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C(3)-C(2)-C(1)	107.5(3)	C(10)-C(9)-C(8)	108.6(2)
C(3)-C(2)-Ru	71.34(18)	C(10)-C(9)-Ru	75.17(15)
C(1)-C(2)-Ru	70.55(17)	C(8)-C(9)-Ru	71.00(16)
C(2)-C(3)-C(4)	108.5(3)	C(9)-C(10)-C(6)	107.5(3)
C(2)-C(3)-Ru	72.22(17)	C(9)-C(10)-Ru	67.61(15)
C(4)-C(3)-Ru	71.77(18)	C(6)-C(10)-Ru	85.58(14)
C(5)-C(4)-C(3)	108.3(4)	C(11)-S(1)-Ru	110.60(8)
C(5)-C(4)-Ru	72.3(2)	N(2)-C(11)-N(1)	120.0(2)
C(3)-C(4)-Ru	71.33(17)	N(2)-C(11)-S(1)	116.84(17)
C(4)-C(5)-C(1)	108.2(3)	N(1)-C(11)-S(1)	123.19(18)
C(4)-C(5)-Ru	71.50(17)	O(4)-S(2)-O(3)	117.44(14)
C(1)-C(5)-Ru	70.54(18)	O(4)-S(2)-O(2)	113.21(14)
O(1)-C(6)-C(10)	128.1(2)	O(3)-S(2)-O(2)	112.93(13)
O(1)-C(6)-C(7)	128.7(2)	O(4)-S(2)-C(12)	104.44(15)
C(10)-C(6)-C(7)	103.1(2)	O(3)-S(2)-C(12)	103.34(13)
O(1)-C(6)-Ru	139.36(17)	O(2)-S(2)-C(12)	103.46(15)
C(10)-C(6)-Ru	60.05(12)	F(1)-C(12)-F(3)	108.1(3)
C(7)-C(6)-Ru	60.39(12)	F(1)-C(12)-F(2)	106.6(3)
C(8)-C(7)-C(6)	108.2(2)	F(3)-C(12)-F(2)	106.2(3)
C(8)-C(7)-Ru	67.79(15)	F(1)-C(12)-S(2)	112.1(3)
C(6)-C(7)-Ru	84.93(14)	F(3)-C(12)-S(2)	111.3(2)
C(7)-C(8)-C(9)	107.9(3)	F(2)-C(12)-S(2)	112.2(2)
C(7)-C(8)-Ru	75.52(15)	N(3)-C(13)-C(14)	179.1(5)
C(9)-C(8)-Ru	70.35(16)		

Symmetry transformations used to generate equivalent atoms: $1 x+1, y, z-1, $2 -x+1, -y+1, -z+1, $3 -x+2, -y, -z

Supporting Table S38. Least-squares planes data for $[Ru(\eta^4\text{-}C_5H_4O)(\eta^5\text{-}C_5H_5)(SC(NH_2)_2]CF_3SO_3\cdot CH_3CN$ (**4**·CH_3CN).

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

```
6.2904 (0.0072) x - 3.6206 (0.0161) y + 4.8373 (0.0164) z = 1.5449 (0.0071)
*    0.0124 (0.0019)  C1
*   -0.0102 (0.0018)  C2
*    0.0042 (0.0018)  C3
*    0.0037 (0.0019)  C4
*   -0.0100 (0.0019)  C5
     1.8615 (0.0014)  Ru
     2.7231 (0.0038)  S1
Rms deviation of fitted atoms =   0.0088

 3.9205 (0.0125) x - 2.6932 (0.0153) y + 9.6930 (0.0122) z = 5.1760 (0.0069)
Angle to previous plane (with approximate esd) = 34.40 ( 0.18 )
*    0.0014 (0.0010)  C7
*   -0.0023 (0.0016)  C8
*    0.0023 (0.0016)  C9
*   -0.0014 (0.0010)  C10
    -1.8657 (0.0015)  Ru
    -2.4164 (0.0052)  S1
Rms deviation of fitted atoms =   0.0019

 1.9328 (0.0099) x - 1.8129 (0.0183) y + 10.9676 (0.0066) z = 4.3213 (0.0089)
Angle to previous plane (with approximate esd) = 18.90 ( 0.17 )
*   -0.0105 (0.0008)  O1
*    0.0247 (0.0020)  C6
*   -0.0071 (0.0006)  C7
*   -0.0071 (0.0006)  C10
    -1.6038 (0.0030)  Ru
    -0.0294 (0.0278)  H7
    -0.0323 (0.0301)  H10
Rms deviation of fitted atoms =   0.0143

 6.2904 (0.0072) x - 3.6206 (0.0161) y + 4.8373 (0.0164) z = 1.5449 (0.0071)
Angle to previous plane (with approximate esd) = 53.29 ( 0.14 )
*    0.0124 (0.0019)  C1
*   -0.0102 (0.0018)  C2
*    0.0042 (0.0018)  C3
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*    0.0037 (0.0019)  C4
*   -0.0100 (0.0019)  C5
Rms deviation of fitted atoms =   0.0088

 5.1433 (0.0055) x - 2.6574 (0.0108) y + 8.4130 (0.0115) z = 3.6286 (0.0044)
Angle to previous plane (with approximate esd) = 22.50 ( 0.16 )
*   -0.0016 (0.0005)  S1
*    0.0058 (0.0018)  C11
*   -0.0022 (0.0007)  N1
*   -0.0020 (0.0006)  N2
Rms deviation of fitted atoms =   0.0034
