-Ru(1)	118.20(9)
C(11)-P(1)-Ru(1)	128.44(8)
C(7)-P(2)-C(9)	102.02(13)
C(7)-P(2)-C(8)	96.97(12)
C(9)-P(2)-C(8)	96.25(12)
C(7)-P(2)-Ru(1)	107.91(8)
C(9)-P(2)-Ru(1)	112.72(8)
C(8)-P(2)-Ru(1)	135.91(9)
C(19)-P(3)-C(20)	98.54(12)
C(19)-P(3)-C(21)	98.22(12)
C(20)-P(3)-C(21)	94.97(12)
C(19)-P(3)-Ru(1)	124.73(8)

C(20)-P(3)-Ru(1)	119.67(9)
C(21)-P(3)-Ru(1)	114.92(9)
C(2)-C(1)-C(6)	116.47(19)
C(2)-C(1)-Ru(1)	117.20(15)
C(6)-C(1)-Ru(1)	116.03(15)
C(2)-C(1)-Ru(2)	72.89(13)
C(6)-C(1)-Ru(2)	76.00(13)
Ru(1)-C(1)-Ru(2)	88.97(8)
C(1)-Ru(2)-C(2)	38.69(8)
C(1)-Ru(2)-P(4)	156.02(6)
C(2)-Ru(2)-P(4)	164.95(6)
C(1)-Ru(2)-C(3)	69.44(9)
C(2)-Ru(2)-C(3)	37.60(8)
P(4)-Ru(2)-C(3)	129.53(7)
C(1)-Ru(2)-C(4)	81.45(9)
C(2)-Ru(2)-C(4)	66.69(9)
P(4)-Ru(2)-C(4)	106.11(7)
C(3)-Ru(2)-C(4)	36.19(9)
C(1)-Ru(2)-C(6)	38.28(8)
C(2)-Ru(2)-C(6)	66.61(8)
P(4)-Ru(2)-C(6)	123.71(6)
C(3)-Ru(2)-C(6)	77.67(9)
C(4)-Ru(2)-C(6)	65.43(9)
C(1)-Ru(2)-C(5)	67.79(8)
C(2)-Ru(2)-C(5)	77.75(9)
P(4)-Ru(2)-C(5)	104.56(6)
C(3)-Ru(2)-C(5)	65.04(9)
C(4)-Ru(2)-C(5)	36.39(9)
C(6)-Ru(2)-C(5)	35.54(8)
C(1)-Ru(2)-Ru(1)	45.12(6)
C(2)-Ru(2)-Ru(1)	70.34(6)
P(4)-Ru(2)-Ru(1)	122.255(17)
C(3)-Ru(2)-Ru(1)	107.84(6)
C(4)-Ru(2)-Ru(1)	126.54(7)
C(6)-Ru(2)-Ru(1)	69.30(5)
C(5)-Ru(2)-Ru(1)	104.83(6)

C(1)-Ru(2)-H(1B)	83.1(11)
C(2)-Ru(2)-H(1B)	105.9(10)
P(4)-Ru(2)-H(1B)	84.7(11)
C(3)-Ru(2)-H(1B)	142.6(10)
C(4)-Ru(2)-H(1B)	161.8(10)
C(6)-Ru(2)-H(1B)	96.5(10)
C(5)-Ru(2)-H(1B)	127.5(10)
Ru(1)-Ru(2)-H(1B)	38.5(11)
C(1)-Ru(2)-H(2)	121.2(13)
C(2)-Ru(2)-H(2)	94.1(13)
P(4)-Ru(2)-H(2)	76.8(13)
C(3)-Ru(2)-H(2)	91.9(12)
C(4)-Ru(2)-H(2)	115.5(12)
C(6)-Ru(2)-H(2)	159.2(13)
C(5)-Ru(2)-H(2)	151.7(12)
Ru(1)-Ru(2)-H(2)	97.6(13)
H(1B)-Ru(2)-H(2)	80.8(16)
C(22)-P(4)-C(24)	100.65(12)
C(22)-P(4)-C(23)	99.91(12)
C(24)-P(4)-C(23)	97.37(12)
C(22)-P(4)-Ru(2)	123.80(8)
C(24)-P(4)-Ru(2)	116.51(9)
C(23)-P(4)-Ru(2)	114.25(9)
C(3)-C(2)-C(1)	120.7(2)
C(3)-C(2)-C(10)	120.2(2)
C(1)-C(2)-C(10)	118.46(19)
C(3)-C(2)-Ru(2)	72.53(13)
C(1)-C(2)-Ru(2)	68.42(12)
C(10)-C(2)-Ru(2)	124.70(16)
C(4)-C(3)-C(2)	120.3(2)
C(4)-C(3)-Ru(2)	72.82(13)
C(2)-C(3)-Ru(2)	69.87(12)
C(4)-C(3)-H(3A)	119.3
C(2)-C(3)-H(3A)	119.3
Ru(2)-C(3)-H(3A)	119.3
C(3)-C(4)-C(5)	119.8(2)

C(3)-C(4)-Ru(2)	70.98(13)
C(5)-C(4)-Ru(2)	73.62(13)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
Ru(2)-C(4)-H(4A)	119.8
C(6)-C(5)-C(4)	120.4(2)
C(6)-C(5)-Ru(2)	71.14(13)
C(4)-C(5)-Ru(2)	69.99(14)
C(6)-C(5)-H(5A)	118.9
C(4)-C(5)-H(5A)	118.9
Ru(2)-C(5)-H(5A)	118.9
C(5)-C(6)-C(1)	121.0(2)
C(5)-C(6)-C(7)	121.0(2)
C(1)-C(6)-C(7)	117.8(2)
C(5)-C(6)-Ru(2)	73.32(15)
C(1)-C(6)-Ru(2)	65.73(12)
C(7)-C(6)-Ru(2)	130.14(17)
C(6)-C(7)-P(2)	106.25(15)
C(6)-C(7)-H(7A)	110.5
P(2)-C(7)-H(7A)	110.5
C(6)-C(7)-H(7B)	110.5
P(2)-C(7)-H(7B)	110.5
H(7A)-C(7)-H(7B)	108.7
F(8C)-C(8)-F(8B)	108.5(2)
F(8C)-C(8)-F(8A)	107.0(2)
F(8B)-C(8)-F(8A)	107.1(2)
F(8C)-C(8)-P(2)	109.61(16)
F(8B)-C(8)-P(2)	112.92(16)
F(8A)-C(8)-P(2)	111.48(18)
F(9B)-C(9)-F(9C)	107.6(2)
F(9B)-C(9)-F(9A)	106.8(2)
F(9C)-C(9)-F(9A)	106.6(2)
F(9B)-C(9)-P(2)	111.91(19)
F(9C)-C(9)-P(2)	110.00(19)
F(9A)-C(9)-P(2)	113.64(17)
C(2)-C(10)-P(1)	104.94(15)

C(2)-C(10)-H(10A)	110.8
P(1)-C(10)-H(10A)	110.8
C(2)-C(10)-H(10B)	110.8
P(1)-C(10)-H(10B)	110.8
H(10A)-C(10)-H(10B)	108.8
F(11A)-C(11)-F(11C)	106.9(2)
F(11A)-C(11)-F(11B)	106.53(19)
F(11C)-C(11)-F(11B)	106.6(2)
F(11A)-C(11)-P(1)	112.63(17)
F(11C)-C(11)-P(1)	109.43(15)
F(11B)-C(11)-P(1)	114.35(19)
F(12C)-C(12)-F(12B)	106.8(2)
F(12C)-C(12)-F(12A)	107.1(2)
F(12B)-C(12)-F(12A)	106.5(2)
F(12C)-C(12)-P(1)	109.28(17)
F(12B)-C(12)-P(1)	113.19(19)
F(12A)-C(12)-P(1)	113.60(19)
C(18)-C(13)-C(14)	121.4(2)
C(18)-C(13)-H(13A)	119.3
C(14)-C(13)-H(13A)	119.3
C(15)-C(14)-C(13)	118.9(2)
C(15)-C(14)-C(22)	121.0(2)
C(13)-C(14)-C(22)	120.1(2)
C(16)-C(15)-C(14)	120.2(3)
C(16)-C(15)-H(15A)	119.9
C(14)-C(15)-H(15A)	119.9
C(17)-C(16)-C(15)	120.2(2)
C(17)-C(16)-H(16A)	119.9
C(15)-C(16)-H(16A)	119.9
C(16)-C(17)-C(18)	120.5(2)
C(16)-C(17)-H(17A)	119.7
C(18)-C(17)-H(17A)	119.7
C(13)-C(18)-C(17)	118.6(2)
C(13)-C(18)-C(19)	120.2(2)
C(17)-C(18)-C(19)	121.2(2)
C(18)-C(19)-P(3)	111.71(16)

C(18)-C(19)-H(19A)	109.3
P(3)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19B)	109.3
P(3)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	107.9
F(20A)-C(20)-F(20C)	107.9(2)
F(20A)-C(20)-F(20B)	106.9(2)
F(20C)-C(20)-F(20B)	106.5(2)
F(20A)-C(20)-P(3)	110.54(17)
F(20C)-C(20)-P(3)	110.20(18)
F(20B)-C(20)-P(3)	114.51(18)
F(21C)-C(21)-F(21A)	108.5(2)
F(21C)-C(21)-F(21B)	106.8(2)
F(21A)-C(21)-F(21B)	106.1(2)
F(21C)-C(21)-P(3)	112.72(19)
F(21A)-C(21)-P(3)	109.19(19)
F(21B)-C(21)-P(3)	113.30(19)
C(14)-C(22)-P(4)	111.98(17)
C(14)-C(22)-H(22A)	109.2
P(4)-C(22)-H(22A)	109.2
C(14)-C(22)-H(22B)	109.2
P(4)-C(22)-H(22B)	109.2
H(22A)-C(22)-H(22B)	107.9
F(23B)-C(23)-F(23A)	107.3(2)
F(23B)-C(23)-F(23C)	107.1(2)
F(23A)-C(23)-F(23C)	107.1(2)
F(23B)-C(23)-P(4)	108.95(18)
F(23A)-C(23)-P(4)	111.41(19)
F(23C)-C(23)-P(4)	114.70(19)
F(24B)-C(24)-F(24C)	107.5(2)
F(24B)-C(24)-F(24A)	107.1(2)
F(24C)-C(24)-F(24A)	106.4(2)
F(24B)-C(24)-P(4)	111.58(19)
F(24C)-C(24)-P(4)	109.29(17)
F(24A)-C(24)-P(4)	114.65(18)
C(25)-Ru(3)-P(6)	79.39(6)

C(25)-Ru(3)-P(5)	78.85(6)
P(6)-Ru(3)-P(5)	148.14(2)
C(25)-Ru(3)-P(7)	167.79(6)
P(6)-Ru(3)-P(7)	100.28(2)
P(5)-Ru(3)-P(7)	105.83(2)
C(25)-Ru(3)-Ru(4)	45.70(6)
P(6)-Ru(3)-Ru(4)	87.110(15)
P(5)-Ru(3)-Ru(4)	94.051(16)
P(7)-Ru(3)-Ru(4)	122.166(16)
C(25)-Ru(3)-H(3)	107.8(12)
P(6)-Ru(3)-H(3)	82.0(11)
P(5)-Ru(3)-H(3)	82.9(11)
P(7)-Ru(3)-H(3)	84.1(12)
Ru(4)-Ru(3)-H(3)	153.1(12)
C(25)-Ru(3)-H(3B)	79.4(9)
P(6)-Ru(3)-H(3B)	102.5(9)
P(5)-Ru(3)-H(3B)	96.1(9)
P(7)-Ru(3)-H(3B)	88.8(9)
Ru(4)-Ru(3)-H(3B)	34.5(9)
H(3)-Ru(3)-H(3B)	172.2(15)
C(31)-P(5)-C(33)	102.51(13)
C(31)-P(5)-C(32)	96.65(12)
C(33)-P(5)-C(32)	95.65(13)
C(31)-P(5)-Ru(3)	108.14(8)
C(33)-P(5)-Ru(3)	111.71(9)
C(32)-P(5)-Ru(3)	137.13(9)
C(34)-P(6)-C(36)	100.30(12)
C(34)-P(6)-C(35)	101.07(11)
C(36)-P(6)-C(35)	95.98(11)
C(34)-P(6)-Ru(3)	110.04(8)
C(36)-P(6)-Ru(3)	117.75(8)
C(35)-P(6)-Ru(3)	127.49(8)
C(46)-P(7)-C(47)	98.87(12)
C(46)-P(7)-C(48)	97.24(11)
C(47)-P(7)-C(48)	95.32(11)
C(46)-P(7)-Ru(3)	125.34(8)

