Table 1. Crystal data and structure refinement for $[Ru(dppe)(CO)(CH_3CN)_3][OTf]_2.2(CHCl_3)$ (**2**).

Identification code	k00mkw2
Empirical formula	C37 H35 Cl6 F6 N3 O7 P2 Ru S2
Formula weight	1187.51
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.2606(3)Å α = 90°
	b = 13.8259(3)Å β = 99.5870(10)°
	c = 29.5038(5)Å γ = 90°
Volume	4931.45(18) $Å^3$
Z	4
Density (calculated)	1.599 Mg/m^3
Absorption coefficient	0.863 mm^{-1}
F(000)	2384
Crystal size	0.37 x 0.20 x 0.13 mm
Theta range for data collection	1.71 to 26.37°
Index ranges	-15<=h<=15; -16<=k<=17; -32<=l<=34
Reflections collected	20389
Independent reflections	9648 [R(int) = 0.0329]
Reflections observed (>2σ)	7901
Data Completeness	0.958
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.03 and 0.99
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9648 / 15 / 609
Goodness-of-fit on F^2	1.034
Final R indices [I>2σ(I)]	R_1 = 0.0383 wR_2 = 0.1042
R indices (all data)	R_1 = 0.0541 wR_2 = 0.1191
Largest diff. peak and hole	0.744 and -0.727 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppe)(CO)(CH_3CN)_3][OTf]_2.2(CHCl_3)$ (**2**).U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1048(1)	2114(1)	-1766(1)	21(1)
P(1)	1751(1)	3033(1)	-2304(1)	23(1)
P(2)	2758(1)	2368(1)	-1317(1)	25(1)
S(1)	-3928(1)	3948(1)	-2425(1)	32(1)
S(2)	114(1)	-2451(1)	15(1)	37(1)
N(2)	252(2)	3325(2)	-1546(1)	26(1)
O(1)	2032(2)	298(2)	-2086(1)	39(1)
O(2)	-4535(2)	4750(2)	-2285(1)	52(1)
O(3)	-2762(2)	3960(2)	-2265(1)	56(1)
O(4)	-4448(2)	3021(2)	-2405(1)	43(1)
O(5)	429(2)	-3124(2)	383(1)	52(1)
O(6)	895(2)	-1680(2)	-2(1)	59(1)
O(7)	-1012(2)	-2152(2)	-59(1)	55(1)
N(1)	-484(2)	1910(2)	-2199(1)	25(1)
N(3)	467(2)	1306(2)	-1246(1)	29(1)
F(1)	1233(3)	-3447(2)	-502(1)	95(1)
F(2)	-67(3)	-2617(3)	-873(1)	95(1)
F(3)	-434(3)	-3922(3)	-511(1)	123(1)
F(4)	-3527(2)	4961(2)	-3136(1)	52(1)
F(5)	-5076(2)	4198(2)	-3251(1)	60(1)
F(6)	-3556(2)	3432(2)	-3240(1)	66(1)
Cl(1)	-4457(1)	7251(1)	-407(1)	54(1)
Cl(2)	-3200(1)	8063(1)	-1057(1)	80(1)
Cl(3)	-3334(1)	5993(1)	-955(1)	67(1)
Cl(4)	-1192(2)	7466(2)	-4514(1)	90(1)
Cl(5)	-2003(2)	7620(2)	-3649(1)	89(1)
Cl(6)	-2084(2)	5809(1)	-4121(1)	80(1)
Cl(4')	-1767(7)	8452(7)	-4029(6)	175(6)
Cl(5')	-2643(8)	6998(11)	-3671(3)	151(5)
Cl(6')	-1069(9)	6624(16)	-4273(6)	240(11)
C(1)	940(2)	4107(2)	-2488(1)	24(1)
C(2)	1092(3)	4979(2)	-2249(1)	35(1)
C(3)	422(3)	5767(2)	-2394(1)	42(1)
C(4)	-406(3)	5688(3)	-2773(1)	44(1)
C(5)	-573(3)	4828(3)	-3001(1)	45(1)
C(6)	93(3)	4033(2)	-2864(1)	35(1)
C(7)	1896(3)	2448(2)	-2843(1)	26(1)
C(8)	2610(3)	2839(2)	-3116(1)	38(1)
C(9)	2698(4)	2430(3)	-3534(1)	49(1)
C(10)	2068(3)	1626(3)	-3689(1)	47(1)
C(11)	1340(3)	1245(2)	-3429(1)	36(1)
C(12)	1258(3)	1645(2)	-3005(1)	29(1)
C(13)	3139(2)	3437(2)	-2045(1)	30(1)

C(14)	3690(3)	2631(2)	-1726(1)	30(1)
C(15)	2903(3)	3390(2)	-920(1)	27(1)
C(16)	2066(3)	3584(2)	-668(1)	32(1)
C(17)	2184(3)	4328(2)	-345(1)	38(1)
C(18)	3134(3)	4884(2)	-282(1)	43(1)
C(19)	3968(3)	4695(2)	-529(1)	39(1)
C(20)	3864(3)	3954(2)	-846(1)	34(1)
C(21)	3275(3)	1324(2)	-973(1)	32(1)
C(22)	3868(3)	601(3)	-1150(1)	46(1)
C(23)	4156(4)	-236(3)	-897(2)	60(1)
C(24)	3866(4)	-346(3)	-475(2)	63(1)
C(25)	3265(4)	363(3)	-297(1)	63(1)
C(26)	2973(3)	1200(3)	-543(1)	45(1)
C(27)	-1292(3)	1769(2)	-2437(1)	29(1)
C(28)	-2324(3)	1570(3)	-2748(1)	41(1)
C(29)	-319(3)	3913(2)	-1459(1)	30(1)
C(30)	-1057(3)	4668(3)	-1343(1)	50(1)
C(31)	248(3)	766(2)	-986(1)	36(1)
C(32)	-8(5)	42(3)	-659(1)	66(1)
C(33)	1668(2)	991(2)	-1969(1)	27(1)
C(34)	-4020(3)	4138(2)	-3041(1)	38(1)
C(35)	215(4)	-3140(4)	-493(2)	63(1)
C(36)	-3289(3)	7116(3)	-671(1)	45(1)
C(37)	-2180(3)	7127(3)	-4187(1)	63(1)

Table 3. Bond lengths [Å] and angles [°] for $[Ru(dppe)(CO)(CH_3CN)_3][OTf]_2.2(CHCl_3)$ (**2**).