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Good quality crystals of **18** in the form of several mm long yellow monoclinic prisms were obtained by diffusion of diethylether in an acetone solution. These crystals were crystallographically outstanding in showing pseudomerohedral contact twinning with [101] as the twin dyad and $B22_12$ as the pseudospace group. The metric prerequisite for this feature is that *a* and *c* axes are similar in size and that the monoclinic crystal structure is distinctly pseudosymmetric orthorhombic in (010) projections but not in threedimensional space. The monoclinic unit cell, space group $P2_1/n$, contains two crystallographically independent but stereochemically closely similar $[Ru(\eta^5\text{-}C_5H_5)(\eta(1,2,3)\text{-}1\text{-}PMe_3\text{-}2\text{-buten-}1\text{-yl})(PMe_3)]PF_6$ complexes the differences showing are essentially in the torsion angles of the PMe_3 groups. The pseudomerohedral twinning was only detected after having collected with a twinned crystal a first data set that did not provide a reasonable solution of the crystal structure. After dividing another crystal into two halves under a polarizing microscope (only weak optical indications for contact twinning were seen) and using this for a further data collection, the true monoclinic symmetry became apparent and the structure was readily solved. With these structural data it was possible to refine the structure also with the reflection data of the previous twin (*hkl* transformation matrices 100/010/001 and 001/0-10/100) yielding a refined twin volume ratio of 51:49, an R1 = 0.058 for all 5792 available data, and a structure agreeing well with that of the single crystal. The crystals of **18** were crystallographically outstanding in showing pseudomerohedral contact twinning with [101] as the twin dyad and $B22_12$ as the pseudospace group. The metric prerequisite for this feature is that *a* and *c* axes are similar in size and that the monoclinic crystal structure is distinctly pseudosymmetric orthorhombic in (010) projections but not in threedimensional space. The monoclinic unit cell, space group $P2_1/n$, contains two crystallographically independent but stereochemically closely similar $[Ru(\eta^5\text{-}C_5H_5)(\eta(1,2,3)\text{-}1\text{-}PMe_3\text{-}2\text{-buten-}1\text{-yl})(PMe_3)]PF_6$ complexes the differences showing are essentially in the torsion angles of the PMe_3 groups. The pseudomerohedral twinning was only detected after having collected with a twinned crystal a first data set that did not provide a reasonable solution of the crystal structure. After dividing another crystal into two halves under a polarizing microscope (only weak optical indications for contact twinning were seen) and using this for a further data collection, the true monoclinic symmetry became apparent and the structure was readily solved. With these structural data it was possible to refine the structure also with the reflection data of the previous twin (*hkl* transformation matrices 100/010/001 and 001/0-10/100) yielding a refined twin volume ratio of 51:49, an R1 = 0.058 for all 5792 available data, and a structure agreeing well with that of the single crystal.