C(47)-P(7)-Ru(3)	117.81(8)
C(48)-P(7)-Ru(3)	116.46(9)
C(25)-Ru(4)-C(26)	38.50(8)
C(25)-Ru(4)-P(8)	156.01(6)
C(26)-Ru(4)-P(8)	165.13(6)
C(25)-Ru(4)-C(27)	68.86(9)
C(26)-Ru(4)-C(27)	37.33(9)
P(8)-Ru(4)-C(27)	129.98(7)
C(25)-Ru(4)-C(28)	81.06(9)
C(26)-Ru(4)-C(28)	66.53(9)
P(8)-Ru(4)-C(28)	106.34(7)
C(27)-Ru(4)-C(28)	36.10(9)
C(25)-Ru(4)-C(30)	38.17(8)
C(26)-Ru(4)-C(30)	66.42(8)
P(8)-Ru(4)-C(30)	123.72(6)
C(27)-Ru(4)-C(30)	77.14(9)
C(28)-Ru(4)-C(30)	65.14(9)
C(25)-Ru(4)-C(29)	67.72(8)
C(26)-Ru(4)-C(29)	77.68(9)
P(8)-Ru(4)-C(29)	104.51(7)
C(27)-Ru(4)-C(29)	64.75(9)
C(28)-Ru(4)-C(29)	36.19(10)
C(30)-Ru(4)-C(29)	35.57(9)
C(25)-Ru(4)-Ru(3)	45.07(6)
C(26)-Ru(4)-Ru(3)	70.10(6)
P(8)-Ru(4)-Ru(3)	122.389(17)
C(27)-Ru(4)-Ru(3)	107.31(6)
C(28)-Ru(4)-Ru(3)	126.09(7)
C(30)-Ru(4)-Ru(3)	69.17(6)
C(29)-Ru(4)-Ru(3)	104.73(6)
C(25)-Ru(4)-H(3B)	83.2(10)
C(26)-Ru(4)-H(3B)	106.9(10)
P(8)-Ru(4)-H(3B)	83.9(10)
C(27)-Ru(4)-H(3B)	143.6(10)
C(28)-Ru(4)-H(3B)	160.5(10)
C(30)-Ru(4)-H(3B)	95.4(10)

C(29)-Ru(4)-H(3B)	125.9(10)
Ru(3)-Ru(4)-H(3B)	39.1(10)
C(25)-Ru(4)-H(4)	118.0(10)
C(26)-Ru(4)-H(4)	91.5(11)
P(8)-Ru(4)-H(4)	79.9(11)
C(27)-Ru(4)-H(4)	91.1(11)
C(28)-Ru(4)-H(4)	116.1(11)
C(30)-Ru(4)-H(4)	155.9(11)
C(29)-Ru(4)-H(4)	152.3(11)
Ru(3)-Ru(4)-H(4)	95.1(11)
H(3B)-Ru(4)-H(4)	81.6(15)
C(43)-P(8)-C(44)	100.04(12)
C(43)-P(8)-C(45)	98.68(12)
C(44)-P(8)-C(45)	96.03(13)
C(43)-P(8)-Ru(4)	124.02(8)
C(44)-P(8)-Ru(4)	117.77(9)
C(45)-P(8)-Ru(4)	115.25(10)
C(26)-C(25)-C(30)	116.8(2)
C(26)-C(25)-Ru(3)	117.19(15)
C(30)-C(25)-Ru(3)	116.11(16)
C(26)-C(25)-Ru(4)	72.91(13)
C(30)-C(25)-Ru(4)	76.32(13)
Ru(3)-C(25)-Ru(4)	89.24(8)
C(27)-C(26)-C(25)	120.9(2)
C(27)-C(26)-C(34)	120.0(2)
C(25)-C(26)-C(34)	118.7(2)
C(27)-C(26)-Ru(4)	73.27(14)
C(25)-C(26)-Ru(4)	68.59(12)
C(34)-C(26)-Ru(4)	125.19(15)
C(28)-C(27)-C(26)	120.5(2)
C(28)-C(27)-Ru(4)	72.86(14)
C(26)-C(27)-Ru(4)	69.39(13)
C(28)-C(27)-H(27A)	119.1
C(26)-C(27)-H(27A)	119.1
Ru(4)-C(27)-H(27A)	119.1
C(27)-C(28)-C(29)	119.5(2)

C(27)-C(28)-Ru(4)	71.04(13)
C(29)-C(28)-Ru(4)	73.14(13)
C(27)-C(28)-H(28A)	120.0
C(29)-C(28)-H(28A)	120.0
Ru(4)-C(28)-H(28A)	120.0
C(30)-C(29)-C(28)	120.7(2)
C(30)-C(29)-Ru(4)	71.50(13)
C(28)-C(29)-Ru(4)	70.68(13)
C(30)-C(29)-H(29A)	119.0
C(28)-C(29)-H(29A)	119.0
Ru(4)-C(29)-H(29A)	119.0
C(29)-C(30)-C(25)	120.5(2)
C(29)-C(30)-C(31)	121.4(2)
C(25)-C(30)-C(31)	117.8(2)
C(29)-C(30)-Ru(4)	72.93(14)
C(25)-C(30)-Ru(4)	65.50(11)
C(31)-C(30)-Ru(4)	130.39(17)
C(30)-C(31)-P(5)	106.15(15)
C(30)-C(31)-H(31A)	110.5
P(5)-C(31)-H(31A)	110.5
C(30)-C(31)-H(31B)	110.5
P(5)-C(31)-H(31B)	110.5
H(31A)-C(31)-H(31B)	108.7
F(32B)-C(32)-F(32C)	109.0(2)
F(32B)-C(32)-F(32A)	107.1(2)
F(32C)-C(32)-F(32A)	105.4(2)
F(32B)-C(32)-P(5)	114.19(19)
F(32C)-C(32)-P(5)	108.97(17)
F(32A)-C(32)-P(5)	111.8(2)
F(33A)-C(33)-F(33B)	107.1(2)
F(33A)-C(33)-F(33C)	107.7(2)
F(33B)-C(33)-F(33C)	106.4(2)
F(33A)-C(33)-P(5)	111.7(2)
F(33B)-C(33)-P(5)	109.90(19)
F(33C)-C(33)-P(5)	113.71(19)
C(26)-C(34)-P(6)	104.49(15)

C(26)-C(34)-H(34A)	110.9
P(6)-C(34)-H(34A)	110.9
C(26)-C(34)-H(34B)	110.9
P(6)-C(34)-H(34B)	110.9
H(34A)-C(34)-H(34B)	108.9
F(35B)-C(35)-F(35C)	107.2(2)
F(35B)-C(35)-F(35A)	106.38(19)
F(35C)-C(35)-F(35A)	107.23(19)
F(35B)-C(35)-P(6)	110.10(15)
F(35C)-C(35)-P(6)	110.83(16)
F(35A)-C(35)-P(6)	114.73(17)
F(36C)-C(36)-F(36A)	107.7(2)
F(36C)-C(36)-F(36B)	106.8(2)
F(36A)-C(36)-F(36B)	106.9(2)
F(36C)-C(36)-P(6)	112.94(19)
F(36A)-C(36)-P(6)	109.30(18)
F(36B)-C(36)-P(6)	112.88(17)
C(42)-C(37)-C(38)	121.1(2)
C(42)-C(37)-H(37A)	119.4
C(38)-C(37)-H(37A)	119.4
C(39)-C(38)-C(37)	119.3(2)
C(39)-C(38)-C(46)	121.2(2)
C(37)-C(38)-C(46)	119.4(2)
C(40)-C(39)-C(38)	119.4(2)
C(40)-C(39)-H(39A)	120.3
C(38)-C(39)-H(39A)	120.3
C(41)-C(40)-C(39)	120.8(2)
C(41)-C(40)-H(40A)	119.6
C(39)-C(40)-H(40A)	119.6
C(40)-C(41)-C(42)	120.3(2)
C(40)-C(41)-H(41A)	119.8
C(42)-C(41)-H(41A)	119.8
C(37)-C(42)-C(41)	118.8(2)
C(37)-C(42)-C(43)	120.3(2)
C(41)-C(42)-C(43)	120.9(2)
C(42)-C(43)-P(8)	112.78(15)

C(42)-C(43)-H(43A)	109.0
P(8)-C(43)-H(43A)	109.0
C(42)-C(43)-H(43B)	109.0
P(8)-C(43)-H(43B)	109.0
H(43A)-C(43)-H(43B)	107.8
F(44A)-C(44)-F(44B)	106.3(2)
F(44A)-C(44)-F(44C)	107.6(2)
F(44B)-C(44)-F(44C)	106.4(2)
F(44A)-C(44)-P(8)	111.4(2)
F(44B)-C(44)-P(8)	114.57(19)
F(44C)-C(44)-P(8)	110.16(19)
F(45A)-C(45)-F(45C)	106.9(3)
F(45A)-C(45)-F(45B)	106.3(2)
F(45C)-C(45)-F(45B)	108.2(3)
F(45A)-C(45)-P(8)	111.76(19)
F(45C)-C(45)-P(8)	109.47(18)
F(45B)-C(45)-P(8)	114.0(2)
C(38)-C(46)-P(7)	111.11(15)
C(38)-C(46)-H(46A)	109.4
P(7)-C(46)-H(46A)	109.4
C(38)-C(46)-H(46B)	109.4
P(7)-C(46)-H(46B)	109.4
H(46A)-C(46)-H(46B)	108.0
F(47B)-C(47)-F(47A)	106.9(2)
F(47B)-C(47)-F(47C)	108.0(2)
F(47A)-C(47)-F(47C)	106.6(2)
F(47B)-C(47)-P(7)	109.89(16)
F(47A)-C(47)-P(7)	115.17(18)
F(47C)-C(47)-P(7)	110.02(18)
F(48C)-C(48)-F(48B)	107.2(2)
F(48C)-C(48)-F(48A)	106.4(2)
F(48B)-C(48)-F(48A)	106.3(2)
F(48C)-C(48)-P(7)	113.00(17)
F(48B)-C(48)-P(7)	108.96(16)
F(48A)-C(48)-P(7)	114.53(18)
C(49)#1-C(49)-C(50)	130.5(11)

C(49)#1-C(49)-H(49A)	104.7
C(50)-C(49)-H(49A)	104.7
C(49)#1-C(49)-H(49C)	104.6
C(50)-C(49)-H(49C)	104.6
H(49A)-C(49)-H(49C)	105.7
C(49)-C(50)-C(51)	121.0(11)
C(49)-C(50)-H(50A)	107.1
C(51)-C(50)-H(50A)	107.1
C(49)-C(50)-H(50B)	107.1
C(51)-C(50)-H(50B)	107.1
H(50A)-C(50)-H(50B)	106.8
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table 1e. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Ru_2H_2(CO)_2(pcp)(\mu\text{-}H)(\mu\text{-}pcpH)$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	12(1)	15(1)	15(1)	-2(1)	1(1)	0(1)
P(1)	14(1)	23(1)	20(1)	-3(1)	3(1)	-3(1)
P(2)	13(1)	24(1)	16(1)	-2(1)	-1(1)	-1(1)
P(3)	18(1)	17(1)	22(1)	-3(1)	1(1)	3(1)
C(1)	18(1)	18(1)	19(1)	2(1)	2(1)	0(1)
Ru(2)	18(1)	15(1)	18(1)	-2(1)	4(1)	1(1)
P(4)	21(1)	23(1)	16(1)	-4(1)	3(1)	-2(1)
C(2)	25(1)	17(1)	20(1)	2(1)	3(1)	0(1)
C(3)	35(1)	16(1)	28(1)	-1(1)	4(1)	0(1)
C(4)	35(1)	17(1)	34(1)	-2(1)	8(1)	7(1)
C(5)	24(1)	23(1)	37(1)	2(1)	8(1)	9(1)
C(6)	19(1)	22(1)	26(1)	2(1)	1(1)	6(1)
C(7)	18(1)	32(1)	37(1)	-7(1)	-4(1)	6(1)
C(8)	20(1)	36(1)	28(1)	-5(1)	2(1)	-9(1)
F(8A)	16(1)	58(1)	46(1)	-4(1)	-5(1)	-7(1)
F(8B)	36(1)	36(1)	46(1)	-15(1)	-3(1)	-10(1)
F(8C)	36(1)	51(1)	29(1)	1(1)	8(1)	-15(1)
C(9)	21(1)	56(2)	22(1)	3(1)	-2(1)	-1(1)
F(9A)	27(1)	117(2)	24(1)	7(1)	-11(1)	-3(1)
F(9B)	47(1)	66(1)	26(1)	-17(1)	9(1)	0(1)
F(9C)	45(1)	66(1)	30(1)	21(1)	2(1)	-5(1)
C(10)	25(1)	22(1)	32(1)	-1(1)	6(1)	-6(1)
C(11)	16(1)	36(1)	28(1)	-8(1)	0(1)	-4(1)
F(11A)	27(1)	51(1)	46(1)	-13(1)	-7(1)	14(1)
F(11B)	26(1)	49(1)	68(1)	-4(1)	-13(1)	-16(1)
F(11C)	27(1)	78(1)	23(1)	-6(1)	-3(1)	-3(1)
C(12)	29(1)	38(1)	29(1)	-3(1)	11(1)	-6(1)
F(12A)	50(1)	86(2)	49(1)	-11(1)	25(1)	-41(1)
F(12B)	47(1)	57(1)	32(1)	-3(1)	17(1)	14(1)
F(12C)	50(1)	58(1)	27(1)	14(1)	9(1)	7(1)
C(13)	24(1)	23(1)	24(1)	2(1)	-6(1)	0(1)