Ru(1)-C(33)	1.870(3)	Ru(1)-N(2)	2.095(2)
Ru(1)-N(1)	2.109(3)	Ru(1)-N(3)	2.115(3)
Ru(1)-P(1)	2.3092(8)	Ru(1)-P(2)	2.3126(8)
P(1)-C(1)	1.819(3)	P(1)-C(7)	1.819(3)
P(1)-C(13)	1.833(3)	P(2)-C(21)	1.816(3)
P(2)-C(15)	1.824(3)	P(2)-C(14)	1.833(3)
S(1)-O(3)	1.429(3)	S(1)-O(2)	1.434(2)
S(1)-O(4)	1.438(2)	S(1)-C(34)	1.823(3)
S(2)-O(7)	1.423(3)	S(2)-O(5)	1.433(3)
S(2)-O(6)	1.440(3)	S(2)-C(35)	1.799(4)
N(2)-C(29)	1.131(4)	O(1)-C(33)	1.135(4)
N(1)-C(27)	1.131(4)	N(3)-C(31)	1.133(4)
F(1)-C(35)	1.322(5)	F(2)-C(35)	1.331(6)
F(3)-C(35)	1.338(6)	F(4)-C(34)	1.339(4)
F(5)-C(34)	1.341(4)	F(6)-C(34)	1.317(4)
Cl(1)-C(36)	1.749(4)	Cl(2)-C(36)	1.749(4)
Cl(3)-C(36)	1.761(4)	Cl(4)-C(37)	1.735(5)
Cl(5)-C(37)	1.707(4)	Cl(6)-C(37)	1.833(5)
C(1)-C(6)	1.390(4)	C(1)-C(2)	1.394(4)
C(2)-C(3)	1.388(5)	C(3)-C(4)	1.383(5)
C(4)-C(5)	1.364(5)	C(5)-C(6)	1.389(5)
C(7)-C(8)	1.395(4)	C(7)-C(12)	1.396(4)
C(8)-C(9)	1.376(5)	C(9)-C(10)	1.387(5)
C(10)-C(11)	1.375(5)	C(11)-C(12)	1.386(4)
C(13)-C(14)	1.541(4)	C(15)-C(16)	1.390(4)
C(15)-C(20)	1.399(4)	C(16)-C(17)	1.394(4)
C(17)-C(18)	1.382(5)	C(18)-C(19)	1.377(5)
C(19)-C(20)	1.378(5)	C(21)-C(22)	1.389(5)
C(21)-C(26)	1.389(5)	C(22)-C(23)	1.390(5)
C(23)-C(24)	1.358(6)	C(24)-C(25)	1.382(6)
C(25)-C(26)	1.380(5)	C(27)-C(28)	1.459(4)
C(29)-C(30)	1.459(4)	C(31)-C(32)	1.461(5)
C(33)-Ru(1)-N(2)	176.20(11)	C(33)-Ru(1)-N(1)	93.59(11)
N(2)-Ru(1)-N(1)	83.13(9)	C(33)-Ru(1)-N(3)	89.95(11)
N(2)-Ru(1)-N(3)	88.12(9)	N(1)-Ru(1)-N(3)	89.74(10)
C(33)-Ru(1)-P(1)	91.04(9)	N(2)-Ru(1)-P(1)	91.06(7)
N(1)-Ru(1)-P(1)	93.06(7)	N(3)-Ru(1)-P(1)	176.96(7)
C(33)-Ru(1)-P(2)	86.12(9)	N(2)-Ru(1)-P(2)	97.24(7)
N(1)-Ru(1)-P(2)	177.54(7)	N(3)-Ru(1)-P(2)	92.71(7)
P(1)-Ru(1)-P(2)	84.49(3)	C(1)-P(1)-C(7)	103.27(13)
C(1)-P(1)-C(13)	107.42(14)	C(7)-P(1)-C(13)	106.27(14)
C(1)-P(1)-Ru(1)	114.03(9)	C(7)-P(1)-Ru(1)	117.26(10)
C(13)-P(1)-Ru(1)	107.97(10)	C(21)-P(2)-C(15)	105.65(14)
C(21)-P(2)-C(14)	109.15(15)	C(15)-P(2)-C(14)	105.31(14)
C(21)-P(2)-Ru(1)	113.46(11)	C(15)-P(2)-Ru(1)	117.87(10)
C(14)-P(2)-Ru(1)	104.93(10)	O(3)-S(1)-O(2)	115.75(18)
O(3)-S(1)-O(4)	115.03(17)	O(2)-S(1)-O(4)	114.98(15)