Supporting Table S39. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $[Ru(\eta^5\text{-}C_5H_5)(\eta^3\text{-}CH_3\text{-}C_3H_3\text{-}PMe_3)(PMe_3)]PF_6$ (**18**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	0.35173(1)	0.54977(3)	0.32823(1)	41(1)
P(1)	0.49267(4)	0.71344(11)	0.35714(4)	43(1)
P(2)	0.34845(4)	0.36608(12)	0.40252(4)	44(1)
C(1)	0.3078(3)	0.7330(7)	0.2700(3)	90(2)
C(2)	0.2649(3)	0.6139(7)	0.2780(4)	99(2)
C(3)	0.2571(2)	0.6077(7)	0.3385(4)	98(2)
C(4)	0.2944(3)	0.7218(7)	0.3691(3)	90(2)
C(5)	0.3244(2)	0.7978(6)	0.3258(4)	86(2)
C(6)	0.4509(2)	0.5446(4)	0.3357(2)	41(1)
C(7)	0.4247(2)	0.5234(5)	0.2754(2)	48(1)
C(8)	0.3876(2)	0.3896(5)	0.2624(2)	55(1)
C(9)	0.4082(2)	0.2267(5)	0.2775(2)	66(1)
C(10)	0.5722(2)	0.6764(6)	0.3707(2)	67(1)
C(11)	0.4692(2)	0.7858(6)	0.4260(2)	70(1)
C(12)	0.4852(2)	0.8602(5)	0.3010(2)	66(1)
C(13)	0.4167(2)	0.2780(8)	0.4388(3)	96(2)
C(14)	0.2991(3)	0.1992(6)	0.3858(2)	72(1)
C(15)	0.3153(3)	0.4348(7)	0.4688(2)	85(2)
Ru(2)	0.66784(2)	0.47264(4)	0.15017(1)	48(1)
P(3)	0.65127(5)	0.61764(12)	0.00678(5)	47(1)
P(4)	0.59356(5)	0.28343(13)	0.14722(5)	50(1)
C(16)	0.7165(5)	0.6783(10)	0.1911(4)	132(3)
C(17)	0.7183(5)	0.5591(10)	0.2318(3)	125(3)
C(18)	0.6609(5)	0.5232(8)	0.2450(3)	116(3)
C(19)	0.6206(4)	0.6292(10)	0.2079(4)	121(3)

C(20)	0.6573(6)	0.7187(8)	0.1772(3)	122(3)
C(21)	0.6704(2)	0.4579(4)	0.0530(2)	42(1)
C(22)	0.7290(2)	0.4429(5)	0.0849(2)	52(1)
C(23)	0.7399(2)	0.3147(5)	0.1245(2)	56(1)
C(24)	0.7295(2)	0.1491(5)	0.1062(2)	62(1)
C(25)	0.6619(3)	0.5799(6)	-0.0702(2)	82(2)
C(26)	0.5729(2)	0.6602(8)	0.0087(3)	92(2)
C(27)	0.6952(3)	0.7858(5)	0.0267(2)	75(1)
C(28)	0.5723(2)	0.1682(7)	0.0806(2)	83(2)
C(29)	0.6031(3)	0.1338(6)	0.2044(2)	82(2)
C(30)	0.5187(3)	0.3551(9)	0.1610(4)	115(3)
P(5)	0.60431(5)	0.19819(14)	0.40901(5)	56(1)
F(1)	0.5765(1)	0.3343(3)	0.4456(1)	82(1)
F(2)	0.6310(2)	0.0638(4)	0.3714(2)	108(1)
F(3)	0.6482(2)	0.1548(6)	0.4662(2)	125(1)
F(4)	0.5628(2)	0.2501(6)	0.3526(2)	143(2)
F(5)	0.5537(2)	0.0903(5)	0.4296(3)	150(2)
F(6)	0.6554(2)	0.3097(5)	0.3906(2)	131(2)
P(6)	0.41411(6)	0.87030(2)	0.10717(5)	64(1)
F(7)	0.4382(3)	0.9759(7)	0.0598(2)	186(3)
F(8)	0.3930(4)	0.7520(9)	0.1497(2)	252(5)
F(9)	0.4739(3)	0.8923(9)	0.1467(3)	202(3)
F(10)	0.3537(2)	0.8513(7)	0.0672(3)	162(2)
F(11)	0.4335(3)	0.7303(6)	0.0683(3)	168(2)
F(12)	0.3922(4)	1.0048(11)	0.1401(5)	311(6)

Supporting Table S40. Hydrogen coordinates and isotropic displacement parameters ($Å^2 \times 10^3$) for [Ru(η^5-C_5H_5)(η^3-CH_3-C_3H_3-PMe_3)(PMe_3)]PF_6 (**18**).