C(14)	30(1)	30(1)	17(1)	1(1)	-5(1)	0(1)
C(15)	42(2)	36(1)	26(1)	8(1)	1(1)	-4(1)
C(16)	50(2)	29(1)	36(2)	11(1)	1(1)	-5(1)
C(17)	41(2)	22(1)	34(2)	4(1)	-3(1)	2(1)
C(18)	25(1)	24(1)	24(1)	2(1)	-7(1)	3(1)
C(19)	23(1)	24(1)	30(1)	0(1)	-4(1)	8(1)
C(20)	34(1)	22(1)	33(1)	-3(1)	-2(1)	-3(1)
F(20A)	31(1)	35(1)	42(1)	4(1)	1(1)	-12(1)
F(20B)	56(1)	18(1)	56(1)	2(1)	-8(1)	-2(1)
F(20C)	54(1)	36(1)	34(1)	-11(1)	-10(1)	-10(1)
C(21)	40(2)	28(1)	38(2)	-3(1)	14(1)	12(1)
F(21A)	29(1)	63(1)	70(1)	-7(1)	22(1)	5(1)
F(21B)	86(2)	32(1)	72(1)	0(1)	38(1)	28(1)
F(21C)	66(1)	58(1)	29(1)	-9(1)	16(1)	18(1)
C(22)	32(1)	31(1)	18(1)	-1(1)	0(1)	-2(1)
C(23)	40(1)	32(1)	28(1)	-8(1)	12(1)	1(1)
F(23A)	54(1)	61(1)	46(1)	-9(1)	9(1)	30(1)
F(23B)	67(1)	37(1)	44(1)	-21(1)	17(1)	-16(1)
F(23C)	60(1)	49(1)	30(1)	-10(1)	24(1)	-2(1)
C(24)	29(1)	37(1)	27(1)	0(1)	2(1)	-10(1)
F(24A)	48(1)	57(1)	32(1)	-3(1)	17(1)	-25(1)
F(24B)	30(1)	65(1)	85(2)	16(1)	-19(1)	-10(1)
F(24C)	59(1)	42(1)	32(1)	-13(1)	10(1)	-26(1)
Ru(3)	12(1)	14(1)	17(1)	0(1)	0(1)	-1(1)
P(5)	16(1)	18(1)	26(1)	3(1)	-2(1)	-4(1)
P(6)	15(1)	17(1)	23(1)	0(1)	-2(1)	-1(1)
P(7)	18(1)	19(1)	20(1)	-4(1)	2(1)	2(1)
Ru(4)	18(1)	18(1)	16(1)	0(1)	4(1)	2(1)
P(8)	18(1)	17(1)	23(1)	0(1)	1(1)	2(1)
C(25)	18(1)	19(1)	17(1)	4(1)	2(1)	-1(1)
C(26)	24(1)	25(1)	14(1)	1(1)	2(1)	-2(1)
C(27)	35(1)	29(1)	17(1)	-4(1)	6(1)	-1(1)
C(28)	36(1)	34(1)	21(1)	-3(1)	12(1)	6(1)
C(29)	22(1)	38(1)	22(1)	3(1)	9(1)	6(1)
C(30)	20(1)	28(1)	22(1)	4(1)	6(1)	-2(1)
C(31)	17(1)	34(1)	37(1)	-1(1)	6(1)	-5(1)

C(32)	24(1)	33(1)	40(2)	-2(1)	-6(1)	-8(1)
F(32A)	21(1)	47(1)	59(1)	2(1)	-6(1)	-16(1)
F(32B)	41(1)	56(1)	57(1)	-26(1)	-4(1)	-13(1)
F(32C)	37(1)	55(1)	44(1)	14(1)	-19(1)	-8(1)
C(33)	28(1)	25(1)	57(2)	17(1)	-1(1)	-7(1)
F(33A)	63(1)	22(1)	88(2)	5(1)	10(1)	9(1)
F(33B)	51(1)	52(1)	56(1)	34(1)	-8(1)	-4(1)
F(33C)	37(1)	41(1)	108(2)	37(1)	-5(1)	-18(1)
C(34)	24(1)	30(1)	18(1)	-2(1)	-3(1)	-3(1)
C(35)	16(1)	24(1)	32(1)	-4(1)	0(1)	-2(1)
F(35A)	28(1)	48(1)	42(1)	-8(1)	-6(1)	-18(1)
F(35B)	29(1)	25(1)	50(1)	11(1)	-2(1)	-6(1)
F(35C)	29(1)	31(1)	60(1)	-8(1)	20(1)	-2(1)
C(36)	29(1)	24(1)	42(2)	2(1)	-16(1)	0(1)
F(36A)	52(1)	40(1)	49(1)	23(1)	-9(1)	0(1)
F(36B)	49(1)	38(1)	75(1)	1(1)	-43(1)	4(1)
F(36C)	40(1)	28(1)	64(1)	1(1)	-4(1)	14(1)
C(37)	23(1)	22(1)	18(1)	2(1)	3(1)	-4(1)
C(38)	27(1)	24(1)	20(1)	1(1)	7(1)	-3(1)
C(39)	47(2)	28(1)	20(1)	1(1)	6(1)	-4(1)
C(40)	52(2)	36(1)	18(1)	5(1)	-2(1)	-7(1)
C(41)	34(1)	26(1)	31(1)	12(1)	-5(1)	-3(1)
C(42)	26(1)	19(1)	25(1)	5(1)	4(1)	-3(1)
C(43)	25(1)	17(1)	30(1)	6(1)	3(1)	1(1)
C(44)	30(1)	38(1)	32(1)	5(1)	-4(1)	-8(1)
F(44A)	39(1)	104(2)	55(1)	9(1)	2(1)	-40(1)
F(44B)	45(1)	64(1)	62(1)	22(1)	-30(1)	-9(1)
F(44C)	62(1)	51(1)	64(1)	-24(1)	-18(1)	-10(1)
C(45)	31(1)	28(1)	49(2)	-4(1)	7(1)	12(1)
F(45A)	41(1)	56(1)	83(2)	-13(1)	30(1)	12(1)
F(45B)	100(2)	54(1)	71(2)	4(1)	0(1)	56(1)
F(45C)	43(1)	49(1)	99(2)	-45(1)	7(1)	0(1)
C(46)	25(1)	27(1)	23(1)	-1(1)	8(1)	-1(1)
C(47)	31(1)	27(1)	26(1)	-8(1)	-2(1)	0(1)
F(47A)	51(1)	44(1)	23(1)	-12(1)	3(1)	0(1)
F(47B)	28(1)	42(1)	33(1)	-4(1)	-9(1)	3(1)

F(47C)	48(1)	26(1)	44(1)	-9(1)	-5(1)	-7(1)
C(48)	27(1)	27(1)	34(1)	-8(1)	1(1)	7(1)
F(48A)	48(1)	45(1)	39(1)	-13(1)	12(1)	19(1)
F(48B)	24(1)	50(1)	74(1)	-20(1)	-6(1)	13(1)
F(48C)	52(1)	26(1)	45(1)	-1(1)	1(1)	17(1)
C(49)	261(15)	190(8)	78(5)	-24(5)	-78(8)	20(10)
C(50)	227(13)	370(20)	100(7)	-38(10)	-3(9)	6(14)
C(51)	237(12)	141(7)	134(8)	37(6)	-2(8)	2(8)

Table 1f. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(H)(μ-H)(μ,η^6,κ^3-^{CF_3}PCP)Ru(H) (**1**).

	x	y	z	U(eq)
H(1)	2470(30)	3073(16)	4714(8)	34(8)
H(1B)	3280(30)	2834(17)	3846(8)	39(8)
H(2)	2460(30)	1988(19)	3509(10)	52(10)
H(3A)	2631	487	3767	32
H(4A)	4844	522	3637	34
H(5A)	6261	1369	3954	33
H(7A)	6495	2461	4340	35
H(7B)	6126	2092	4715	35
H(10A)	1111	994	4446	31
H(10B)	827	1127	4022	31
H(13A)	1792	3227	3408	29
H(15A)	4204	4255	2747	41
H(16A)	3573	5393	2974	46
H(17A)	2183	5443	3448	39
H(19A)	336	4010	3769	31
H(19B)	717	4855	3837	31
H(22A)	4014	2954	2708	32
H(22B)	2736	2587	2851	32
H(3)	9050(30)	4040(16)	1394(8)	37(8)
H(3B)	10360(30)	2361(17)	1634(9)	43(9)
H(4)	9690(30)	1397(16)	1331(8)	32(8)
H(27A)	9950	1332	563	32
H(28A)	12208	1203	671	36
H(29A)	13401	2170	974	33
H(31A)	12898	3870	1017	35
H(31B)	13360	3315	1334	35
H(34A)	7988	1947	726	29
H(34B)	8126	2720	517	29
H(37A)	8993	1587	1927	25
H(39A)	9040	2450	2932	38

H(40A)	10667	1620	3107	43
H(41A)	11568	850	2687	37
H(43A)	10224	340	1872	29
H(43B)	11523	283	2115	29
H(46A)	7521	2915	2482	30
H(46B)	7280	2459	2116	30
H(49A)	4103	-531	4954	215
H(49C)	4121	230	4748	215
H(50A)	3496	823	5216	280
H(50B)	3651	110	5462	280
H(51A)	1593	363	5343	257
H(51B)	1948	-412	5167	257
H(51C)	1792	306	4920	257

[(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (2)

Crystallographic data. The X-ray diffraction data were measured at 150 K on a Bruker SMART APEX II CCD area detector system equipped with a graphite monochromator and a Mo Kα fine-focus sealed tube operated at 1.5 kW power (50 kV, 30 mA). A colorless rectangular prism of [(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (**2**) of approximate dimensions 0.32 × 0.12 × 0.10 mm^3 was glued to a glass fiber using Paratone N oil. The detector was placed at a distance of 5.127 cm from the crystal during the data collection.

A series of narrow frames of data were collected with a scan width of 0.5° in ω or ϕ and an exposure time of 10 s per frame. The frames were integrated with the Bruker SAINT Software package[1] using a narrow-frame integration algorithm. The integration of the data using a triclinic unit cell yielded a total of 24941 reflections in the θ range of 1.86 to 29.57° of which 9083 were independent with $I \geq 2\sigma(I)$ (R_{int} = 0.0289). The data were corrected for absorption effects by the multi-scan method (SADABS). Crystallographic data collection parameters and refinement data are collected below in Table 1. The structure was solved by the direct methods using the Bruker SHELXTL (V. 6.14) Software Package.[1] All non-hydrogen atoms were located in successive Fourier maps and refined anisotropically. As the [(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (**2**) complex molecule is located on a two-fold symmetry axis, the asymmetric unit consists of a half of the molecule. All non-hydrogen atoms are located on general positions and well ordered. The hydride hydrogen atom was also located in the Fourier maps and refined isotropically. The rest of the hydrogen atoms were placed in calculated positions and refined isotropically. The final refinement parameters are R_1 = 0.0448 and wR_2 = 0.1223 for data with $F > 4\sigma(F)$ giving the data to parameter ratio of 19. The refinement data for all data are R_1 = 0.0558 and wR_2 = 0.1307.

Table 2a. Crystallographic Data for $[(^{CF_3}PCP)Ru(H)]_2(\mu\text{-}^{CF_3}PCP)_2$ (**2**)

compound	$[(^{CF_3}PCP)Ru(H)]_2(\mu\text{-}^{CF_3}PCP)_2$ (**2**)		color
chemical formula	$C_{48}H_{32}F_{48}P_8Ru_2$	fw	1970.64
T, K	150(2)	λ, Å	0.71073
space group	$P\bar{1}$	*a*, Å	9.7406(3)
b, Å	10.9574(3)	*c*, Å	15.5252(4)
α, °	91.681(1)	β, °	97.886(1)
γ, °	93.194(2)	*V*, Å^3	1637.66(8)
Z	1	D_{calc}, Mg m^{-3}	1.998
μ, mm^{-1}	0.830	goodness of fit	1.044
$R1[I > 2\sigma(I)]$[a]	0.0448	$wR2[I > 2\sigma(I)]$[b]	0.1223

[a] $R1 = \sum||F_o| - |F_c||/\sum|F_o|$; [b] $_wR2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2]\}^{1/2}$

Table 2b. Crystal data and structure refinement for $[(^{CF_3}PCP)Ru(H)]_2(\mu\text{-}^{CF_3}PCP)_2$ (**2**).