O(3)-S(1)-C(34)	102.78(16)	O(2)-S(1)-C(34)	103.18(15)
O(4)-S(1)-C(34)	102.39(16)	O(7)-S(2)-O(5)	115.95(17)
O(7)-S(2)-O(6)	114.42(18)	O(5)-S(2)-O(6)	114.34(17)
O(7)-S(2)-C(35)	103.0(2)	O(5)-S(2)-C(35)	103.9(2)
O(6)-S(2)-C(35)	102.9(2)	C(29)-N(2)-Ru(1)	169.6(3)
C(27)-N(1)-Ru(1)	177.5(3)	C(31)-N(3)-Ru(1)	169.8(3)
C(6)-C(1)-C(2)	119.1(3)	C(6)-C(1)-P(1)	118.5(2)
C(2)-C(1)-P(1)	122.3(2)	C(3)-C(2)-C(1)	120.0(3)
C(2)-C(3)-C(4)	120.3(3)	C(5)-C(4)-C(3)	119.7(3)
C(4)-C(5)-C(6)	120.9(4)	C(5)-C(6)-C(1)	119.9(3)
C(8)-C(7)-C(12)	118.7(3)	C(8)-C(7)-P(1)	119.7(2)
C(12)-C(7)-P(1)	121.5(2)	C(9)-C(8)-C(7)	120.5(3)
C(8)-C(9)-C(10)	120.3(3)	C(11)-C(10)-C(9)	119.9(3)
C(10)-C(11)-C(12)	120.2(3)	C(11)-C(12)-C(7)	120.3(3)
C(14)-C(13)-P(1)	108.4(2)	C(13)-C(14)-P(2)	106.7(2)
C(16)-C(15)-C(20)	119.1(3)	C(16)-C(15)-P(2)	119.4(2)
C(20)-C(15)-P(2)	121.5(2)	C(17)-C(16)-C(15)	120.4(3)
C(18)-C(17)-C(16)	119.5(3)	C(19)-C(18)-C(17)	120.4(3)
C(20)-C(19)-C(18)	120.5(3)	C(19)-C(20)-C(15)	120.1(3)
C(22)-C(21)-C(26)	119.4(3)	C(22)-C(21)-P(2)	121.2(3)
C(26)-C(21)-P(2)	119.1(2)	C(23)-C(22)-C(21)	120.0(3)
C(24)-C(23)-C(22)	120.2(4)	C(23)-C(24)-C(25)	120.4(4)
C(26)-C(25)-C(24)	120.2(4)	C(25)-C(26)-C(21)	119.9(3)
N(1)-C(27)-C(28)	178.8(4)	N(2)-C(29)-C(30)	179.5(4)
N(3)-C(31)-C(32)	177.8(4)	O(1)-C(33)-Ru(1)	178.4(3)
F(6)-C(34)-F(4)	107.1(3)	F(6)-C(34)-F(5)	107.2(3)
F(4)-C(34)-F(5)	106.7(3)	F(6)-C(34)-S(1)	112.2(2)
F(4)-C(34)-S(1)	112.0(2)	F(5)-C(34)-S(1)	111.3(2)
F(1)-C(35)-F(3)	107.3(4)	F(1)-C(35)-F(2)	105.8(4)
F(3)-C(35)-F(2)	109.6(4)	F(1)-C(35)-S(2)	112.5(4)
F(3)-C(35)-S(2)	109.8(3)	F(2)-C(35)-S(2)	111.8(3)
Cl(2)-C(36)-Cl(1)	110.7(2)	Cl(2)-C(36)-Cl(3)	110.5(2)
Cl(1)-C(36)-Cl(3)	110.0(2)	Cl(5)-C(37)-Cl(4)	114.6(3)
Cl(5)-C(37)-Cl(6)	107.6(2)	Cl(4)-C(37)-Cl(6)	106.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Ru(dppe)(CO)(CH_3CN)_3][OTf]_2.2(CHCl_3)$ (**2**). The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	19(1)	22(1)	-1(1)	5(1)	1(1)
P(1)	24(1)	21(1)	24(1)	-2(1)	5(1)	-1(1)
P(2)	25(1)	26(1)	25(1)	-2(1)	2(1)	3(1)
S(1)	35(1)	27(1)	36(1)	2(1)	10(1)	-2(1)
S(2)	36(1)	40(1)	33(1)	-2(1)	2(1)	4(1)
N(2)	29(1)	26(1)	25(1)	-2(1)	5(1)	1(1)
O(1)	47(2)	24(1)	47(1)	-5(1)	14(1)	8(1)
O(2)	74(2)	33(1)	57(2)	-3(1)	34(1)	5(1)
O(3)	39(2)	76(2)	49(2)	10(1)	-3(1)	-11(1)
O(4)	50(2)	27(1)	53(2)	6(1)	14(1)	-5(1)
O(5)	48(2)	59(2)	46(2)	18(1)	3(1)	-1(1)
O(6)	60(2)	42(2)	67(2)	7(1)	-10(1)	-10(1)
O(7)	42(2)	74(2)	49(2)	-8(1)	5(1)	18(1)
N(1)	26(1)	22(1)	28(1)	-1(1)	7(1)	-2(1)
N(3)	34(2)	27(1)	27(1)	0(1)	7(1)	2(1)
F(1)	107(2)	93(2)	99(2)	8(2)	57(2)	50(2)
F(2)	107(3)	145(3)	33(1)	-1(2)	12(1)	34(2)
F(3)	157(4)	105(3)	118(3)	-74(2)	58(3)	-62(2)
F(4)	60(1)	44(1)	56(1)	15(1)	24(1)	-2(1)
F(5)	50(1)	70(2)	55(1)	15(1)	-5(1)	-2(1)
F(6)	106(2)	51(1)	47(1)	0(1)	28(1)	30(1)
Cl(1)	55(1)	53(1)	59(1)	-3(1)	20(1)	5(1)
Cl(2)	81(1)	87(1)	75(1)	39(1)	20(1)	1(1)
Cl(3)	61(1)	74(1)	66(1)	-19(1)	13(1)	12(1)
Cl(4)	70(1)	116(2)	83(1)	-4(1)	12(1)	-27(1)
Cl(5)	81(1)	116(2)	62(1)	-41(1)	-13(1)	25(1)
Cl(6)	96(1)	76(1)	61(1)	8(1)	-7(1)	18(1)
Cl(4')	57(5)	98(7)	363(19)	-49(10)	13(8)	9(5)
Cl(5')	82(6)	263(15)	97(6)	86(8)	-17(5)	-9(8)
Cl(6')	86(7)	400(30)	209(14)	-222(17)	-47(8)	117(12)
C(1)	29(2)	19(1)	28(2)	2(1)	11(1)	-1(1)
C(2)	36(2)	26(2)	44(2)	-5(1)	12(2)	-4(1)
C(3)	55(2)	20(2)	59(2)	-4(2)	29(2)	0(2)
C(4)	48(2)	32(2)	56(2)	14(2)	23(2)	15(2)
C(5)	45(2)	43(2)	45(2)	9(2)	6(2)	12(2)
C(6)	42(2)	28(2)	34(2)	2(1)	4(2)	5(1)
C(7)	30(2)	23(1)	24(2)	1(1)	6(1)	3(1)
C(8)	46(2)	32(2)	37(2)	-5(1)	15(2)	-10(2)
C(9)	66(3)	50(2)	38(2)	-9(2)	28(2)	-10(2)
C(10)	56(2)	54(2)	33(2)	-14(2)	14(2)	-2(2)
C(11)	38(2)	34(2)	34(2)	-8(1)	3(1)	0(1)
C(12)	30(2)	27(2)	29(2)	-2(1)	4(1)	1(1)
C(13)	27(2)	32(2)	29(2)	-2(1)	5(1)	-7(1)
C(14)	23(2)	36(2)	33(2)	-6(1)	5(1)	0(1)

C(15)	30(2)	26(2)	24(2)	0(1)	0(1)	2(1)
C(16)	34(2)	33(2)	26(2)	-1(1)	-1(1)	2(1)
C(17)	52(2)	35(2)	26(2)	-2(1)	4(2)	9(2)
C(18)	64(3)	28(2)	32(2)	-4(1)	-4(2)	3(2)
C(19)	45(2)	32(2)	35(2)	3(2)	-5(2)	-8(2)
C(20)	37(2)	33(2)	29(2)	3(1)	1(1)	1(1)
C(21)	30(2)	31(2)	32(2)	-1(1)	-2(1)	4(1)
C(22)	49(2)	42(2)	48(2)	5(2)	12(2)	17(2)
C(23)	70(3)	45(2)	67(3)	11(2)	15(2)	30(2)
C(24)	79(3)	43(2)	63(3)	21(2)	3(2)	25(2)
C(25)	91(4)	56(3)	40(2)	17(2)	7(2)	20(2)
C(26)	60(3)	40(2)	33(2)	1(2)	5(2)	16(2)
C(27)	31(2)	23(1)	33(2)	1(1)	11(1)	1(1)
C(28)	32(2)	40(2)	46(2)	-1(2)	-4(2)	1(2)
C(29)	34(2)	29(2)	25(2)	-4(1)	3(1)	1(1)
C(30)	49(2)	42(2)	56(2)	-17(2)	3(2)	17(2)
C(31)	53(2)	28(2)	28(2)	0(1)	11(2)	2(2)
C(32)	122(4)	38(2)	43(2)	12(2)	31(2)	0(2)
C(33)	28(2)	26(2)	26(2)	1(1)	6(1)	-3(1)
C(34)	42(2)	31(2)	43(2)	3(2)	13(2)	7(2)
C(35)	66(3)	67(3)	58(3)	-10(2)	21(2)	3(2)
C(36)	38(2)	52(2)	43(2)	5(2)	2(2)	2(2)
C(37)	36(2)	97(4)	51(3)	-6(2)	-8(2)	10(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppe)(CO)(CH_3CN)_3][OTf]_2.2(CHCl_3)$ (**2**).