	x	y	z	U_{iso}
H(1)	0.3221(3)	0.7622(7)	0.2340(3)	108
H(2)	0.2457(3)	0.5516(7)	0.2481(4)	119
H(3)	0.2315(2)	0.5397(7)	0.3562(4)	118
H(4)	0.2980(3)	0.7417(7)	0.4101(3)	107
H(5)	0.3515(2)	0.8796(6)	0.3331(4)	103
H(6)	0.4683(2)	0.4496(4)	0.3542(2)	49
H(7)	0.4318(2)	0.5987(5)	0.2440(2)	57
H(8)	0.3647(2)	0.3962(5)	0.2230(2)	66
H(9A)	0.3762(2)	0.1553(5)	0.2648(2)	98
H(9B)	0.4180(2)	0.2177(5)	0.3200(2)	98
H(9C)	0.4434(2)	0.2031(5)	0.2572(2)	98
H(10A)	0.5930(2)	0.7710(6)	0.3822(2)	101
H(10B)	0.5873(2)	0.6366(6)	0.3349(2)	101
H(10C)	0.5792(2)	0.6016(6)	0.4024(2)	101
H(11A)	0.4920(2)	0.8776(6)	0.4375(2)	106
H(11B)	0.4763(2)	0.7084(6)	0.4566(2)	106
H(11C)	0.4268(2)	0.8105(6)	0.4209(2)	106
H(12A)	0.5086(2)	0.9494(5)	0.3146(2)	99
H(12B)	0.4433(2)	0.8889(5)	0.2934(2)	99
H(12C)	0.4998(2)	0.8215(5)	0.2648(2)	99
H(13A)	0.4402(2)	0.2346(8)	0.4090(3)	144
H(13B)	0.4058(2)	0.1975(8)	0.4654(3)	144
H(13C)	0.4403(2)	0.3554(8)	0.4613(3)	144
H(14A)	0.2611(3)	0.2336(6)	0.3661(2)	109
H(14B)	0.2922(3)	0.1471(6)	0.4224(2)	109
H(14C)	0.3181(3)	0.1291(6)	0.3599(2)	109
H(15A)	0.2776(3)	0.4861(7)	0.4571(2)	128
H(15B)	0.3427(3)	0.5063(7)	0.4902(2)	128
H(15C)	0.3082(3)	0.3484(7)	0.4943(2)	128
H(16)	0.7499(5)	0.7235(10)	0.1756(4)	158
H(17)	0.7534(5)	0.5100(10)	0.2481(3)	151
H(18)	0.6496(5)	0.4481(8)	0.2716(3)	139
H(19)	0.5785(4)	0.6335(10)	0.2059(4)	145
H(20)	0.6441(6)	0.7968(8)	0.1505(3)	147
H(21)	0.6544(2)	0.3596(4)	0.0362(2)	50
H(22)	0.7609(2)	0.5197(5)	0.0800(2)	62
H(23)	0.7776(2)	0.3273(5)	0.1506(2)	68

H(24A)	0.7398(2)	0.0827(5)	0.1400(2)	93
H(24B)	0.7544(2)	0.1238(5)	0.0747(2)	93
H(24C)	0.6875(2)	0.1346(5)	0.0921(2)	93
H(25A)	0.6509(3)	0.6703(6)	-0.0938(2)	123
H(25B)	0.6367(3)	0.4943(6)	-0.0843(2)	123
H(25C)	0.7036(3)	0.5549(6)	-0.0737(2)	123
H(26A)	0.5623(2)	0.7477(8)	-0.0166(3)	138
H(26B)	0.5649(2)	0.6838(8)	0.0491(3)	138
H(26C)	0.5492(2)	0.5720(8)	-0.0053(3)	138
H(27A)	0.6827(3)	0.8690(5)	-0.0002(2)	113
H(27B)	0.7374(3)	0.7636(5)	0.0239(2)	113
H(27C)	0.6893(3)	0.8155(5)	0.0670(2)	113
H(28A)	0.5658(2)	0.2354(7)	0.0464(2)	124
H(28B)	0.5357(2)	0.1122(7)	0.0857(2)	124
H(28C)	0.6042(2)	0.0963(7)	0.0744(2)	124
H(29A)	0.6147(3)	0.1808(6)	0.2426(2)	124
H(29B)	0.6342(3)	0.0628(6)	0.1947(2)	124
H(29C)	0.5656(3)	0.0788(6)	0.2060(2)	124
H(30A)	0.5071(3)	0.4372(9)	0.1334(4)	172
H(30B)	0.5197(3)	0.3937(9)	0.2013(4)	172
H(30C)	0.4897(3)	0.2722(9)	0.1557(4)	172

Hydrogen atoms were inserted in idealized positions and were refined riding with the atoms to which they were bonded. All hydrogen atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms

Supporting Table S41.. Anisotropic displacement parameters ($Å^2$ x 10^3) for [Ru(η^5-C_5H_5)(η^3-CH_3-C_3H_3-PMe_3)(PMe_3)]PF_6 (**18**). 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)	41(1)	35(1)	47(1)	-2(1)	-1(1)	7(1)
P(1)	47(1)	41(1)	42(1)	2(1)	8(1)	-1(1)
P(2)	43(1)	50(1)	41(1)	-2(1)	6(1)	-3(1)
C(1)	85(4)	74(4)	109(5)	37(4)	-8(3)	35(3)
C(2)	65(3)	72(4)	150(6)	19(4)	-42(4)	11(3)
C(3)	45(3)	76(4)	175(7)	31(4)	17(4)	23(3)
C(4)	69(3)	73(4)	130(5)	-15(4)	26(3)	32(3)
C(5)	63(3)	40(2)	154(6)	0(3)	4(4)	17(2)
C(6)	44(2)	35(2)	43(2)	2(2)	9(2)	4(2)
C(7)	62(2)	44(2)	38(2)	-3(2)	15(2)	3(2)
C(8)	75(3)	50(2)	40(2)	-11(2)	5(2)	0(2)
C(9)	84(3)	47(2)	69(3)	-17(2)	26(2)	0(2)
C(10)	47(2)	66(3)	88(3)	6(3)	4(2)	-4(2)
C(11)	74(3)	82(3)	56(3)	-24(2)	15(2)	-23(3)
C(12)	82(3)	46(2)	69(3)	14(2)	0(2)	-4(2)
C(13)	61(3)	139(6)	87(4)	67(4)	3(3)	9(3)
C(14)	89(4)	57(3)	72(3)	-2(2)	10(3)	-19(3)
C(15)	109(4)	90(4)	62(3)	-17(3)	36(3)	-19(3)
Ru(2)	61(1)	39(1)	43(1)	-6(1)	-4(1)	0(1)
P(3)	43(1)	44(1)	55(1)	10(1)	3(1)	-8(1)
P(4)	48(1)	59(1)	45(1)	6(1)	12(1)	0(1)
C(16)	194(10)	87(5)	111(6)	-52(5)	-2(6)	-50(6)
C(17)	197(10)	102(6)	67(4)	-27(4)	-41(5)	-25(6)
C(18)	235(10)	67(4)	49(3)	-19(3)	31(5)	-4(5)
C(19)	168(8)	107(6)	93(5)	-54(5)	37(5)	25(6)
C(20)	238(11)	49(3)	80(5)	-21(3)	16(6)	20(5)
C(21)	41(2)	37(2)	48(2)	3(2)	7(2)	-6(2)
C(22)	36(2)	50(2)	69(3)	7(2)	5(2)	-5(2)
C(23)	42(2)	56(2)	69(3)	6(2)	-3(2)	3(2)
C(24)	67(3)	51(2)	70(3)	7(2)	20(2)	14(2)
C(25)	124(5)	65(3)	57(3)	12(2)	14(3)	-20(3)
C(26)	52(3)	106(5)	117(5)	52(4)	7(3)	14(3)
C(27)	93(4)	44(2)	85(3)	13(2)	-6(3)	-20(2)
C(28)	73(3)	108(4)	67(3)	-7(3)	4(2)	-46(3)
C(29)	108(4)	76(3)	63(3)	18(3)	7(3)	-17(3)
C(30)	70(4)	128(6)	155(7)	29(5)	56(4)	23(4)
P(5)	43(1)	60(1)	66(1)	-13(1)	4(1)	1(1)
F(1)	94(2)	70(2)	85(2)	-15(2)	29(2)	3(2)

F(2)	88(2)	102(3)	132(3)	-53(2)	1(2)	32(2)
F(3)	120(3)	152(4)	98(3)	2(3)	-22(2)	43(3)
F(4)	129(3)	206(5)	87(2)	-43(3)	-35(2)	91(3)
F(5)	112(3)	84(3)	264(6)	-38(3)	79(4)	-42(2)
F(6)	103(3)	133(3)	165(4)	-9(3)	69(3)	-34(3)
P(6)	69(1)	68(1)	54(1)	2(1)	3(1)	-12(1)
F(7)	239(6)	183(5)	128(4)	53(4)	-23(4)	-130(5)
F(8)	380(10)	293(9)	83(3)	57(4)	13(4)	-190(8)
F(9)	142(4)	296(8)	151(4)	67(5)	-74(4)	-89(5)
F(10)	100(3)	192(5)	184(5)	5(4)	-46(3)	-35(3)
F(11)	190(5)	136(4)	186(5)	-36(4)	63(4)	9(4)
F(12)	242(9)	304(10)	383(13)	-261(10)	7(8)	61(7)

Supporting Table S42. Complete bond lengths [Å] and angles [deg] for $[Ru(\eta^5\text{-}C_5H_5)(\eta^3\text{-}CH_3\text{-}C_3H_3\text{-}PMe_3)(PMe_3)]PF_6$ **(18)**.