Identification code	bcg10	
Empirical formula	C48 H32 F48 P8 Ru2	
Formula weight	1970.64	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.7406(3) Å	□= 91.681(1)°.
	b = 10.9574(3) Å	□= 97.886(1)°.
	c = 15.5252(4) Å	□ = 93.194(2)°.
Volume	1637.66(8) $Å^3$	
Z	1	
Density (calculated)	1.998 Mg/m^3	
Absorption coefficient	0.831 mm^{-1}	
F(000)	960	
Crystal size	0.32 x 0.12 x 0.10 mm^3	
Theta range for data collection	1.86 to 29.57°.	
Index ranges	-13<=h<=13, -15<=k<=15, -21<=l<=21	
Reflections collected	24941	
Independent reflections	9083 [R(int) = 0.0289]	
Completeness to theta = 29.57°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.6254	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9083 / 0 / 482	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1223	
R indices (all data)	R1 = 0.0558, wR2 = 0.1307	
Largest diff. peak and hole	1.562 and -0.814 e.$Å^{-3}$	

Table 2c. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	4119(1)	2340(1)	2292(1)	26(1)
P(1)	2206(1)	2860(1)	1395(1)	31(1)
P(2)	5913(1)	1096(1)	2334(1)	38(1)
P(3)	3198(1)	2049(1)	3629(1)	31(1)
P(4)	5363(1)	4209(1)	2641(1)	33(1)
C(1)	3114(3)	574(3)	1799(2)	31(1)
C(2)	3809(4)	-516(3)	1858(3)	41(1)
C(3)	3170(5)	-1623(4)	1515(3)	54(1)
C(4)	1818(5)	-1683(4)	1112(3)	59(1)
C(5)	1094(4)	-645(3)	1053(3)	47(1)
C(6)	1732(3)	472(3)	1385(2)	33(1)
C(7)	916(3)	1599(3)	1316(2)	37(1)
C(8)	1010(5)	4165(4)	1420(3)	50(1)
F(8A)	674(3)	4290(3)	2218(2)	72(1)
F(8B)	1587(3)	5225(2)	1221(2)	75(1)
F(8C)	-174(3)	3969(3)	885(2)	71(1)
C(9)	2457(4)	2963(4)	205(2)	47(1)
F(9A)	1325(4)	3145(5)	-305(2)	106(1)
F(9B)	2853(5)	1921(4)	-81(2)	108(1)
F(9C)	3387(5)	3783(4)	79(2)	116(2)
C(10)	5266(4)	-486(3)	2337(3)	49(1)
C(11)	6749(5)	1079(5)	1300(3)	58(1)
F(11A)	7379(3)	2131(3)	1168(2)	73(1)
F(11B)	5795(3)	792(4)	624(2)	88(1)
F(11C)	7702(3)	239(3)	1317(3)	89(1)
C(12)	7621(4)	1038(4)	3088(3)	57(1)
F(12A)	7515(3)	1376(4)	3906(2)	82(1)
F(12B)	8608(2)	1822(3)	2863(2)	64(1)
F(12C)	8123(3)	-53(3)	3101(3)	105(1)
C(13)	2246(4)	521(3)	3778(2)	43(1)

F(13A)	1093(3)	394(2)	3210(2)	57(1)
F(13B)	1886(4)	396(3)	4568(2)	71(1)
F(13C)	3008(3)	-421(2)	3641(2)	58(1)
C(14)	4504(4)	1956(4)	4638(2)	41(1)
F(14A)	5357(3)	2964(2)	4736(2)	60(1)
F(14B)	3996(3)	1820(3)	5381(1)	60(1)
F(14C)	5279(3)	1012(2)	4547(2)	56(1)
C(15)	1910(3)	3104(3)	3958(2)	38(1)
C(16)	1678(3)	3335(3)	4897(2)	37(1)
C(17)	693(4)	2634(4)	5276(3)	54(1)
C(18)	477(5)	2903(5)	6118(3)	63(1)
C(19)	1193(4)	3878(4)	6590(3)	54(1)
C(20)	2172(4)	4605(3)	6227(2)	39(1)
C(21)	2384(3)	4324(3)	5377(2)	36(1)
C(22)	2885(4)	5739(3)	6703(2)	40(1)
C(23)	4526(4)	5479(3)	3177(2)	41(1)
F(23A)	5162(3)	6584(2)	3181(2)	57(1)
F(23B)	4485(3)	5204(2)	4008(1)	51(1)
F(23C)	3221(3)	5581(2)	2811(2)	62(1)
C(24)	5767(5)	5098(4)	1671(2)	49(1)
F(24A)	6337(4)	4399(3)	1138(2)	76(1)
F(24B)	6602(4)	6092(3)	1871(2)	78(1)
F(24C)	4617(3)	5483(3)	1232(2)	70(1)

Table 2d. Bond lengths [Å] and angles [°] for [(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (**2**).

Ru(1)-C(1)	2.188(3)
Ru(1)-P(2)	2.2708(9)
Ru(1)-P(1)	2.2776(9)
Ru(1)-P(4)	2.3309(8)
Ru(1)-P(3)	2.3940(8)
Ru(1)-Ru(1)#1	9.9827(5)
Ru(1)-H(1)	1.47(4)
P(1)-C(7)	1.806(3)
P(1)-C(8)	1.897(4)
P(1)-C(9)	1.902(4)
P(2)-C(10)	1.812(4)
P(2)-C(11)	1.896(4)
P(2)-C(12)	1.904(4)
P(3)-C(15)	1.863(4)
P(3)-C(14)	1.887(4)
P(3)-C(13)	1.904(4)
P(4)-C(22)#1	1.861(4)
P(4)-C(23)	1.881(4)
P(4)-C(24)	1.891(4)
C(1)-C(2)	1.405(5)
C(1)-C(6)	1.407(4)
C(2)-C(3)	1.390(5)
C(2)-C(10)	1.507(5)
C(3)-C(4)	1.375(6)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.370(6)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.392(5)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.504(5)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-F(8B)	1.324(5)
C(8)-F(8A)	1.329(5)

C(8)-F(8C)	1.329(5)
C(9)-F(9C)	1.278(5)
C(9)-F(9A)	1.295(5)
C(9)-F(9B)	1.311(5)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-F(11A)	1.310(6)
C(11)-F(11B)	1.322(6)
C(11)-F(11C)	1.340(5)
C(12)-F(12C)	1.316(5)
C(12)-F(12A)	1.332(6)
C(12)-F(12B)	1.342(5)
C(13)-F(13A)	1.328(5)
C(13)-F(13B)	1.329(4)
C(13)-F(13C)	1.333(5)
C(14)-F(14B)	1.325(4)
C(14)-F(14C)	1.330(5)
C(14)-F(14A)	1.337(4)
C(15)-C(16)	1.523(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(21)	1.389(4)
C(16)-C(17)	1.399(5)
C(17)-C(18)	1.378(6)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.377(6)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.397(5)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.392(5)
C(20)-C(22)	1.511(5)
C(21)-H(21A)	0.9300
C(22)-P(4)#1	1.861(4)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-F(23A)	1.328(4)

C(23)-F(23C)	1.331(4)
C(23)-F(23B)	1.339(4)
C(24)-F(24A)	1.311(5)
C(24)-F(24B)	1.326(4)
C(24)-F(24C)	1.326(6)

C(1)-Ru(1)-P(2)	76.54(9)
C(1)-Ru(1)-P(1)	76.43(9)
P(2)-Ru(1)-P(1)	141.10(3)
C(1)-Ru(1)-P(4)	171.55(8)
P(2)-Ru(1)-P(4)	99.43(3)
P(1)-Ru(1)-P(4)	103.34(3)
C(1)-Ru(1)-P(3)	89.07(8)
P(2)-Ru(1)-P(3)	105.41(3)
P(1)-Ru(1)-P(3)	101.59(3)
P(4)-Ru(1)-P(3)	99.20(3)
C(1)-Ru(1)-Ru(1)#1	141.05(8)
P(2)-Ru(1)-Ru(1)#1	106.79(2)
P(1)-Ru(1)-Ru(1)#1	111.85(2)
P(4)-Ru(1)-Ru(1)#1	47.07(2)
P(3)-Ru(1)-Ru(1)#1	52.220(19)
C(1)-Ru(1)-H(1)	81.6(14)
P(2)-Ru(1)-H(1)	84.2(15)
P(1)-Ru(1)-H(1)	64.5(15)
P(4)-Ru(1)-H(1)	90.7(14)
P(3)-Ru(1)-H(1)	164.7(15)
Ru(1)#1-Ru(1)-H(1)	137.1(14)
C(7)-P(1)-C(8)	98.61(18)
C(7)-P(1)-C(9)	100.05(17)
C(8)-P(1)-C(9)	96.80(19)
C(7)-P(1)-Ru(1)	108.35(12)
C(8)-P(1)-Ru(1)	133.27(13)
C(9)-P(1)-Ru(1)	114.49(14)
C(10)-P(2)-C(11)	100.6(2)
C(10)-P(2)-C(12)	100.2(2)
C(11)-P(2)-C(12)	94.5(2)

C(10)-P(2)-Ru(1)	109.75(13)
C(11)-P(2)-Ru(1)	113.62(16)
C(12)-P(2)-Ru(1)	133.12(15)
C(15)-P(3)-C(14)	104.42(16)
C(15)-P(3)-C(13)	99.57(17)
C(14)-P(3)-C(13)	94.71(17)
C(15)-P(3)-Ru(1)	119.63(12)
C(14)-P(3)-Ru(1)	116.43(12)
C(13)-P(3)-Ru(1)	118.03(11)
C(22)#1-P(4)-C(23)	101.81(16)
C(22)#1-P(4)-C(24)	100.31(18)
C(23)-P(4)-C(24)	96.14(18)
C(22)#1-P(4)-Ru(1)	120.16(12)
C(23)-P(4)-Ru(1)	119.53(12)
C(24)-P(4)-Ru(1)	114.72(12)
C(2)-C(1)-C(6)	116.1(3)
C(2)-C(1)-Ru(1)	122.4(2)
C(6)-C(1)-Ru(1)	121.5(2)
C(3)-C(2)-C(1)	121.6(3)
C(3)-C(2)-C(10)	119.4(3)
C(1)-C(2)-C(10)	118.9(3)
C(4)-C(3)-C(2)	120.4(4)
C(4)-C(3)-H(3A)	119.8
C(2)-C(3)-H(3A)	119.8
C(5)-C(4)-C(3)	119.8(3)
C(5)-C(4)-H(4A)	120.1
C(3)-C(4)-H(4A)	120.1
C(4)-C(5)-C(6)	120.2(4)
C(4)-C(5)-H(5A)	119.9
C(6)-C(5)-H(5A)	119.9
C(5)-C(6)-C(1)	121.9(3)
C(5)-C(6)-C(7)	119.3(3)
C(1)-C(6)-C(7)	118.9(3)
C(6)-C(7)-P(1)	104.9(2)
C(6)-C(7)-H(7A)	110.8
P(1)-C(7)-H(7A)	110.8

C(6)-C(7)-H(7B)	110.8
P(1)-C(7)-H(7B)	110.8
H(7A)-C(7)-H(7B)	108.8
F(8B)-C(8)-F(8A)	107.9(3)
F(8B)-C(8)-F(8C)	107.1(3)
F(8A)-C(8)-F(8C)	106.7(4)
F(8B)-C(8)-P(1)	113.0(3)
F(8A)-C(8)-P(1)	108.7(3)
F(8C)-C(8)-P(1)	113.1(3)
F(9C)-C(9)-F(9A)	108.6(4)
F(9C)-C(9)-F(9B)	106.7(4)
F(9A)-C(9)-F(9B)	104.5(4)
F(9C)-C(9)-P(1)	113.0(3)
F(9A)-C(9)-P(1)	113.4(3)
F(9B)-C(9)-P(1)	110.0(3)
C(2)-C(10)-P(2)	105.0(3)
C(2)-C(10)-H(10A)	110.7
P(2)-C(10)-H(10A)	110.7
C(2)-C(10)-H(10B)	110.7
P(2)-C(10)-H(10B)	110.7
H(10A)-C(10)-H(10B)	108.8
F(11A)-C(11)-F(11B)	108.5(4)
F(11A)-C(11)-F(11C)	106.8(4)
F(11B)-C(11)-F(11C)	107.2(4)
F(11A)-C(11)-P(2)	112.9(3)
F(11B)-C(11)-P(2)	109.7(3)
F(11C)-C(11)-P(2)	111.6(4)
F(12C)-C(12)-F(12A)	107.4(5)
F(12C)-C(12)-F(12B)	107.0(4)
F(12A)-C(12)-F(12B)	104.3(4)
F(12C)-C(12)-P(2)	113.2(3)
F(12A)-C(12)-P(2)	112.5(3)
F(12B)-C(12)-P(2)	111.9(3)
F(13A)-C(13)-F(13B)	107.5(3)
F(13A)-C(13)-F(13C)	107.5(3)
F(13B)-C(13)-F(13C)	106.2(3)

F(13A)-C(13)-P(3)	109.4(3)
F(13B)-C(13)-P(3)	113.9(3)
F(13C)-C(13)-P(3)	112.1(3)
F(14B)-C(14)-F(14C)	106.5(3)
F(14B)-C(14)-F(14A)	107.1(3)
F(14C)-C(14)-F(14A)	107.2(3)
F(14B)-C(14)-P(3)	116.5(3)
F(14C)-C(14)-P(3)	109.4(2)
F(14A)-C(14)-P(3)	109.7(2)
C(16)-C(15)-P(3)	123.5(3)
C(16)-C(15)-H(15A)	106.4
P(3)-C(15)-H(15A)	106.4
C(16)-C(15)-H(15B)	106.4
P(3)-C(15)-H(15B)	106.4
H(15A)-C(15)-H(15B)	106.5
C(21)-C(16)-C(17)	118.5(3)
C(21)-C(16)-C(15)	119.6(3)
C(17)-C(16)-C(15)	121.8(3)
C(18)-C(17)-C(16)	120.0(3)
C(18)-C(17)-H(17A)	120.0
C(16)-C(17)-H(17A)	120.0
C(19)-C(18)-C(17)	120.9(4)
C(19)-C(18)-H(18A)	119.5
C(17)-C(18)-H(18A)	119.5
C(18)-C(19)-C(20)	120.4(3)
C(18)-C(19)-H(19A)	119.8
C(20)-C(19)-H(19A)	119.8
C(21)-C(20)-C(19)	118.1(3)
C(21)-C(20)-C(22)	120.2(3)
C(19)-C(20)-C(22)	121.4(3)
C(16)-C(21)-C(20)	122.0(3)
C(16)-C(21)-H(21A)	119.0
C(20)-C(21)-H(21A)	119.0
C(20)-C(22)-P(4)#1	124.2(3)
C(20)-C(22)-H(22A)	106.3
P(4)#1-C(22)-H(22A)	106.3