Atom	x	y	z	U(eq)
H(2)	1653	5034	-1987	41
H(3)	532	6362	-2233	51
H(4)	-856	6231	-2874	52
H(5)	-1154	4772	-3256	53
H(6)	-29	3440	-3027	42
H(8)	3039	3393	-3013	45
H(9)	3192	2698	-3716	59
H(10)	2139	1339	-3975	56
H(11)	893	707	-3540	43
H(12)	764	1371	-2824	34
H(13A)	3584	3573	-2289	35
H(13B)	3090	4038	-1867	35
H(14A)	4419	2848	-1562	36
H(14B)	3800	2045	-1907	36
H(16)	1410	3206	-716	38
H(17)	1615	4453	-170	46
H(18)	3212	5400	-66	51
H(19)	4620	5078	-481	46
H(20)	4445	3827	-1014	40
H(22)	4077	678	-1444	55
H(23)	4558	-732	-1019	72
H(24)	4077	-914	-302	75
H(25)	3051	275	-5	75
H(26)	2567	1690	-419	53
H(28A)	-2918	1965	-2659	61
H(28B)	-2511	883	-2728	61
H(28C)	-2235	1727	-3063	61
H(30A)	-1150	4598	-1021	75
H(30B)	-1779	4610	-1541	75
H(30C)	-739	5304	-1388	75
H(32A)	-540	-424	-818	99
H(32B)	-327	361	-415	99
H(32C)	672	-296	-524	99
H(36)	-2616	7132	-428	54
H(37)	-2931	7301	-4355	76

Table 6. Crystal data and structure refinement for $[Ru(dppe)(CO)(DMSO)_3][OTf]_2$ (**3**).

Identification code	k01mkw8
Empirical formula	C38 H48 F6 O11 P2 Ru S5
Formula weight	1118.07
Temperature	150(2) K
Wavelength	0.71070 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 11.53960(10)Å α = 90°
	b = 20.25930(10)Å β = 90°
	c = 20.42650(10)Å γ = 90°
Volume	4775.39(5) $Å^3$
Z	4
Density (calculated)	1.555 Mg/m^3
Absorption coefficient	0.691 mm^{-1}
F(000)	2288
Crystal size	0.28 x 0.25 x 0.25 mm
Theta range for data collection	4.60 to 30.03°
Index ranges	-15<=h<=16; -28<=k<=27; -28<=l<=28
Reflections collected	92137
Independent reflections	13879 [R(int) = 0.0377]
Reflections observed (>2σ)	13626
Data Completeness	0.992
Max. and min. transmission	0.8462 and 0.8300
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13879 / 0 / 603
Goodness-of-fit on F^2	1.105
Final R indices [I>2σ(I)]	R_1 = 0.0339 wR_2 = 0.0739
R indices (all data)	R_1 = 0.0350 wR_2 = 0.0743
Absolute structure parameter	0.000(17)
Largest diff. peak and hole	0.816 and -0.819 $eÅ^{-3}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppe)(CO)(DMSO)_3][OTf]_2$ (**3**).U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	9702(1)	9985(1)	7225(1)	19(1)
S(1)	6996(1)	10376(1)	6991(1)	55(1)
S(2)	9489(1)	11547(1)	7272(1)	24(1)
S(3)	9430(1)	10285(1)	5610(1)	36(1)
S(4)	4608(1)	10589(1)	8995(1)	40(1)
S(5)	7411(1)	12579(1)	6112(1)	26(1)
F(1)	4926(2)	11849(1)	9261(1)	66(1)
F(2)	5927(2)	11194(1)	9851(1)	55(1)
F(3)	6396(2)	11364(1)	8846(1)	60(1)
F(4)	5965(2)	13532(1)	6421(1)	50(1)
F(5)	5226(2)	12784(1)	5798(1)	48(1)
F(6)	5508(2)	12587(1)	6819(1)	56(1)
P(1)	11611(1)	9742(1)	7024(1)	19(1)
P(2)	10098(1)	9654(1)	8272(1)	19(1)
C(1)	9278(2)	9134(1)	7044(1)	27(1)
C(2)	12388(7)	10346(4)	6537(3)	24(1)
C(3)	12860(8)	10900(5)	6836(3)	20(2)
C(4)	13426(8)	11374(4)	6461(5)	29(3)
C(5)	13518(7)	11293(3)	5787(4)	37(2)
C(6)	13046(6)	10738(3)	5488(3)	51(2)
C(7)	12480(5)	10265(3)	5863(3)	42(2)
C(2A)	12495(9)	10331(5)	6540(4)	24(1)
C(3A)	12678(10)	10966(7)	6776(5)	21(2)
C(4A)	13331(11)	11413(5)	6414(7)	32(3)
C(5A)	13800(9)	11224(4)	5816(6)	57(4)
C(6A)	13616(8)	10589(4)	5580(4)	66(4)
C(7A)	12963(8)	10143(4)	5942(4)	48(3)
C(8)	11943(2)	8960(1)	6626(1)	23(1)
C(9)	11282(2)	8756(1)	6094(1)	29(1)
C(10)	11564(3)	8189(1)	5749(1)	32(1)
C(11)	12511(3)	7821(1)	5928(1)	36(1)
C(12)	13186(3)	8015(2)	6457(2)	47(1)
C(13)	12900(2)	8586(1)	6808(2)	36(1)
C(14)	12329(2)	9723(1)	7821(1)	23(1)
C(15)	11570(2)	9321(1)	8295(1)	22(1)
C(16)	9174(2)	9030(1)	8637(1)	22(1)
C(17)	9602(2)	8606(1)	9120(1)	26(1)
C(18)	8856(3)	8155(1)	9415(1)	33(1)
C(19)	7700(2)	8129(1)	9246(1)	34(1)
C(20)	7271(3)	8552(2)	8773(1)	38(1)
C(21)	8008(2)	9002(1)	8469(1)	34(1)
C(22)	10058(2)	10315(1)	8878(1)	22(1)
C(23)	11071(2)	10565(1)	9157(1)	32(1)