Bond lengths

Ru(1)-C(7)	2.101(4)
Ru(1)-C(3)	2.186(5)
Ru(1)-C(6)	2.187(4)
Ru(1)-C(2)	2.205(5)
Ru(1)-C(4)	2.205(5)
Ru(1)-C(1)	2.215(5)
Ru(1)-C(8)	2.220(4)
Ru(1)-C(5)	2.222(5)
Ru(1)-P(2)	2.3037(11)
P(1)-C(6)	1.767(4)
P(1)-C(12)	1.781(4)
P(1)-C(11)	1.785(4)
P(1)-C(10)	1.788(4)
P(2)-C(13)	1.815(5)
P(2)-C(15)	1.816(5)
P(2)-C(14)	1.824(5)
C(1)-C(5)	1.387(9)
C(1)-C(2)	1.421(9)
C(2)-C(3)	1.382(10)
C(3)-C(4)	1.420(9)
C(4)-C(5)	1.390(9)
C(6)-C(7)	1.431(5)
C(7)-C(8)	1.430(6)
C(8)-C(9)	1.505(6)
P(5)-F(4)	1.558(4)
P(5)-F(5)	1.559(4)
P(5)-F(6)	1.568(4)
P(5)-F(2)	1.578(3)
P(5)-F(3)	1.579(4)
P(5)-F(1)	1.588(3)
P(6)-F(12)	1.481(6)
P(6)-F(8)	1.499(5)
P(6)-F(7)	1.530(5)
P(6)-F(9)	1.536(4)
P(6)-F(10)	1.548(4)
P(6)-F(11)	1.572(5)

Bond angles

C(7)-Ru(1)-C(3)	151.4(3)
C(7)-Ru(1)-C(6)	38.9(2)
C(3)-Ru(1)-C(6)	164.1(2)
C(7)-Ru(1)-C(2)	114.8(3)
C(3)-Ru(1)-C(2)	36.7(3)
C(6)-Ru(1)-C(2)	149.9(2)
C(7)-Ru(1)-C(4)	143.9(2)
C(3)-Ru(1)-C(4)	37.7(2)
C(6)-Ru(1)-C(4)	126.4(2)
C(2)-Ru(1)-C(4)	62.3(3)
C(7)-Ru(1)-C(1)	93.7(2)
C(3)-Ru(1)-C(1)	61.7(2)
C(6)-Ru(1)-C(1)	116.3(2)
C(2)-Ru(1)-C(1)	37.5(2)
C(4)-Ru(1)-C(1)	61.8(3)
C(7)-Ru(1)-C(8)	38.5(2)
C(3)-Ru(1)-C(8)	128.1(3)
C(6)-Ru(1)-C(8)	67.7(2)
C(2)-Ru(1)-C(8)	99.5(3)
C(4)-Ru(1)-C(8)	161.7(2)
C(1)-Ru(1)-C(8)	102.6(2)
C(7)-Ru(1)-C(5)	108.2(2)
C(3)-Ru(1)-C(5)	61.4(2)
C(6)-Ru(1)-C(5)	106.9(2)
C(2)-Ru(1)-C(5)	61.6(2)
C(4)-Ru(1)-C(5)	36.6(2)
C(1)-Ru(1)-C(5)	36.4(2)
C(8)-Ru(1)-C(5)	134.1(2)
C(7)-Ru(1)-P(2)	14.19(11)
C(3)-Ru(1)-P(2)	89.2(2)
C(6)-Ru(1)-P(2)	10.67(10)
C(2)-Ru(1)-P(2)	117.2(2)
C(4)-Ru(1)-P(2)	96.0(2)
C(1)-Ru(1)-P(2)	151.0(2)
C(8)-Ru(1)-P(2)	5.11(12)
C(5)-Ru(1)-P(2)	130.7(2)
C(6)-P(1)-C(12)	112.5(2)
C(6)-P(1)-C(11)	109.7(2)
C(12)-P(1)-C(11)	110.3(3)
C(6)-P(1)-C(10)	112.4(2)
C(12)-P(1)-C(10)	105.8(2)
C(11)-P(1)-C(10)	106.0(2)
C(13)-P(2)-C(15)	98.8(3)
C(13)-P(2)-C(14)	102.7(3)
C(15)-P(2)-C(14)	98.4(3)
C(13)-P(2)-Ru(1)	122.1(2)
C(15)-P(2)-Ru(1)	114.1(2)
C(14)-P(2)-Ru(1)	116.9(2)
C(5)-C(1)-C(2)	107.6(6)
C(5)-C(1)-Ru(1)	72.1(3)
C(2)-C(1)-Ru(1)	70.8(3)
C(3)-C(2)-C(1)	107.3(6)
C(3)-C(2)-Ru(1)	70.9(3)
C(1)-C(2)-Ru(1)	71.6(3)
C(2)-C(3)-C(4)	109.1(6)
C(2)-C(3)-Ru(1)	72.4(3)
C(4)-C(3)-Ru(1)	71.9(3)
C(5)-C(4)-C(3)	106.5(6)
C(5)-C(4)-Ru(1)	72.4(3)
C(3)-C(4)-Ru(1)	70.4(3)
C(1)-C(5)-C(4)	109.6(6)

C(1)-C(5)-Ru(1)	71.5(3)	C(20)-C(16)-C(17)	108.1(9)
C(4)-C(5)-Ru(1)	71.1(3)	C(20)-C(16)-Ru(2)	72.1(4)
C(7)-C(6)-P(1)	121.2(3)	C(17)-C(16)-Ru(2)	70.2(4)