C(20)-C(22)-H(22B)	106.3
P(4)#1-C(22)-H(22B)	106.3
H(22A)-C(22)-H(22B)	106.4
F(23A)-C(23)-F(23C)	106.6(3)
F(23A)-C(23)-F(23B)	107.1(3)
F(23C)-C(23)-F(23B)	107.1(3)
F(23A)-C(23)-P(4)	116.0(3)
F(23C)-C(23)-P(4)	111.6(2)
F(23B)-C(23)-P(4)	108.1(2)
F(24A)-C(24)-F(24B)	108.0(4)
F(24A)-C(24)-F(24C)	107.5(3)
F(24B)-C(24)-F(24C)	105.6(4)
F(24A)-C(24)-P(4)	110.2(3)
F(24B)-C(24)-P(4)	114.4(3)
F(24C)-C(24)-P(4)	110.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 2e. Anisotropic displacement parameters (Å^2 × 10^3) for [(^{CF_3}PCP)Ru(H)]$_2$(μ-^{CF_3}PCP)$_2$ (**2**). The anisotropic displacement factor exponent takes the form: -2□^{2}[h^2 a*^{2}U^{11} + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	28(1)	24(1)	26(1)	-1(1)	2(1)	1(1)
P(1)	34(1)	29(1)	29(1)	2(1)	0(1)	3(1)
P(2)	26(1)	35(1)	53(1)	-3(1)	2(1)	3(1)
P(3)	34(1)	31(1)	26(1)	1(1)	2(1)	-2(1)
P(4)	40(1)	29(1)	30(1)	-2(1)	6(1)	-5(1)
C(1)	31(2)	27(1)	34(2)	-2(1)	2(1)	1(1)
C(2)	38(2)	32(2)	52(2)	-2(1)	2(2)	2(1)
C(3)	55(2)	28(2)	77(3)	-4(2)	1(2)	4(2)
C(4)	62(3)	30(2)	77(3)	-9(2)	-10(2)	-7(2)
C(5)	42(2)	36(2)	57(2)	-2(2)	-10(2)	-7(2)
C(6)	35(2)	30(2)	33(2)	1(1)	1(1)	-1(1)
C(7)	30(2)	38(2)	41(2)	3(1)	0(1)	0(1)
C(8)	56(2)	36(2)	55(2)	1(2)	-9(2)	14(2)
F(8A)	75(2)	79(2)	67(2)	-5(1)	11(1)	44(2)
F(8B)	84(2)	34(1)	100(2)	14(1)	-14(2)	8(1)
F(8C)	57(2)	60(2)	88(2)	-2(1)	-26(1)	24(1)
C(9)	57(2)	52(2)	29(2)	4(1)	-2(2)	-5(2)
F(9A)	81(2)	191(4)	42(2)	25(2)	-14(2)	11(3)
F(9B)	194(4)	92(3)	48(2)	-3(2)	39(2)	37(3)
F(9C)	152(4)	142(3)	42(2)	12(2)	14(2)	-86(3)
C(10)	36(2)	32(2)	76(3)	2(2)	-2(2)	4(1)
C(11)	43(2)	64(3)	69(3)	-14(2)	18(2)	10(2)
F(11A)	70(2)	68(2)	89(2)	3(2)	38(2)	0(1)
F(11B)	68(2)	129(3)	64(2)	-40(2)	14(2)	-2(2)
F(11C)	66(2)	77(2)	132(3)	-16(2)	44(2)	25(2)
C(12)	29(2)	54(2)	85(3)	1(2)	-3(2)	8(2)
F(12A)	46(2)	129(3)	66(2)	18(2)	-9(1)	4(2)
F(12B)	31(1)	72(2)	87(2)	-10(1)	5(1)	-5(1)
F(12C)	48(2)	57(2)	198(4)	1(2)	-31(2)	21(1)
C(13)	51(2)	38(2)	39(2)	3(1)	8(2)	-10(2)
F(13A)	44(1)	56(2)	67(2)	6(1)	-2(1)	-15(1)

F(13B)	107(2)	61(2)	48(1)	8(1)	30(1)	-22(2)
F(13C)	72(2)	35(1)	66(2)	7(1)	9(1)	-1(1)
C(14)	47(2)	45(2)	30(2)	1(1)	-1(1)	1(2)
F(14A)	65(2)	55(1)	50(1)	0(1)	-15(1)	-16(1)
F(14B)	63(2)	87(2)	30(1)	9(1)	6(1)	11(1)
F(14C)	55(1)	62(2)	50(1)	8(1)	0(1)	19(1)
C(15)	32(2)	43(2)	35(2)	-5(1)	1(1)	0(1)
C(16)	31(2)	44(2)	36(2)	-7(1)	4(1)	-3(1)
C(17)	45(2)	61(3)	56(2)	-19(2)	15(2)	-22(2)
C(18)	57(3)	71(3)	62(3)	-16(2)	30(2)	-33(2)
C(19)	49(2)	64(3)	49(2)	-15(2)	22(2)	-18(2)
C(20)	33(2)	42(2)	41(2)	-7(1)	7(1)	-6(1)
C(21)	30(2)	40(2)	38(2)	-3(1)	6(1)	-4(1)
C(22)	41(2)	37(2)	41(2)	-7(1)	9(1)	-4(1)
C(23)	44(2)	34(2)	42(2)	-4(1)	2(1)	0(1)
F(23A)	72(2)	31(1)	68(2)	-5(1)	7(1)	-6(1)
F(23B)	59(1)	53(1)	43(1)	-8(1)	15(1)	0(1)
F(23C)	51(1)	54(1)	74(2)	-16(1)	-11(1)	14(1)
C(24)	71(3)	39(2)	36(2)	3(1)	10(2)	-15(2)
F(24A)	117(3)	58(2)	63(2)	10(1)	52(2)	4(2)
F(24B)	110(2)	66(2)	53(2)	9(1)	10(2)	-49(2)
F(24C)	89(2)	64(2)	54(2)	21(1)	1(1)	1(2)

Table 2f. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[(^{CF_3}PCP)Ru(H)]_2(\mu\text{-}^{CF_3}PCP)_2$ (**2**).

	x	y	z	U(eq)
H(1)	4300(40)	2450(30)	1370(20)	34(9)
H(3A)	3660	-2329	1557	65
H(4A)	1396	-2426	881	71
H(5A)	175	-686	791	56
H(7A)	355	1654	1785	44
H(7B)	311	1590	765	44
H(10A)	5835	-1015	2042	59
H(10B)	5263	-750	2928	59
H(15A)	2143	3896	3735	45
H(15B)	1017	2820	3640	45
H(17A)	183	1986	4960	65
H(18A)	-162	2418	6371	76
H(19A)	1023	4054	7154	64
H(21A)	3017	4812	5123	43
H(22A)	2257	6022	7090	48
H(22B)	2929	6354	6269	48

(^{CF_3}PCP)Ru(cod)H (3)

Crystallographic data. The X-ray diffraction data were measured at 150 K on a Bruker SMART APEX II CCD area detector system equipped with a graphite monochromator and a Mo Kα fine-focus sealed tube operated at 1.5 kW power (50 kV, 30 mA). A colorless rectangular prism of (^{CF_3}PCP)Ru(cod)H (**3**) of approximate dimensions 0.32 × 0.12 × 0.10 mm^3 was glued to a glass fiber using Paratone N oil. The detector was placed at a distance of 5.127 cm from the crystal during the data collection.

A series of narrow frames of data were collected with a scan width of 0.5° in ω or ϕ and an exposure time of 10 s per frame. The frames were integrated with the Bruker SAINT Software package[1] using a narrow-frame integration algorithm. The integration of the data using a monoclinic unit cell yielded a total of 27653 reflections in the θ range of 1.89 to 33.73° of which 9161 were independent with $I \geq 2\sigma(I)$ (R_{int} = 0.0285). The data were corrected for absorption effects by the multi-scan method (SADABS). Crystallographic data collection parameters and refinement data are collected below in Table 1. The structure was solved by the direct methods using the Bruker SHELXTL (V. 6.14) Software Package.[1] All non-hydrogen atoms were located in successive Fourier maps and refined anisotropically. The asymmetric unit consists of a (^{CF_3}PCP)Ru(cod)H (**3**) molecule. All non-hydrogen atoms are located on general positions and well ordered. All of the hydrogen atoms were also located in the Fourier maps, and were refined isotropically. The final refinement parameters are R_1 = 0.0425 and wR_2 = 0.0979 for data with $F > 4\sigma(F)$ giving the data to parameter ratio of 23. The refinement data for all data are R_1 = 0.0589 and wR_2 = 0.1069.

Table 3a. Crystallographic Data for (^{CF_3}PCP)Ru(cod)H (**3**)

compound	(^{CF_3}PCP)Ru(cod)H (**3**)	color	colorless
chemical formula	$C_{20}H_{20}F_{12}P_2Ru$	fw	651.37
T, K	150(2)	λ, Å	0.71073
space group	$P2_1/c$	a, Å	9.5162(1)
b, Å	18.0336(2)	c, Å	13.7718(2)
β, °	103.584(1)	V, Å^3	2297.28(5)
Z	4	D_{calc}, Mg m^{-3}	1.883
μ, mm^{-1}	0.926	goodness of fit	1.031
$R1[I > 2\sigma(I)]$[a]	0.0425	$wR2[I > 2\sigma(I)]$[b]	0.0979

[a] $R1 = \sum||F_o| - |F_c||/\sum|F_o|$; [b] $_wR2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2]\}^{1/2}$

Table 3b. Crystal data and structure refinement for (^{CF_3}PCP)Ru(cod)H (**3**).

Identification code	bcg11	
Empirical formula	C20 H20 F12 P2 Ru	
Formula weight	651.37	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.5162(1) Å	α= 90°.
	b = 18.0336(2) Å	β= 103.584(1)°.
	c = 13.7718(2) Å	γ = 90°.
Volume	2297.28(5) Å^3	
Z	4	
Density (calculated)	1.883 Mg/m^3	
Absorption coefficient	0.926 mm^{-1}	
F(000)	1288	
Crystal size	0.38 × 0.24 × 0.14 mm^3	
Theta range for data collection	1.89 to 33.73°.	
Index ranges	-14<=h<=14, -27<=k<=28, -21<=l<=20	
Reflections collected	27653	
Independent reflections	9161 [R(int) = 0.0285]	
Completeness to theta = 33.73°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8812 and 0.7215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9161 / 0 / 396	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.0979	
R indices (all data)	R1 = 0.0589, wR2 = 0.1069	
Largest diff. peak and hole	1.569 and -0.660 e.Å^{-3}	

Table 3c. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for RuH(pcp)(cod). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3023(1)	679(1)	2898(1)	19(1)
P(1)	2326(1)	1808(1)	3268(1)	25(1)
P(2)	2031(1)	-448(1)	2882(1)	21(1)
C(1)	900(2)	822(1)	1938(2)	23(1)
C(13)	3863(3)	376(2)	1528(2)	31(1)
C(14)	3840(3)	1142(2)	1594(2)	31(1)
C(17)	5387(3)	971(2)	3647(2)	36(1)
C(18)	5304(3)	212(2)	3588(2)	36(1)
C(2)	48(2)	215(1)	1493(2)	25(1)
C(3)	-1286(3)	312(2)	826(2)	33(1)
C(4)	-1813(3)	1012(2)	560(2)	40(1)
C(5)	-1017(3)	1621(2)	980(2)	38(1)
C(6)	310(3)	1530(2)	1662(2)	30(1)
C(7)	1130(4)	2198(2)	2164(2)	39(1)
C(8)	1142(4)	1834(2)	4195(3)	46(1)
F(8A)	62(3)	1363(1)	3941(2)	76(1)
F(8B)	1866(3)	1661(2)	5100(2)	90(1)
F(8C)	559(4)	2491(1)	4273(2)	94(1)
C(9)	3424(4)	2643(2)	3813(3)	47(1)
F(9A)	4316(4)	2824(2)	3264(3)	141(2)
F(9B)	2661(3)	3254(1)	3851(2)	75(1)
F(9C)	4182(3)	2526(2)	4728(2)	99(1)
C(10)	593(3)	-558(2)	1766(2)	31(1)
C(11)	2892(3)	-1393(2)	2910(3)	40(1)
F(11A)	3531(2)	-1428(1)	2130(2)	58(1)
F(11B)	1979(2)	-1959(1)	2734(2)	59(1)
F(11C)	3859(3)	-1526(1)	3731(2)	67(1)
C(12)	1021(3)	-640(2)	3886(2)	28(1)
F(12A)	-4(2)	-146(1)	3844(2)	57(1)
F(12B)	1858(2)	-609(2)	4790(2)	62(1)
F(12C)	355(3)	-1294(1)	3785(2)	72(1)

C(15)	5191(4)	1601(2)	1939(3)	41(1)
C(16)	6109(4)	1419(2)	2961(3)	50(1)
C(19)	5898(3)	-240(2)	2873(3)	51(1)
C(20)	5273(4)	-63(2)	1774(3)	44(1)

Table 3d. Bond lengths [Å] and angles [°] for (^{CF_3}PCP)Ru(cod)H (**3**).