C(24)	11009(3)	11040(2)	9648(1)	40(1)
C(25)	9959(3)	11266(2)	9863(1)	42(1)
C(26)	8946(3)	11031(2)	9580(2)	41(1)
C(27)	8994(2)	10557(1)	9087(1)	32(1)
C(28)	5899(3)	9807(2)	7259(2)	66(1)
C(29)	6289(3)	11121(2)	7214(3)	73(1)
C(30)	9307(5)	12014(2)	7999(2)	65(1)
C(31)	10497(3)	12066(2)	6865(2)	57(1)
C(32)	7990(4)	10321(2)	5306(2)	63(1)
C(33)	9978(5)	11000(2)	5211(2)	79(2)
C(34)	5504(3)	11276(1)	9252(2)	38(1)
C(35)	5962(2)	12882(1)	6296(1)	32(1)
C(57)	6847(3)	7917(2)	6418(2)	55(1)
C(61)	6598(5)	7573(4)	7034(2)	101(2)
C(63)	7618(5)	7609(3)	5944(2)	83(2)
O(2)	7967(2)	10311(1)	7497(1)	30(1)
O(3)	10231(2)	10956(1)	7500(1)	24(1)
O(4)	9329(2)	10500(1)	6328(1)	33(1)
O(5)	3785(2)	10534(2)	9518(1)	65(1)
O(6)	4160(2)	10809(2)	8378(1)	61(1)
O(7)	5431(3)	10063(1)	8955(1)	64(1)
O(8)	7759(2)	12990(1)	5576(1)	46(1)
O(9)	8010(2)	12696(1)	6721(1)	36(1)
O(10)	7216(2)	11895(1)	5953(1)	41(1)
O(1)	9009(2)	8595(1)	6962(1)	41(1)
O(11)	6432(4)	8446(2)	6303(2)	129(2)

Table 8. Bond lengths [Å] and angles [°] for $[Ru(dppe)(CO)(DMSO)_3][OTf]_2$ (**3**).

Ru(1)-C(1)	1.831(2)	Ru(1)-O(3)	2.1350(16)
Ru(1)-O(4)	2.1524(17)	Ru(1)-O(2)	2.1810(17)
Ru(1)-P(2)	2.2866(5)	Ru(1)-P(1)	2.2941(6)
S(1)-O(2)	1.5305(18)	S(1)-C(29)	1.775(4)
S(1)-C(28)	1.798(4)	S(2)-O(3)	1.5444(16)
S(2)-C(31)	1.773(3)	S(2)-C(30)	1.774(3)
S(3)-O(4)	1.5345(18)	S(3)-C(32)	1.776(4)
S(3)-C(33)	1.780(4)	S(4)-O(7)	1.430(3)
S(4)-O(5)	1.434(3)	S(4)-O(6)	1.433(2)
S(4)-C(34)	1.812(3)	S(5)-O(8)	1.432(2)
S(5)-O(10)	1.440(2)	S(5)-O(9)	1.4426(19)
S(5)-C(35)	1.822(3)	F(1)-C(34)	1.338(4)
F(2)-C(34)	1.329(3)	F(3)-C(34)	1.333(4)
F(4)-C(35)	1.340(3)	F(5)-C(35)	1.340(3)
F(6)-C(35)	1.331(3)	P(1)-C(2)	1.813(7)
P(1)-C(8)	1.822(2)	P(1)-C(14)	1.828(2)
P(1)-C(2A)	1.855(8)	P(2)-C(16)	1.814(2)
P(2)-C(22)	1.824(2)	P(2)-C(15)	1.828(2)
C(1)-O(1)	1.148(3)	C(2)-C(3)	1.3900
C(2)-C(7)	1.3900	C(3)-C(4)	1.3900
C(4)-C(5)	1.3900	C(5)-C(6)	1.3900
C(6)-C(7)	1.3900	C(2A)-C(3A)	1.3900
C(2A)-C(7A)	1.3900	C(3A)-C(4A)	1.3900
C(4A)-C(5A)	1.3900	C(5A)-C(6A)	1.3900
C(6A)-C(7A)	1.3900	C(8)-C(13)	1.390(3)
C(8)-C(9)	1.390(3)	C(9)-C(10)	1.387(3)
C(10)-C(11)	1.372(4)	C(11)-C(12)	1.389(5)
C(12)-C(13)	1.400(4)	C(14)-C(15)	1.539(3)
C(16)-C(21)	1.389(3)	C(16)-C(17)	1.398(3)
C(17)-C(18)	1.393(3)	C(18)-C(19)	1.379(4)
C(19)-C(20)	1.383(4)	C(20)-C(21)	1.393(4)
C(22)-C(27)	1.389(3)	C(22)-C(23)	1.395(3)
C(23)-C(24)	1.393(4)	C(24)-C(25)	1.367(5)
C(25)-C(26)	1.389(5)	C(26)-C(27)	1.393(4)
C(57)-O(11)	1.197(5)	C(57)-C(63)	1.456(6)
C(57)-C(61)	1.465(6)		
C(1)-Ru(1)-O(3)	176.17(9)	C(1)-Ru(1)-O(4)	103.35(9)
O(3)-Ru(1)-O(4)	80.48(7)	C(1)-Ru(1)-O(2)	95.21(9)
O(3)-Ru(1)-O(2)	85.21(7)	O(4)-Ru(1)-O(2)	83.48(7)
C(1)-Ru(1)-P(2)	88.07(8)	O(3)-Ru(1)-P(2)	88.12(4)
O(4)-Ru(1)-P(2)	168.01(5)	O(2)-Ru(1)-P(2)	91.94(5)
C(1)-Ru(1)-P(1)	91.05(8)	O(3)-Ru(1)-P(1)	88.33(5)
O(4)-Ru(1)-P(1)	98.24(6)	O(2)-Ru(1)-P(1)	172.95(5)
P(2)-Ru(1)-P(1)	85.03(2)	O(2)-S(1)-C(29)	103.65(19)
O(2)-S(1)-C(28)	104.74(16)	C(29)-S(1)-C(28)	98.23(19)
O(3)-S(2)-C(31)	103.71(13)	O(3)-S(2)-C(30)	103.04(13)
C(31)-S(2)-C(30)	98.9(2)	O(4)-S(3)-C(32)	104.61(15)