C(7)-C(6)-Ru(1)	67.3(2)	C(18)-C(17)-C(16)	110.1(9)
P(1)-C(6)-Ru(1)	120.0(2)	C(18)-C(17)-Ru(2)	71.9(4)
C(8)-C(7)-C(6)	118.0(4)	C(16)-C(17)-Ru(2)	73.6(4)
C(8)-C(7)-Ru(1)	75.2(2)	C(17)-C(18)-C(19)	105.2(7)
C(6)-C(7)-Ru(1)	73.8(2)	C(17)-C(18)-Ru(2)	71.7(4)
C(7)-C(8)-C(9)	123.5(4)	C(19)-C(18)-Ru(2)	70.7(3)
C(7)-C(8)-Ru(1)	66.2(2)	C(20)-C(19)-C(18)	106.2(8)
C(9)-C(8)-Ru(1)	123.5(3)	C(20)-C(19)-Ru(2)	73.2(4)
		C(18)-C(19)-Ru(2)	69.9(3)
C(22)-Ru(2)-C(17)	108.2(3)	C(19)-C(20)-C(16)	110.4(8)
C(22)-Ru(2)-C(21)	38.9(2)	C(19)-C(20)-Ru(2)	71.1(4)
C(17)-Ru(2)-C(21)	142.7(3)	C(16)-C(20)-Ru(2)	72.3(4)
C(22)-Ru(2)-C(18)	143.9(3)	C(19)-C(20)-H(20)	124.8(7)
C(17)-Ru(2)-C(18)	36.4(3)	C(16)-C(20)-H(20)	124.8(6)
C(21)-Ru(2)-C(18)	171.4(2)	Ru(2)-C(20)-H(20)	123.4(2)
C(22)-Ru(2)-C(19)	149.0(3)	C(22)-C(21)-P(3)	121.7(3)
C(17)-Ru(2)-C(19)	62.1(4)	C(22)-C(21)-Ru(2)	67.2(2)
C(21)-Ru(2)-C(19)	132.7(3)	P(3)-C(21)-Ru(2)	121.1(2)
C(18)-Ru(2)-C(19)	39.4(3)	C(23)-C(22)-C(21)	118.3(4)
C(22)-Ru(2)-C(23)	38.4(2)	C(23)-C(22)-Ru(2)	75.2(3)
C(17)-Ru(2)-C(23)	95.9(3)	C(21)-C(22)-Ru(2)	73.8(2)
C(21)-Ru(2)-C(23)	67.7(2)	C(22)-C(23)-C(24)	123.9(4)
C(18)-Ru(2)-C(23)	119.5(3)	C(22)-C(23)-Ru(2)	66.4(2)
C(19)-Ru(2)-C(23)	157.5(3)	C(24)-C(23)-Ru(2)	124.2(3)
C(22)-Ru(2)-C(20)	113.4(3)		
C(17)-Ru(2)-C(20)	60.3(3)	F(4)-P(5)-F(5)	91.4(3)
C(21)-Ru(2)-C(20)	109.9(2)	F(4)-P(5)-F(6)	89.7(3)
C(18)-Ru(2)-C(20)	61.8(3)	F(5)-P(5)-F(6)	177.9(3)
C(19)-Ru(2)-C(20)	35.6(3)	F(4)-P(5)-F(2)	90.0(2)
C(23)-Ru(2)-C(20)	138.9(4)	F(5)-P(5)-F(2)	92.0(2)
C(22)-Ru(2)-C(16)	93.7(3)	F(6)-P(5)-F(2)	89.7(2)
C(17)-Ru(2)-C(16)	36.2(3)	F(4)-P(5)-F(3)	176.7(3)
C(21)-Ru(2)-C(16)	113.6(3)	F(5)-P(5)-F(3)	91.4(3)
C(18)-Ru(2)-C(16)	61.1(3)	F(6)-P(5)-F(3)	87.4(3)
C(19)-Ru(2)-C(16)	60.5(4)	F(2)-P(5)-F(3)	91.5(2)
C(23)-Ru(2)-C(16)	105.3(3)	F(4)-P(5)-F(1)	88.7(2)
C(20)-Ru(2)-C(16)	35.7(3)	F(5)-P(5)-F(1)	87.9(2)
C(22)-Ru(2)-P(4)	13.39(12)	F(6)-P(5)-F(1)	90.4(2)
C(17)-Ru(2)-P(4)	124.9(3)	F(2)-P(5)-F(1)	178.8(2)
C(21)-Ru(2)-P(4)	90.80(10)	F(3)-P(5)-F(1)	89.7(2)
C(18)-Ru(2)-P(4)	93.1(3)		
C(19)-Ru(2)-P(4)	94.3(3)	F(12)-P(6)-F(8)	94.6(6)
C(23)-Ru(2)-P(4)	94.92(12)	F(12)-P(6)-F(7)	91.7(6)
C(20)-Ru(2)-P(4)	126.1(3)	F(8)-P(6)-F(7)	173.6(5)
C(16)-Ru(2)-P(4)	152.7(3)	F(12)-P(6)-F(9)	85.4(5)
C(21)-P(3)-C(26)	109.3(2)	F(8)-P(6)-F(9)	91.1(4)
C(21)-P(3)-C(27)	113.4(2)	F(7)-P(6)-F(9)	89.4(3)
C(26)-P(3)-C(27)	109.7(3)	F(12)-P(6)-F(10)	93.8(4)