Ru(1)-C(1)	2.154(2)
Ru(1)-P(1)	2.2360(6)
Ru(1)-P(2)	2.2392(6)
Ru(1)-C(14)	2.276(2)
Ru(1)-C(13)	2.282(2)
Ru(1)-C(17)	2.305(3)
Ru(1)-C(18)	2.314(3)
Ru(1)-H(1)	1.53(4)
P(1)-C(7)	1.813(3)
P(1)-C(9)	1.886(3)
P(1)-C(8)	1.892(3)
P(2)-C(10)	1.813(3)
P(2)-C(11)	1.888(3)
P(2)-C(12)	1.891(2)
C(1)-C(6)	1.412(3)
C(1)-C(2)	1.413(3)
C(13)-C(14)	1.385(4)
C(13)-C(20)	1.526(4)
C(13)-H(13)	0.97(3)
C(14)-C(15)	1.508(4)
C(14)-H(14)	0.87(3)
C(17)-C(18)	1.372(5)
C(17)-C(16)	1.523(5)
C(17)-H(17)	0.92(4)
C(18)-C(19)	1.489(5)
C(18)-H(18)	0.95(4)
C(2)-C(3)	1.392(3)
C(2)-C(10)	1.503(4)
C(3)-C(4)	1.377(5)
C(3)-H(3)	0.94(3)
C(4)-C(5)	1.381(5)
C(4)-H(4)	0.97(4)
C(5)-C(6)	1.394(4)
C(5)-H(5)	0.83(4)

C(6)-C(7)	1.512(4)
C(7)-H(7A)	1.00(4)
C(7)-H(7B)	0.87(5)
C(8)-F(8B)	1.312(5)
C(8)-F(8A)	1.315(4)
C(8)-F(8C)	1.323(4)
C(9)-F(9A)	1.304(4)
C(9)-F(9C)	1.314(5)
C(9)-F(9B)	1.328(4)
C(10)-H(10A)	0.95(3)
C(10)-H(10B)	0.90(4)
C(11)-F(11C)	1.302(4)
C(11)-F(11B)	1.325(3)
C(11)-F(11A)	1.354(4)
C(12)-F(12B)	1.312(3)
C(12)-F(12A)	1.313(3)
C(12)-F(12C)	1.330(3)
C(15)-C(16)	1.508(5)
C(15)-H(15A)	0.94(4)
C(15)-H(15B)	0.88(5)
C(16)-H(16A)	1.01(5)
C(16)-H(16B)	0.89(4)
C(19)-C(20)	1.525(6)
C(19)-H(19A)	0.93(5)
C(19)-H(19B)	1.04(5)
C(20)-H(20A)	0.88(5)
C(20)-H(20B)	0.95(4)

C(1)-Ru(1)-P(1)	75.27(6)
C(1)-Ru(1)-P(2)	76.67(6)
P(1)-Ru(1)-P(2)	132.93(2)
C(1)-Ru(1)-C(14)	85.26(9)
P(1)-Ru(1)-C(14)	91.18(8)
P(2)-Ru(1)-C(14)	123.15(8)
C(1)-Ru(1)-C(13)	88.94(9)
P(1)-Ru(1)-C(13)	125.95(8)

P(2)-Ru(1)-C(13)	90.19(7)
C(14)-Ru(1)-C(13)	35.40(11)
C(1)-Ru(1)-C(17)	157.48(10)
P(1)-Ru(1)-C(17)	90.07(8)
P(2)-Ru(1)-C(17)	125.21(8)
C(14)-Ru(1)-C(17)	77.93(11)
C(13)-Ru(1)-C(17)	85.99(10)
C(1)-Ru(1)-C(18)	161.71(10)
P(1)-Ru(1)-C(18)	122.52(8)
P(2)-Ru(1)-C(18)	91.50(8)
C(14)-Ru(1)-C(18)	89.80(11)
C(13)-Ru(1)-C(18)	77.04(11)
C(17)-Ru(1)-C(18)	34.55(11)
C(1)-Ru(1)-H(1)	109.2(15)
P(1)-Ru(1)-H(1)	74.4(14)
P(2)-Ru(1)-H(1)	80.3(14)
C(14)-Ru(1)-H(1)	155.5(14)
C(13)-Ru(1)-H(1)	156.7(14)
C(17)-Ru(1)-H(1)	82.3(15)
C(18)-Ru(1)-H(1)	81.9(15)
C(7)-P(1)-C(9)	101.73(17)
C(7)-P(1)-C(8)	101.56(17)
C(9)-P(1)-C(8)	94.20(15)
C(7)-P(1)-Ru(1)	108.90(10)
C(9)-P(1)-Ru(1)	130.64(12)
C(8)-P(1)-Ru(1)	115.62(11)
C(10)-P(2)-C(11)	98.95(14)
C(10)-P(2)-C(12)	100.83(12)
C(11)-P(2)-C(12)	96.43(13)
C(10)-P(2)-Ru(1)	109.89(9)
C(11)-P(2)-Ru(1)	129.74(9)
C(12)-P(2)-Ru(1)	116.43(8)
C(6)-C(1)-C(2)	115.6(2)
C(6)-C(1)-Ru(1)	121.99(18)
C(2)-C(1)-Ru(1)	122.26(17)
C(14)-C(13)-C(20)	122.0(3)

C(14)-C(13)-Ru(1)	72.06(15)
C(20)-C(13)-Ru(1)	113.7(2)
C(14)-C(13)-H(13)	120(2)
C(20)-C(13)-H(13)	115(2)
Ru(1)-C(13)-H(13)	103(2)
C(13)-C(14)-C(15)	122.8(3)
C(13)-C(14)-Ru(1)	72.55(14)
C(15)-C(14)-Ru(1)	112.12(19)
C(13)-C(14)-H(14)	118(2)
C(15)-C(14)-H(14)	114(2)
Ru(1)-C(14)-H(14)	108(2)
C(18)-C(17)-C(16)	121.4(3)
C(18)-C(17)-Ru(1)	73.11(16)
C(16)-C(17)-Ru(1)	112.3(2)
C(18)-C(17)-H(17)	120(2)
C(16)-C(17)-H(17)	115(2)
Ru(1)-C(17)-H(17)	104(2)
C(17)-C(18)-C(19)	124.0(3)
C(17)-C(18)-Ru(1)	72.34(16)
C(19)-C(18)-Ru(1)	113.1(2)
C(17)-C(18)-H(18)	115(2)
C(19)-C(18)-H(18)	116(2)
Ru(1)-C(18)-H(18)	105(2)
C(3)-C(2)-C(1)	122.0(2)
C(3)-C(2)-C(10)	119.3(2)
C(1)-C(2)-C(10)	118.7(2)
C(4)-C(3)-C(2)	120.6(3)
C(4)-C(3)-H(3)	120(2)
C(2)-C(3)-H(3)	120(2)
C(3)-C(4)-C(5)	119.2(3)
C(3)-C(4)-H(4)	122(2)
C(5)-C(4)-H(4)	119(2)
C(4)-C(5)-C(6)	120.6(3)
C(4)-C(5)-H(5)	123(2)
C(6)-C(5)-H(5)	116(3)
C(5)-C(6)-C(1)	121.8(3)

C(5)-C(6)-C(7)	120.2(3)
C(1)-C(6)-C(7)	117.9(2)
C(6)-C(7)-P(1)	103.22(19)
C(6)-C(7)-H(7A)	116(3)
P(1)-C(7)-H(7A)	101(2)
C(6)-C(7)-H(7B)	114(3)
P(1)-C(7)-H(7B)	116(3)
H(7A)-C(7)-H(7B)	106(4)
F(8B)-C(8)-F(8A)	107.6(3)
F(8B)-C(8)-F(8C)	105.9(3)
F(8A)-C(8)-F(8C)	106.5(3)
F(8B)-C(8)-P(1)	111.8(2)
F(8A)-C(8)-P(1)	110.9(2)
F(8C)-C(8)-P(1)	113.8(2)
F(9A)-C(9)-F(9C)	108.1(4)
F(9A)-C(9)-F(9B)	104.6(3)
F(9C)-C(9)-F(9B)	106.2(3)
F(9A)-C(9)-P(1)	110.1(2)
F(9C)-C(9)-P(1)	112.4(3)
F(9B)-C(9)-P(1)	115.0(2)
C(2)-C(10)-P(2)	104.91(17)
C(2)-C(10)-H(10A)	114(2)
P(2)-C(10)-H(10A)	106(2)
C(2)-C(10)-H(10B)	115(2)
P(2)-C(10)-H(10B)	112(2)
H(10A)-C(10)-H(10B)	105(3)
F(11C)-C(11)-F(11B)	108.4(3)
F(11C)-C(11)-F(11A)	108.9(3)
F(11B)-C(11)-F(11A)	102.5(3)
F(11C)-C(11)-P(2)	113.5(2)
F(11B)-C(11)-P(2)	115.4(2)
F(11A)-C(11)-P(2)	107.4(2)
F(12B)-C(12)-F(12A)	107.0(2)
F(12B)-C(12)-F(12C)	107.8(2)
F(12A)-C(12)-F(12C)	105.5(2)
F(12B)-C(12)-P(2)	112.72(17)

F(12A)-C(12)-P(2)	110.03(18)
F(12C)-C(12)-P(2)	113.43(18)
C(16)-C(15)-C(14)	116.0(2)
C(16)-C(15)-H(15A)	112(3)
C(14)-C(15)-H(15A)	108(3)
C(16)-C(15)-H(15B)	108(3)
C(14)-C(15)-H(15B)	111(3)
H(15A)-C(15)-H(15B)	101(4)
C(15)-C(16)-C(17)	116.5(2)
C(15)-C(16)-H(16A)	113(3)
C(17)-C(16)-H(16A)	103(3)
C(15)-C(16)-H(16B)	114(3)
C(17)-C(16)-H(16B)	104(3)
H(16A)-C(16)-H(16B)	106(4)
C(18)-C(19)-C(20)	115.0(3)
C(18)-C(19)-H(19A)	112(3)
C(20)-C(19)-H(19A)	104(3)
C(18)-C(19)-H(19B)	109(3)
C(20)-C(19)-H(19B)	108(3)
H(19A)-C(19)-H(19B)	109(4)
C(19)-C(20)-C(13)	116.5(2)
C(19)-C(20)-H(20A)	109(3)
C(13)-C(20)-H(20A)	106(3)
C(19)-C(20)-H(20B)	108(2)
C(13)-C(20)-H(20B)	110(2)
H(20A)-C(20)-H(20B)	107(4)

Table 3e. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(cod)H (**3**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	19(1)	20(1)	20(1)	0(1)	5(1)	-2(1)
P(1)	29(1)	21(1)	29(1)	-3(1)	11(1)	-3(1)
P(2)	22(1)	20(1)	24(1)	0(1)	10(1)	0(1)
C(1)	21(1)	27(1)	22(1)	-1(1)	7(1)	0(1)
C(13)	28(1)	42(2)	26(1)	-4(1)	14(1)	-7(1)
C(14)	28(1)	39(1)	28(1)	8(1)	13(1)	-2(1)
C(17)	26(1)	43(2)	35(1)	-5(1)	-2(1)	-6(1)
C(18)	23(1)	39(2)	40(2)	3(1)	-4(1)	1(1)
C(2)	22(1)	34(1)	20(1)	-3(1)	6(1)	-2(1)
C(3)	23(1)	53(2)	24(1)	-5(1)	4(1)	-4(1)
C(4)	23(1)	68(2)	26(1)	-4(1)	2(1)	9(1)
C(5)	33(1)	48(2)	32(1)	2(1)	7(1)	18(1)
C(6)	29(1)	31(1)	29(1)	-1(1)	6(1)	8(1)
C(7)	46(2)	26(1)	42(2)	2(1)	7(1)	8(1)
C(8)	58(2)	36(2)	56(2)	-8(1)	37(2)	1(1)
F(8A)	67(2)	74(2)	109(2)	-36(2)	68(2)	-27(1)
F(8B)	101(2)	139(3)	43(1)	3(2)	42(1)	12(2)
F(8C)	134(3)	45(1)	140(3)	-8(2)	106(2)	18(1)
C(9)	50(2)	33(2)	62(2)	-18(1)	21(2)	-12(1)
F(9A)	170(3)	84(2)	224(4)	-90(3)	160(3)	-95(2)
F(9B)	77(2)	29(1)	109(2)	-24(1)	5(2)	0(1)
F(9C)	96(2)	58(2)	109(2)	-35(2)	-46(2)	0(1)
C(10)	35(1)	30(1)	26(1)	-6(1)	6(1)	-10(1)
C(11)	37(2)	24(1)	65(2)	2(1)	25(1)	2(1)
F(11A)	64(1)	40(1)	86(2)	-8(1)	46(1)	8(1)
F(11B)	65(1)	23(1)	97(2)	-2(1)	34(1)	-5(1)
F(11C)	67(2)	47(1)	78(2)	14(1)	-1(1)	26(1)
C(12)	29(1)	30(1)	28(1)	-1(1)	13(1)	-6(1)
F(12A)	50(1)	69(1)	65(1)	15(1)	40(1)	19(1)
F(12B)	46(1)	110(2)	28(1)	17(1)	8(1)	-15(1)
F(12C)	105(2)	54(1)	81(2)	-27(1)	69(2)	-48(1)

C(15)	45(2)	38(2)	47(2)	0(1)	25(1)	-14(1)
C(16)	26(1)	50(2)	71(2)	9(2)	6(1)	-15(1)
C(19)	23(1)	54(2)	73(2)	-10(2)	4(1)	9(1)
C(20)	42(2)	41(2)	61(2)	-2(2)	33(2)	2(1)

Table 3f. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(cod)H (**3**).

	x	y	z	U(eq)
H(1)	2900(40)	630(20)	3990(30)	51(11)
H(13)	3050(40)	119(19)	1100(30)	37(9)
H(14)	3130(40)	1380(20)	1200(30)	38(9)
H(17)	5330(40)	1210(20)	4230(30)	43(10)
H(18)	5220(40)	-30(20)	4190(30)	46(10)
H(3)	-1820(30)	-104(19)	540(20)	31(8)
H(4)	-2720(40)	1090(20)	70(30)	51(10)
H(5)	-1270(40)	2060(20)	830(30)	38(9)
H(7A)	1840(50)	2430(30)	1820(30)	66(13)
H(7B)	570(50)	2560(30)	2260(30)	68(13)
H(10A)	1020(40)	-782(17)	1280(30)	32(8)
H(10B)	-80(40)	-880(20)	1850(30)	44(10)
H(15A)	4930(40)	2100(20)	1880(30)	56(12)
H(15B)	5750(50)	1570(30)	1520(40)	75(14)
H(16A)	6980(50)	1110(30)	2930(30)	66(13)
H(16B)	6450(50)	1820(30)	3330(30)	63(13)
H(19A)	6890(60)	-170(30)	2960(40)	98(18)
H(19B)	5710(60)	-800(30)	2990(40)	98(19)
H(20A)	5900(50)	200(30)	1540(40)	86(16)
H(20B)	5160(40)	-520(20)	1420(30)	51(11)

(^{CF_3}PCP)Ru(dfepe)H (4)

Crystallographic data. The X-ray diffraction data were measured at 150 K on a Bruker SMART APEX II CCD area detector system equipped with a graphite monochromator and a Mo Kα fine-focus sealed tube operated at 1.5 kW power (50 kV, 30 mA). A colorless rectangular prism of (^{CF_3}PCP)Ru(dfepe)H (**4**) of approximate dimensions 0.49 × 0.27 × 0.19 mm^3 was glued to a glass fiber using Paratone N oil. The detector was placed at a distance of 5.127 cm from the crystal during the data collection.