O(4)-S(3)-C(33)	103.50(15)	C(32)-S(3)-C(33)	98.0(3)
O(7)-S(4)-O(5)	115.20(18)	O(7)-S(4)-O(6)	114.88(18)
O(5)-S(4)-O(6)	116.09(17)	O(7)-S(4)-C(34)	102.15(15)
O(5)-S(4)-C(34)	102.80(16)	O(6)-S(4)-C(34)	102.79(15)
O(8)-S(5)-O(10)	115.57(14)	O(8)-S(5)-O(9)	115.42(13)
O(10)-S(5)-O(9)	115.23(12)	O(8)-S(5)-C(35)	102.67(14)
O(10)-S(5)-C(35)	103.14(13)	O(9)-S(5)-C(35)	101.88(12)
C(2)-P(1)-C(8)	103.8(3)	C(2)-P(1)-C(14)	106.2(3)
C(8)-P(1)-C(14)	106.46(11)	C(2)-P(1)-C(2A)	3.7(6)
C(8)-P(1)-C(2A)	102.0(4)	C(14)-P(1)-C(2A)	103.9(3)
C(2)-P(1)-Ru(1)	115.4(3)	C(8)-P(1)-Ru(1)	117.93(8)
C(14)-P(1)-Ru(1)	106.24(7)	C(2A)-P(1)-Ru(1)	119.0(3)
C(16)-P(2)-C(22)	102.57(10)	C(16)-P(2)-C(15)	106.15(10)
C(22)-P(2)-C(15)	106.08(11)	C(16)-P(2)-Ru(1)	118.09(8)
C(22)-P(2)-Ru(1)	114.48(7)	C(15)-P(2)-Ru(1)	108.55(7)
O(1)-C(1)-Ru(1)	176.8(2)	C(3)-C(2)-C(7)	120.0
C(3)-C(2)-P(1)	119.9(5)	C(7)-C(2)-P(1)	120.1(5)
C(4)-C(3)-C(2)	120.0	C(3)-C(4)-C(5)	120.0
C(4)-C(5)-C(6)	120.0	C(7)-C(6)-C(5)	120.0
C(6)-C(7)-C(2)	120.0	C(3A)-C(2A)-C(7A)	120.0
C(3A)-C(2A)-P(1)	119.6(6)	C(7A)-C(2A)-P(1)	120.4(6)
C(4A)-C(3A)-C(2A)	120.0	C(5A)-C(4A)-C(3A)	120.0
C(4A)-C(5A)-C(6A)	120.0	C(7A)-C(6A)-C(5A)	120.0
C(6A)-C(7A)-C(2A)	120.0	C(13)-C(8)-C(9)	118.9(2)
C(13)-C(8)-P(1)	121.48(19)	C(9)-C(8)-P(1)	119.43(18)
C(10)-C(9)-C(8)	121.0(2)	C(11)-C(10)-C(9)	120.1(3)
C(10)-C(11)-C(12)	120.0(2)	C(11)-C(12)-C(13)	120.0(3)
C(8)-C(13)-C(12)	120.1(3)	C(15)-C(14)-P(1)	108.33(15)
C(14)-C(15)-P(2)	108.46(14)	C(21)-C(16)-C(17)	119.4(2)
C(21)-C(16)-P(2)	119.75(18)	C(17)-C(16)-P(2)	120.66(18)
C(18)-C(17)-C(16)	119.4(2)	C(19)-C(18)-C(17)	120.9(2)
C(18)-C(19)-C(20)	119.9(2)	C(19)-C(20)-C(21)	119.9(3)
C(16)-C(21)-C(20)	120.5(2)	C(27)-C(22)-C(23)	119.2(2)
C(27)-C(22)-P(2)	119.29(18)	C(23)-C(22)-P(2)	121.46(18)
C(24)-C(23)-C(22)	120.1(3)	C(25)-C(24)-C(23)	120.5(3)
C(24)-C(25)-C(26)	119.9(2)	C(25)-C(26)-C(27)	120.3(3)
C(22)-C(27)-C(26)	120.0(3)	F(2)-C(34)-F(3)	107.8(3)
F(2)-C(34)-F(1)	106.2(2)	F(3)-C(34)-F(1)	106.2(3)
F(2)-C(34)-S(4)	112.3(2)	F(3)-C(34)-S(4)	111.3(2)
F(1)-C(34)-S(4)	112.7(2)	F(6)-C(35)-F(4)	106.8(2)
F(6)-C(35)-F(5)	107.1(2)	F(4)-C(35)-F(5)	107.0(2)
F(6)-C(35)-S(5)	112.1(2)	F(4)-C(35)-S(5)	111.61(19)
F(5)-C(35)-S(5)	111.94(19)	O(11)-C(57)-C(63)	119.8(5)
O(11)-C(57)-C(61)	121.1(5)	C(63)-C(57)-C(61)	119.1(5)
S(1)-O(2)-Ru(1)	121.73(10)	S(2)-O(3)-Ru(1)	118.47(10)
S(3)-O(4)-Ru(1)	131.34(11)		

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Ru(dppe)(CO)(DMSO)_3][OTf]_2$ (**3**). The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	19(1)	17(1)	1(1)	-2(1)	3(1)
S(1)	26(1)	110(1)	28(1)	7(1)	-4(1)	15(1)
S(2)	27(1)	19(1)	27(1)	2(1)	1(1)	3(1)
S(3)	58(1)	29(1)	20(1)	1(1)	-2(1)	8(1)
S(4)	34(1)	51(1)	36(1)	5(1)	-6(1)	-16(1)
S(5)	25(1)	26(1)	27(1)	-2(1)	-2(1)	2(1)
F(1)	83(2)	45(1)	71(1)	-2(1)	3(1)	13(1)
F(2)	54(1)	63(1)	49(1)	-6(1)	-16(1)	-10(1)
F(3)	48(1)	62(1)	68(1)	-6(1)	11(1)	-25(1)
F(4)	43(1)	30(1)	76(1)	-19(1)	-14(1)	12(1)
F(5)	31(1)	50(1)	63(1)	-16(1)	-18(1)	5(1)
F(6)	51(1)	65(1)	53(1)	-1(1)	23(1)	-10(1)
P(1)	22(1)	17(1)	19(1)	1(1)	1(1)	0(1)
P(2)	19(1)	19(1)	19(1)	2(1)	-1(1)	0(1)
C(1)	24(1)	31(1)	27(1)	-5(1)	0(1)	0(1)
C(2)	30(2)	21(1)	22(1)	4(1)	2(1)	-5(1)
C(3)	16(3)	23(3)	21(2)	7(2)	-2(2)	2(2)
C(4)	32(5)	26(4)	27(4)	-4(3)	2(3)	4(3)
C(5)	53(4)	27(3)	30(4)	6(2)	9(3)	-12(3)
C(6)	92(6)	39(4)	22(2)	2(2)	11(3)	-21(4)
C(7)	73(6)	34(3)	19(2)	1(2)	2(3)	-21(3)
C(2A)	30(2)	21(1)	22(1)	4(1)	2(1)	-5(1)
C(3A)	20(4)	12(3)	31(4)	1(3)	-7(3)	3(3)
C(4A)	30(6)	21(5)	45(6)	14(4)	-4(5)	-12(4)
C(5A)	88(10)	47(6)	37(6)	6(5)	18(5)	-35(6)
C(6A)	121(11)	45(5)	32(4)	-2(4)	35(6)	-28(6)
C(7A)	87(8)	30(4)	28(4)	-4(3)	24(5)	-25(5)
C(8)	25(1)	18(1)	25(1)	1(1)	5(1)	0(1)
C(9)	39(1)	21(1)	27(1)	0(1)	0(1)	3(1)
C(10)	47(2)	24(1)	26(1)	-2(1)	2(1)	2(1)
C(11)	47(2)	24(1)	38(1)	-4(1)	9(1)	6(1)
C(12)	45(2)	36(2)	58(2)	-10(1)	-3(1)	17(1)
C(13)	30(1)	32(1)	45(2)	-8(1)	-2(1)	8(1)
C(14)	21(1)	25(1)	23(1)	1(1)	1(1)	0(1)
C(15)	22(1)	23(1)	22(1)	6(1)	-1(1)	3(1)
C(16)	24(1)	21(1)	21(1)	1(1)	1(1)	-2(1)
C(17)	29(1)	25(1)	24(1)	4(1)	1(1)	0(1)
C(18)	43(2)	28(1)	28(1)	6(1)	4(1)	-1(1)
C(19)	37(1)	34(1)	30(1)	0(1)	9(1)	-12(1)
C(20)	28(1)	47(2)	40(1)	5(1)	3(1)	-13(1)
C(21)	26(1)	40(1)	35(1)	10(1)	-4(1)	-6(1)
C(22)	26(1)	22(1)	17(1)	2(1)	0(1)	-1(1)
C(23)	29(1)	37(1)	29(1)	-7(1)	-1(1)	-1(1)
C(24)	44(2)	42(2)	33(1)	-13(1)	-3(1)	-9(1)