C(21)-P(3)-C(25)	112.4(2)	F(8)-P(6)-F(10)	89.6(4)
C(26)-P(3)-C(25)	106.0(3)	F(7)-P(6)-F(10)	90.0(3)
C(27)-P(3)-C(25)	105.8(3)	F(9)-P(6)-F(10)	179.0(4)
C(29)-P(4)-C(28)	101.3(3)	F(12)-P(6)-F(11)	175.6(5)
C(29)-P(4)-C(30)	99.8(3)	F(8)-P(6)-F(11)	86.9(4)
C(28)-P(4)-C(30)	98.9(3)	F(7)-P(6)-F(11)	86.7(3)
C(29)-P(4)-Ru(2)	116.4(2)	F(9)-P(6)-F(11)	98.6(4)
C(28)-P(4)-Ru(2)	122.5(2)	F(10)-P(6)-F(11)	82.2(3)
C(30)-P(4)-Ru(2)	114.3(3)		

Supporting Table S43.. Least-squares planes for [Ru(η^5-C_5H_5)(η^3-CH_3-C_3H_3-PMe_3)(PMe_3)]PF_6 (**18**).

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

16.321 (0.037) x - 5.701 (0.016) y + 1.556 (0.060) z = 1.259 (0.028)

* 0.006 (0.003) C1
* -0.002 (0.003) C2

```
*   -0.001 (0.003)  C3
*    0.005 (0.003)  C4
*   -0.006 (0.003)  C5
     1.857 (0.002)  Ru1
     3.269 (0.008)  P1
     2.967 (0.006)  P2
     3.518 (0.005)  C6
     3.116 (0.006)  C7
     3.254 (0.007)  C8
     4.541 (0.007)  C9
     4.800 (0.011)  C10
     2.581 (0.011)  C11
     2.224 (0.011)  C12
     4.640 (0.009)  C13
     3.087 (0.010)  C14
     2.138 (0.012)  C15
Rms deviation of fitted atoms =   0.005

 18.356 (0.045) x - 4.462 (0.040) y - 6.424 (0.109) z = 3.691 (0.026)
Angle to previous plane (with approximate esd) = 22.41 ( 0.42 )
*    0.000 (0.000)  C6
*    0.000 (0.000)  C7
*    0.000 (0.000)  C8
    -1.796 (0.005)  Ru1
    -0.125 (0.008)  P1
     1.007 (0.011)  C9
Rms deviation of fitted atoms =   0.000

 0.036 (0.075) x + 5.746 (0.019) y + 16.631 (0.044) z = 7.099 (0.049)
Angle to previous plane (with approximate esd) = 59.96 ( 0.37 )
*    0.002 (0.004)  C16
*   -0.005 (0.004)  C17
*    0.006 (0.004)  C18
*   -0.005 (0.004)  C19
*    0.002 (0.004)  C20
    -1.862 (0.002)  Ru2
    -3.414 (0.009)  P3
    -3.000 (0.007)  P4
    -3.562 (0.006)  C21
    -3.115 (0.008)  C22
    -3.194 (0.008)  C23
    -4.450 (0.008)  C24
    -4.911 (0.013)  C25
    -3.140 (0.014)  C26
    -2.115 (0.013)  C27
    -4.771 (0.009)  C28
    -2.909 (0.012)  C29
    -2.362 (0.014)  C30
Rms deviation of fitted atoms =   0.004

 8.322 (0.119) x + 4.692 (0.045) y + 17.512 (0.047) z = 2.502 (0.099)
Angle to previous plane (with approximate esd) = 22.89 ( 0.47 )

*    0.000 (0.000)  C21
*    0.000 (0.000)  C22
*    0.000 (0.000)  C23
    -1.791 (0.005)  Ru2
    -8.368 (0.054)  P2
     1.011 (0.012)  C24
Rms deviation of fitted atoms =   0.000
```