A series of narrow frames of data were collected with a scan width of 0.5° in ω or ϕ and an exposure time of 10 s per frame. The frames were integrated with the Bruker SAINT Software package[1] using a narrow-frame integration algorithm. The integration of the data using a monoclinic unit cell yielded a total of 43989 reflections in the θ range of 3.05 to 33.73° of which 13331 were independent with $I \geq 2\sigma(I)$ (R_{int} = 0.0188). The data were corrected for absorption effects by the multi-scan method (SADABS). Crystallographic data collection parameters and refinement data are collected below in Table 1. The structure was solved by the direct methods using the Bruker SHELXTL (V. 6.14) Software Package.[1] All non-hydrogen atoms were located in successive Fourier maps and refined anisotropically. The asymmetric unit consists of one RuH(pcp)(dfepe) molecule. All of the hydrogen atoms were also located in the Fourier maps, and were refined isotropically. All atoms are located on general positions and well ordered. The final refinement parameters are R_1 = 0.0312 and wR_2 = 0.0791 for data with $F > 4\sigma(F)$ giving the data to parameter ratio of 23. The refinement data for all data are R_1 = 0.0368 and wR_2 = 0.0830.

Table 4a. Crystallographic Data for (^{CF_3}PCP)Ru(dfepe)H (**4**)

compound	(^{CF_3}PCP)Ru(dfepe)H (**4**)	color	colorless
chemical formula	$C_{22}H_{12}F_{32}P_4Ru$	fw	1109.27
T, K	150(2)	λ, Å	0.71073
space group	$P2_1/c$	a, Å	19.2841(3)
b, Å	10.0809(2)	c, Å	19.1078(3)
β, °	115.39(1)	V, Å^3	3355.84(10)
Z	4	D_{calc}, Mg m^{-3}	2.196
μ, mm^{-1}	0.857	goodness of fit	1.026
$R1[I > 2\sigma(I)]$[a]	0.0312	$wR2[I > 2\sigma(I)]$[b]	0.0791

[a] $R1 = \sum||F_o| - |F_c||/\sum|F_o|$; [b] $_wR2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2]\}^{1/2}$

Table 4b. Crystal data and structure refinement for (^{CF_3}PCP)Ru(dfepe)H (**4**).

Identification code	bcg12	
Empirical formula	C22 H12 F32 P4 Ru	
Formula weight	1109.27	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 19.2841(3) Å	α= 90°.
	b = 10.0809(2) Å	β= 115.39°.
	c = 19.1078(3) Å	γ = 90°.
Volume	3355.84(10) Å^3	
Z	4	
Density (calculated)	2.196 Mg/m^3	
Absorption coefficient	0.857 mm^{-1}	
F(000)	2144	
Crystal size	0.49 × 0.27 × 0.19 mm^3	
Theta range for data collection	3.05 to 33.73°.	
Index ranges	-30<=h<=30, -15<=k<=13, -29<=l<=29	
Reflections collected	43989	
Independent reflections	13331 [R(int) = 0.0188]	
Completeness to theta = 33.73°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8514 and 0.6779	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13331 / 0 / 580	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0791	
R indices (all data)	R1 = 0.0368, wR2 = 0.0830	
Largest diff. peak and hole	2.019 and -1.048 e.Å^{-3}	

Table 4c. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(dfepe)H (**4**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2583(1)	1644(1)	2932(1)	13(1)
P(1)	3307(1)	3402(1)	3590(1)	18(1)
P(2)	1962(1)	-122(1)	3146(1)	17(1)
P(3)	3298(1)	809(1)	2328(1)	17(1)
P(4)	1846(1)	2548(1)	1688(1)	15(1)
C(1)	1900(1)	2572(2)	3459(1)	16(1)
C(2)	1296(1)	1896(2)	3537(1)	19(1)
C(3)	808(1)	2539(2)	3793(1)	23(1)
C(4)	914(1)	3863(2)	4000(1)	26(1)
C(5)	1528(1)	4538(2)	3974(1)	23(1)
C(6)	2017(1)	3902(2)	3716(1)	19(1)
C(7)	2694(1)	4654(2)	3723(1)	21(1)
C(8)	4033(1)	4505(2)	3423(1)	28(1)
F(8A)	3930(1)	5777(1)	3542(1)	48(1)
F(8B)	4756(1)	4202(1)	3891(1)	38(1)
F(8C)	3962(1)	4401(1)	2699(1)	36(1)
C(9)	3942(1)	3017(2)	4641(1)	30(1)
F(9A)	3518(1)	2505(1)	4976(1)	38(1)
F(9B)	4276(1)	4107(1)	5040(1)	44(1)
F(9C)	4493(1)	2146(2)	4734(1)	42(1)
C(10)	1175(1)	443(2)	3354(1)	23(1)
C(11)	2566(1)	-1055(2)	4069(1)	30(1)
F(11A)	2174(1)	-2017(2)	4227(1)	46(1)
F(11B)	3178(1)	-1613(2)	4043(1)	48(1)
F(11C)	2808(1)	-223(2)	4668(1)	43(1)
C(12)	1484(1)	-1655(2)	2565(1)	25(1)
F(12A)	1015(1)	-2247(1)	2824(1)	37(1)
F(12B)	1994(1)	-2564(1)	2583(1)	34(1)
F(12C)	1053(1)	-1338(1)	1828(1)	31(1)
C(13)	3159(1)	1864(2)	1494(1)	23(1)
C(14)	2298(1)	2134(2)	1033(1)	24(1)

C(15)	4393(1)	770(2)	2824(1)	26(1)
F(15A)	4690(1)	764(1)	2300(1)	38(1)
F(15B)	4590(1)	1941(1)	3202(1)	39(1)
C(16)	4817(1)	-299(2)	3435(1)	39(1)
F(16A)	5544(1)	52(2)	3830(1)	61(1)
F(16B)	4816(1)	-1455(2)	3111(1)	56(1)
F(16C)	4498(1)	-436(2)	3917(1)	59(1)
C(17)	3049(1)	-908(2)	1868(1)	23(1)
F(17A)	2271(1)	-920(1)	1499(1)	29(1)
F(17B)	3264(1)	-1813(1)	2444(1)	32(1)
C(18)	3312(1)	-1440(2)	1263(1)	31(1)
F(18A)	3018(1)	-709(2)	628(1)	57(1)
F(18B)	3066(1)	-2661(1)	1069(1)	50(1)
F(18C)	4059(1)	-1440(2)	1528(1)	59(1)
C(19)	825(1)	2061(2)	992(1)	21(1)
F(19A)	625(1)	2635(1)	291(1)	33(1)
F(19B)	841(1)	739(1)	874(1)	36(1)
C(20)	162(1)	2326(2)	1212(1)	31(1)
F(20A)	-499(1)	2003(2)	640(1)	47(1)
F(20B)	137(1)	3547(2)	1394(2)	82(1)
F(20C)	241(1)	1523(2)	1799(1)	52(1)
C(21)	1772(1)	4441(2)	1604(1)	20(1)
F(21A)	2514(1)	4848(1)	1928(1)	30(1)
F(21B)	1446(1)	4883(1)	2060(1)	30(1)
C(22)	1389(1)	5259(2)	848(1)	34(1)
F(22A)	626(1)	5219(2)	588(1)	57(1)
F(22B)	1578(1)	4854(2)	310(1)	64(1)
F(22C)	1575(1)	6517(1)	994(1)	39(1)

Table 4d. Bond lengths [Å] and angles [°] for (^{CF_3}PCP)Ru(dfepe)H (**4**).

Ru(1)-C(1)	2.1802(14)
Ru(1)-P(1)	2.2725(4)
Ru(1)-P(2)	2.2778(4)
Ru(1)-P(3)	2.3055(4)
Ru(1)-P(4)	2.3666(4)
Ru(1)-H(1)	1.53(3)
P(1)-C(7)	1.8198(17)
P(1)-C(9)	1.8898(19)
P(1)-C(8)	1.9192(18)
P(2)-C(10)	1.8175(17)
P(2)-C(11)	1.8935(19)
P(2)-C(12)	1.8965(17)
P(3)-C(13)	1.8365(17)
P(3)-C(17)	1.9068(17)
P(3)-C(15)	1.9084(17)
P(4)-C(14)	1.8549(16)
P(4)-C(19)	1.9074(16)
P(4)-C(21)	1.9153(16)
C(1)-C(2)	1.411(2)
C(1)-C(6)	1.412(2)
C(2)-C(3)	1.394(2)
C(2)-C(10)	1.501(2)
C(3)-C(4)	1.382(3)
C(3)-H(3)	1.00(2)
C(4)-C(5)	1.385(3)
C(4)-H(4)	0.96(3)
C(5)-C(6)	1.394(2)
C(5)-H(5)	0.91(3)
C(6)-C(7)	1.504(2)
C(7)-H(7A)	0.95(3)
C(7)-H(7B)	1.02(3)
C(8)-F(8B)	1.330(2)
C(8)-F(8A)	1.331(2)
C(8)-F(8C)	1.334(2)

C(9)-F(9C)	1.330(2)
C(9)-F(9B)	1.336(2)
C(9)-F(9A)	1.340(3)
C(10)-H(10A)	0.91(3)
C(10)-H(10B)	0.92(3)
C(11)-F(11B)	1.328(3)
C(11)-F(11C)	1.333(2)
C(11)-F(11A)	1.340(2)
C(12)-F(12C)	1.331(2)
C(12)-F(12B)	1.334(2)
C(12)-F(12A)	1.342(2)
C(13)-C(14)	1.534(2)
C(13)-H(13A)	0.95(3)
C(13)-H(13B)	0.98(3)
C(14)-H(14A)	0.92(3)
C(14)-H(14B)	0.94(3)
C(15)-F(15A)	1.350(2)
C(15)-F(15B)	1.351(2)
C(15)-C(16)	1.541(3)
C(16)-F(16C)	1.316(3)
C(16)-F(16B)	1.319(3)
C(16)-F(16A)	1.324(3)
C(17)-F(17B)	1.350(2)
C(17)-F(17A)	1.3559(19)
C(17)-C(18)	1.545(2)
C(18)-F(18C)	1.307(2)
C(18)-F(18B)	1.314(2)
C(18)-F(18A)	1.322(3)
C(19)-F(19B)	1.354(2)
C(19)-F(19A)	1.355(2)
C(19)-C(20)	1.531(3)
C(20)-F(20B)	1.285(3)
C(20)-F(20A)	1.315(2)
C(20)-F(20C)	1.339(3)
C(21)-F(21B)	1.3507(19)
C(21)-F(21A)	1.3562(18)

C(21)-C(22)	1.548(2)
C(22)-F(22B)	1.295(3)
C(22)-F(22C)	1.314(2)
C(22)-F(22A)	1.338(3)

C(1)-Ru(1)-P(1)	76.10(4)
C(1)-Ru(1)-P(2)	77.60(4)
P(1)-Ru(1)-P(2)	139.078(15)
C(1)-Ru(1)-P(3)	175.76(4)
P(1)-Ru(1)-P(3)	101.760(15)
P(2)-Ru(1)-P(3)	106.123(15)
C(1)-Ru(1)-P(4)	94.43(4)
P(1)-Ru(1)-P(4)	102.568(15)
P(2)-Ru(1)-P(4)	110.230(14)
P(3)-Ru(1)-P(4)	82.422(14)
C(1)-Ru(1)-H(1)	95.0(10)
P(1)-Ru(1)-H(1)	76.0(11)
P(2)-Ru(1)-H(1)	75.7(10)
P(3)-Ru(1)-H(1)	88.0(10)
P(4)-Ru(1)-H(1)	169.8(10)
C(7)-P(1)-C(9)	99.11(8)
C(7)-P(1)-C(8)	100.65(8)
C(9)-P(1)-C(8)	96.23(9)
C(7)-P(1)-Ru(1)	109.61(5)
C(9)-P(1)-Ru(1)	113.12(6)
C(8)-P(1)-Ru(1)	132.79(6)
C(10)-P(2)-C(11)	100.94(9)
C(10)-P(2)-C(12)	98.12(8)
C(11)-P(2)-C(12)	95.21(9)
C(10)-P(2)-Ru(1)	110.26(6)
C(11)-P(2)-Ru(1)	113.27(6)
C(12)-P(2)-Ru(1)	133.88(6)
C(13)-P(3)-C(17)	102.23(8)
C(13)-P(3)-C(15)	99.33(8)
C(17)-P(3)-C(15)	102.54(8)
C(13)-P(3)-Ru(1)	109.04(5)