C(25)	54(2)	40(1)	32(1)	-13(1)	3(1)	-2(1)
C(26)	39(2)	43(2)	42(2)	-12(1)	7(1)	7(1)
C(27)	28(1)	35(1)	32(1)	-6(1)	4(1)	3(1)
C(28)	34(2)	80(3)	84(3)	-25(2)	-13(2)	-4(2)
C(29)	33(2)	77(3)	110(3)	60(3)	10(2)	19(2)
C(30)	116(4)	41(2)	37(2)	-10(1)	-4(2)	39(2)
C(31)	35(2)	37(2)	98(3)	34(2)	15(2)	7(1)
C(32)	76(3)	76(2)	36(2)	-17(2)	-24(2)	22(2)
C(33)	156(5)	46(2)	34(2)	13(1)	8(2)	-21(3)
C(34)	37(2)	37(1)	41(1)	-1(1)	-3(1)	-2(1)
C(35)	28(1)	28(1)	41(1)	-7(1)	-3(1)	-1(1)
C(57)	45(2)	69(2)	50(2)	-9(2)	-15(2)	5(2)
C(61)	88(4)	163(6)	51(2)	7(3)	-3(2)	-54(4)
C(63)	71(3)	118(4)	59(2)	-33(3)	2(2)	-11(3)
O(2)	24(1)	38(1)	26(1)	3(1)	-2(1)	8(1)
O(3)	30(1)	18(1)	25(1)	1(1)	-3(1)	5(1)
O(4)	48(1)	31(1)	19(1)	1(1)	-7(1)	12(1)
O(5)	40(1)	109(2)	46(1)	17(1)	0(1)	-27(1)
O(6)	51(1)	92(2)	38(1)	11(1)	-15(1)	-26(1)
O(7)	87(2)	38(1)	67(2)	-6(1)	-4(1)	-2(2)
O(8)	45(1)	57(1)	36(1)	7(1)	5(1)	-15(1)
O(9)	37(1)	33(1)	36(1)	-6(1)	-15(1)	6(1)
O(10)	54(1)	27(1)	43(1)	-12(1)	-11(1)	9(1)
O(1)	42(1)	32(1)	51(1)	-12(1)	3(1)	-10(1)
O(11)	138(4)	113(3)	135(4)	-22(3)	-73(3)	61(3)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppe)(CO)(DMSO)_3][OTf]_2$ (**3**).

Atom	x	y	z	U(eq)
H(3)	12797	10956	7296	24
H(4)	13749	11753	6665	34
H(5)	13905	11616	5531	44
H(6)	13109	10682	5028	61
H(7)	12157	9886	5659	50
H(3A)	12358	11095	7185	25
H(4A)	13456	11847	6576	38
H(5A)	14245	11529	5568	69
H(6A)	13936	10461	5171	79
H(7A)	12838	9709	5780	58
H(9C)	10627	9009	5965	35
H(10)	11101	8055	5388	39
H(11)	12704	7433	5690	44
H(12)	13843	7761	6580	56
H(13)	13360	8718	7171	43
H(14A)	13103	9516	7780	27
H(14B)	12431	10177	7989	27
H(15A)	11885	9351	8745	27
H(15B)	11564	8851	8164	27
H(17)	10393	8626	9246	31
H(18)	9148	7860	9737	39
H(19)	7199	7822	9454	41
H(20)	6476	8535	8655	46
H(21)	7712	9293	8145	40
H(23)	11805	10410	9011	38
H(24)	11702	11209	9835	48
H(25)	9923	11582	10205	50
H(26)	8217	11194	9723	49
H(27)	8299	10399	8893	38
H(28A)	5760	9867	7729	99
H(28B)	6158	9354	7177	99
H(28C)	5179	9890	7018	99
H(29A)	6834	11490	7177	110
H(29B)	6013	11088	7667	110
H(29C)	5629	11196	6922	110
H(30A)	10054	12055	8224	97
H(30B)	8752	11791	8287	97
H(30C)	9015	12455	7889	97
H(31A)	10742	11856	6455	85
H(31B)	11174	12135	7147	85
H(31C)	10132	12491	6769	85
H(32A)	7638	10743	5429	94
H(32B)	7535	9958	5493	94
H(32C)	8001	10281	4828	94
H(33A)	10801	11054	5317	118

H(33B)	9548	11389	5359	118
H(33C)	9888	10951	4736	118
H(61A)	6056	7836	7295	151
H(61B)	7320	7511	7279	151
H(61C)	6253	7142	6938	151
H(63A)	7725	7906	5570	124
H(63B)	7278	7193	5793	124
H(63C)	8370	7522	6149	124

Table 11. Crystal data and structure refinement for $[Ru(dppe)(CO)(CNCMe_3)_3][OTf]_2.(acetone)$ (**4**).

Identification code	k01mkw6
Empirical formula	C45.50 H54 F6 N3 O7.50 P2 Ru S2
Formula weight	1104.05
Temperature	150(2) K
Wavelength	0.7107 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.11030(10)Å α = 90°
	b = 21.97210(10)Å β = 90.1040(3)°
	c = 19.6937(2)Å γ = 90°
Volume	5240.26(7) $Å^3$
Z	4
Density (calculated)	1.399 Mg/m^3
Absorption coefficient	0.511 mm^{-1}
F(000)	2272
Crystal size	0.30 x 0.20 x 0.10 mm
Theta range for data collection	3.53 to 27.12°
Index ranges	-15<=h<=13; -27<=k<=28; -25<=l<=25
Reflections collected	82263
Independent reflections	11508 [R(int) = 0.0566]
Reflections observed (>2σ)	10152
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.055 and 0.944
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11508 / 3 / 635
Goodness-of-fit on F^2	0.966
Final R indices [I>2σ(I)]	R_1 = 0.0504 wR_2 = 0.1254
R indices (all data)	R_1 = 0.0580 wR_2 = 0.1312
Largest diff. peak and hole	1.873 and -1.750 $eÅ^{-3}$

Notes: Asymmetric unit contains a molecule of acetone with half site occupancy. Triflate based on S2 exhibits some positional disorder approximately along the S(2)–C(44) vector which could not be successfully modelled. C–F distances restrained to be similar in this anion. Gross structure heavily dominated by C–H...O interactions. Disorder in second triflate may be a consequence o the partial occupancy of the solvent, which is implicit in the C–H...O network.