C(17)-P(3)-Ru(1)	118.37(5)
C(15)-P(3)-Ru(1)	122.11(6)
C(14)-P(4)-C(19)	96.57(8)
C(14)-P(4)-C(21)	101.92(8)
C(19)-P(4)-C(21)	100.36(7)
C(14)-P(4)-Ru(1)	109.78(5)
C(19)-P(4)-Ru(1)	126.66(5)
C(21)-P(4)-Ru(1)	117.33(5)
C(2)-C(1)-C(6)	115.96(13)
C(2)-C(1)-Ru(1)	122.00(11)
C(6)-C(1)-Ru(1)	122.00(10)
C(3)-C(2)-C(1)	121.65(15)
C(3)-C(2)-C(10)	118.31(14)
C(1)-C(2)-C(10)	120.03(14)
C(4)-C(3)-C(2)	120.73(15)
C(4)-C(3)-H(3)	123.5(14)
C(2)-C(3)-H(3)	115.8(14)
C(3)-C(4)-C(5)	119.20(15)
C(3)-C(4)-H(4)	120.8(16)
C(5)-C(4)-H(4)	120.0(16)
C(4)-C(5)-C(6)	120.35(16)
C(4)-C(5)-H(5)	118.9(17)
C(6)-C(5)-H(5)	120.8(17)
C(5)-C(6)-C(1)	121.89(14)
C(5)-C(6)-C(7)	118.79(14)
C(1)-C(6)-C(7)	119.31(13)
C(6)-C(7)-P(1)	105.23(11)
C(6)-C(7)-H(7A)	112.1(15)
P(1)-C(7)-H(7A)	111.2(15)
C(6)-C(7)-H(7B)	111.2(15)
P(1)-C(7)-H(7B)	107.2(15)
H(7A)-C(7)-H(7B)	110(2)
F(8B)-C(8)-F(8A)	107.30(15)
F(8B)-C(8)-F(8C)	106.91(15)
F(8A)-C(8)-F(8C)	107.22(18)
F(8B)-C(8)-P(1)	112.65(14)

F(8A)-C(8)-P(1)	110.88(13)
F(8C)-C(8)-P(1)	111.60(12)
F(9C)-C(9)-F(9B)	107.77(16)
F(9C)-C(9)-F(9A)	107.34(17)
F(9B)-C(9)-F(9A)	106.68(17)
F(9C)-C(9)-P(1)	113.19(14)
F(9B)-C(9)-P(1)	111.88(14)
F(9A)-C(9)-P(1)	109.67(13)
C(2)-C(10)-P(2)	107.16(11)
C(2)-C(10)-H(10A)	114.2(18)
P(2)-C(10)-H(10A)	103.4(17)
C(2)-C(10)-H(10B)	114.1(17)
P(2)-C(10)-H(10B)	109.7(16)
H(10A)-C(10)-H(10B)	108(2)
F(11B)-C(11)-F(11C)	107.96(18)
F(11B)-C(11)-F(11A)	107.27(17)
F(11C)-C(11)-F(11A)	106.59(17)
F(11B)-C(11)-P(2)	112.19(14)
F(11C)-C(11)-P(2)	109.68(13)
F(11A)-C(11)-P(2)	112.88(14)
F(12C)-C(12)-F(12B)	108.12(15)
F(12C)-C(12)-F(12A)	106.51(15)
F(12B)-C(12)-F(12A)	106.94(14)
F(12C)-C(12)-P(2)	110.47(12)
F(12B)-C(12)-P(2)	112.09(12)
F(12A)-C(12)-P(2)	112.44(12)
C(14)-C(13)-P(3)	108.77(11)
C(14)-C(13)-H(13A)	111.5(16)
P(3)-C(13)-H(13A)	111.5(15)
C(14)-C(13)-H(13B)	111.2(15)
P(3)-C(13)-H(13B)	104.0(14)
H(13A)-C(13)-H(13B)	110(2)
C(13)-C(14)-P(4)	110.94(11)
C(13)-C(14)-H(14A)	111.3(16)
P(4)-C(14)-H(14A)	112.4(16)
C(13)-C(14)-H(14B)	111.4(16)

P(4)-C(14)-H(14B)	105.6(16)
H(14A)-C(14)-H(14B)	105(2)
F(15A)-C(15)-F(15B)	106.78(16)
F(15A)-C(15)-C(16)	107.66(15)
F(15B)-C(15)-C(16)	105.66(17)
F(15A)-C(15)-P(3)	111.27(13)
F(15B)-C(15)-P(3)	104.18(11)
C(16)-C(15)-P(3)	120.35(14)
F(16C)-C(16)-F(16B)	109.2(2)
F(16C)-C(16)-F(16A)	109.1(2)
F(16B)-C(16)-F(16A)	107.04(18)
F(16C)-C(16)-C(15)	110.38(17)
F(16B)-C(16)-C(15)	111.62(19)
F(16A)-C(16)-C(15)	109.4(2)
F(17B)-C(17)-F(17A)	107.69(14)
F(17B)-C(17)-C(18)	106.85(14)
F(17A)-C(17)-C(18)	104.57(14)
F(17B)-C(17)-P(3)	108.01(12)
F(17A)-C(17)-P(3)	104.63(11)
C(18)-C(17)-P(3)	124.13(13)
F(18C)-C(18)-F(18B)	108.29(18)
F(18C)-C(18)-F(18A)	108.9(2)
F(18B)-C(18)-F(18A)	107.62(19)
F(18C)-C(18)-C(17)	111.76(17)
F(18B)-C(18)-C(17)	109.99(17)
F(18A)-C(18)-C(17)	110.18(16)
F(19B)-C(19)-F(19A)	105.77(14)
F(19B)-C(19)-C(20)	107.36(15)
F(19A)-C(19)-C(20)	106.21(14)
F(19B)-C(19)-P(4)	106.25(11)
F(19A)-C(19)-P(4)	110.55(11)
C(20)-C(19)-P(4)	119.86(12)
F(20B)-C(20)-F(20A)	109.0(2)
F(20B)-C(20)-F(20C)	110.8(2)
F(20A)-C(20)-F(20C)	105.49(16)
F(20B)-C(20)-C(19)	112.02(16)

F(20A)-C(20)-C(19)	110.88(17)
F(20C)-C(20)-C(19)	108.43(16)
F(21B)-C(21)-F(21A)	107.26(13)
F(21B)-C(21)-C(22)	104.97(14)
F(21A)-C(21)-C(22)	104.61(14)
F(21B)-C(21)-P(4)	108.23(10)
F(21A)-C(21)-P(4)	103.74(10)
C(22)-C(21)-P(4)	126.76(12)
F(22B)-C(22)-F(22C)	109.09(19)
F(22B)-C(22)-F(22A)	109.55(19)
F(22C)-C(22)-F(22A)	105.37(18)
F(22B)-C(22)-C(21)	112.84(18)
F(22C)-C(22)-C(21)	109.85(15)
F(22A)-C(22)-C(21)	109.86(17)

Table 4e. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(dfepe)H (**4**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	13(1)	13(1)	15(1)	0(1)	7(1)	-1(1)
P(1)	16(1)	17(1)	19(1)	-3(1)	6(1)	-3(1)
P(2)	20(1)	14(1)	20(1)	1(1)	10(1)	-2(1)
P(3)	15(1)	18(1)	20(1)	-1(1)	9(1)	1(1)
P(4)	15(1)	16(1)	15(1)	0(1)	7(1)	0(1)
C(1)	18(1)	17(1)	16(1)	0(1)	9(1)	0(1)
C(2)	21(1)	19(1)	20(1)	1(1)	11(1)	0(1)
C(3)	24(1)	25(1)	27(1)	2(1)	16(1)	2(1)
C(4)	29(1)	25(1)	30(1)	2(1)	19(1)	6(1)
C(5)	28(1)	19(1)	26(1)	-1(1)	15(1)	4(1)
C(6)	22(1)	17(1)	19(1)	0(1)	10(1)	1(1)
C(7)	24(1)	17(1)	22(1)	-4(1)	11(1)	-3(1)
C(8)	21(1)	26(1)	40(1)	-6(1)	14(1)	-8(1)
F(8A)	44(1)	23(1)	89(1)	-11(1)	40(1)	-13(1)
F(8B)	18(1)	46(1)	45(1)	-15(1)	9(1)	-11(1)
F(8C)	28(1)	44(1)	40(1)	2(1)	18(1)	-12(1)
C(9)	28(1)	30(1)	23(1)	-5(1)	2(1)	-1(1)
F(9A)	47(1)	44(1)	20(1)	0(1)	10(1)	-2(1)
F(9B)	42(1)	41(1)	30(1)	-16(1)	-2(1)	-9(1)
F(9C)	32(1)	46(1)	33(1)	-1(1)	-2(1)	12(1)
C(10)	26(1)	20(1)	31(1)	-1(1)	19(1)	-3(1)
C(11)	34(1)	26(1)	30(1)	10(1)	12(1)	-2(1)
F(11A)	54(1)	36(1)	43(1)	20(1)	16(1)	-10(1)
F(11B)	40(1)	45(1)	54(1)	22(1)	16(1)	18(1)
F(11C)	54(1)	44(1)	21(1)	5(1)	9(1)	-11(1)
C(12)	30(1)	18(1)	30(1)	-3(1)	17(1)	-6(1)
F(12A)	46(1)	28(1)	49(1)	-7(1)	32(1)	-18(1)
F(12B)	43(1)	16(1)	48(1)	-4(1)	25(1)	0(1)
F(12C)	30(1)	32(1)	30(1)	-6(1)	11(1)	-10(1)
C(13)	23(1)	25(1)	26(1)	3(1)	16(1)	2(1)
C(14)	24(1)	31(1)	18(1)	2(1)	12(1)	6(1)

C(15)	17(1)	28(1)	35(1)	-3(1)	12(1)	2(1)
F(15A)	23(1)	49(1)	50(1)	2(1)	24(1)	4(1)
F(15B)	19(1)	34(1)	55(1)	-15(1)	8(1)	-3(1)
C(16)	22(1)	43(1)	43(1)	4(1)	6(1)	9(1)
F(16A)	21(1)	68(1)	69(1)	4(1)	-4(1)	8(1)
F(16B)	45(1)	36(1)	72(1)	5(1)	12(1)	18(1)
F(16C)	46(1)	83(1)	46(1)	29(1)	18(1)	24(1)
C(17)	21(1)	21(1)	28(1)	-3(1)	13(1)	1(1)
F(17A)	21(1)	29(1)	37(1)	-11(1)	13(1)	-4(1)
F(17B)	41(1)	22(1)	38(1)	4(1)	20(1)	3(1)
C(18)	33(1)	29(1)	38(1)	-10(1)	22(1)	0(1)
F(18A)	96(1)	51(1)	38(1)	-2(1)	41(1)	14(1)
F(18B)	64(1)	34(1)	67(1)	-25(1)	43(1)	-10(1)
F(18C)	33(1)	83(1)	73(1)	-37(1)	33(1)	-6(1)
C(19)	20(1)	19(1)	21(1)	0(1)	5(1)	0(1)
F(19A)	28(1)	47(1)	19(1)	3(1)	5(1)	0(1)
F(19B)	32(1)	20(1)	45(1)	-7(1)	6(1)	-2(1)
C(20)	20(1)	39(1)	34(1)	-1(1)	11(1)	-5(1)
F(20A)	18(1)	62(1)	50(1)	8(1)	3(1)	-5(1)
F(20B)	54(1)	47(1)	175(2)	-50(1)	79(1)	-17(1)
F(20C)	36(1)	84(1)	38(1)	12(1)	19(1)	-2(1)
C(21)	21(1)	16(1)	19(1)	1(1)	7(1)	-1(1)
F(21A)	22(1)	24(1)	37(1)	4(1)	5(1)	-7(1)
F(21B)	40(1)	20(1)	37(1)	0(1)	24(1)	4(1)
C(22)	44(1)	22(1)	25(1)	4(1)	6(1)	-4(1)
F(22A)	39(1)	41(1)	58(1)	15(1)	-10(1)	0(1)
F(22B)	131(2)	37(1)	35(1)	12(1)	46(1)	16(1)
F(22C)	54(1)	19(1)	36(1)	8(1)	13(1)	-2(1)

Table 4f. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for (^{CF_3}PCP)Ru(dfepe)H (**4**).

	x	y	z	U(eq)
H(1)	3173(15)	1040(30)	3690(16)	36(7)
H(3)	395(13)	1980(20)	3824(14)	22(5)
H(4)	572(15)	4310(30)	4170(15)	30(6)
H(5)	1608(16)	5400(30)	4132(16)	36(7)
H(7A)	2959(14)	5130(30)	4192(14)	27(6)
H(7B)	2530(15)	5290(30)	3263(15)	31(6)
H(10A)	752(16)	250(30)	2912(16)	33(7)
H(10B)	1154(15)	-60(30)	3746(15)	31(6)
H(13A)	3372(15)	1470(20)	1181(15)	27(6)
H(13B)	3439(14)	2680(30)	1729(14)	27(6)
H(14A)	2210(14)	2770(30)	660(15)	27(6)
H(14B)	2039(15)	1380(30)	758(15)	31(6)