Relevant geometric data for C–H...O interactions appended.

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Ru(dppe)(CO)($CNCMe_3$)$_3$][OTf]$_2$.(acetone) (**4**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	2440(1)	2251(1)	2233(1)	15(1)
S(1)	6841(1)	262(1)	3542(1)	32(1)
S(2)	1833(2)	1438(1)	-669(2)	120(1)
P(1)	4377(1)	2123(1)	2161(1)	15(1)
P(2)	2655(1)	1854(1)	3338(1)	18(1)
O(1)	1976(2)	969(1)	1701(1)	41(1)
O(2)	7524(2)	128(1)	4119(1)	44(1)
O(3)	7162(3)	-42(2)	2930(2)	65(1)
O(4)	6559(3)	895(1)	3468(1)	43(1)
O(5)	2039(8)	771(4)	-1163(4)	176(3)
O(6)	2896(4)	1634(2)	-482(3)	99(2)
O(7)	1100(4)	1810(2)	-1005(2)	96(2)
F(1)	4818(3)	-24(2)	3234(3)	107(2)
F(2)	5073(3)	189(2)	4282(2)	99(1)
F(3)	5630(4)	-667(2)	3890(3)	114(2)
F(4)	348(6)	740(5)	-277(4)	286(7)
F(5)	1908(6)	592(4)	184(4)	224(5)
F(6)	1098(6)	1582(2)	374(3)	141(2)
N(1)	2348(2)	2925(1)	813(1)	25(1)
N(2)	-103(2)	2549(2)	2376(2)	33(1)
N(3)	2718(2)	3601(1)	2785(1)	27(1)
C(1)	4805(2)	1470(1)	1658(1)	20(1)
C(2)	4300(3)	1367(2)	1027(2)	24(1)
C(3)	4596(3)	867(2)	635(2)	31(1)
C(4)	5380(3)	462(2)	874(2)	38(1)
C(5)	5875(3)	553(2)	1500(2)	38(1)
C(6)	5598(3)	1059(2)	1888(2)	28(1)
C(7)	5120(2)	2779(1)	1830(2)	19(1)
C(8)	5315(3)	2823(2)	1133(2)	27(1)
C(9)	5814(3)	3344(2)	867(2)	36(1)
C(10)	6118(3)	3816(2)	1286(2)	36(1)
C(11)	5927(3)	3777(2)	1977(2)	33(1)
C(12)	5429(3)	3260(2)	2254(2)	26(1)
C(13)	1782(3)	1229(1)	3619(2)	23(1)
C(14)	773(3)	1108(2)	3313(2)	34(1)
C(15)	83(3)	664(2)	3572(2)	43(1)
C(16)	398(3)	336(2)	4141(2)	36(1)
C(17)	1402(3)	449(2)	4447(2)	32(1)
C(18)	2095(3)	894(2)	4193(2)	27(1)
C(19)	2450(3)	2406(2)	4013(2)	25(1)
C(20)	1374(3)	2618(2)	4117(2)	33(1)
C(21)	1150(4)	3034(2)	4624(2)	44(1)
C(22)	2001(4)	3235(2)	5038(2)	52(1)

C(23)	3062(4)	3035(2)	4940(2)	54(1)
C(24)	3299(3)	2617(2)	4424(2)	39(1)
C(25)	4876(2)	1998(1)	3030(1)	19(1)
C(26)	4081(2)	1573(1)	3405(2)	21(1)
C(27)	2150(3)	1442(2)	1886(2)	25(1)
C(28)	2389(2)	2651(1)	1305(2)	21(1)
C(29)	2233(3)	3343(2)	233(2)	31(1)
C(30)	3136(4)	3203(2)	-271(2)	52(1)
C(31)	1099(4)	3241(2)	-71(2)	50(1)
C(32)	2341(5)	3980(2)	523(2)	59(1)
C(33)	804(3)	2418(2)	2331(2)	26(1)
C(34)	-1264(3)	2744(2)	2409(2)	45(1)
C(35)	-1695(4)	2720(3)	1688(3)	69(2)
C(36)	-1263(4)	3394(3)	2690(4)	78(2)
C(37)	-1851(4)	2318(4)	2884(4)	90(2)
C(38)	2671(2)	3109(1)	2602(2)	20(1)
C(39)	2758(3)	4244(2)	2992(2)	33(1)
C(40)	3045(5)	4608(2)	2360(2)	51(1)
C(41)	1623(4)	4406(2)	3266(3)	61(1)
C(42)	3641(5)	4293(2)	3538(3)	63(1)
C(43)	5531(5)	-81(2)	3749(3)	66(2)
C(44)	1224(8)	1113(6)	-46(5)	192(7)
O(8)	9353(13)	1319(4)	1451(6)	126(5)
C(45)	8935(10)	262(7)	1904(5)	78(4)
C(46)	9018(14)	812(8)	1405(9)	101(5)
C(47)	8710(30)	502(10)	686(9)	240(20)

Table 13. Bond lengths [Å] and angles [°] for $[Ru(dppe)(CO)(CNCMe_3)_3][OTf]_2$.(acetone) (**4**).

Ru(1)-C(27)	1.937(3)	Ru(1)-C(33)	2.025(3)
Ru(1)-C(28)	2.030(3)	Ru(1)-C(38)	2.041(3)
Ru(1)-P(2)	2.3583(7)	Ru(1)-P(1)	2.3660(7)
S(1)-O(3)	1.433(3)	S(1)-O(2)	1.434(3)
S(1)-O(4)	1.438(3)	S(1)-C(43)	1.804(6)
S(2)-O(7)	1.375(5)	S(2)-O(6)	1.405(5)
S(2)-C(44)	1.601(14)	S(2)-O(5)	1.778(8)
P(1)-C(1)	1.821(3)	P(1)-C(7)	1.822(3)
P(1)-C(25)	1.834(3)	P(2)-C(19)	1.815(3)
P(2)-C(13)	1.820(3)	P(2)-C(26)	1.839(3)
O(1)-C(27)	1.121(4)	F(1)-C(43)	1.337(7)
F(2)-C(43)	1.328(7)	F(3)-C(43)	1.322(6)
F(4)-C(44)	1.415(10)	F(5)-C(44)	1.482(11)
F(6)-C(44)	1.332(8)	N(1)-C(28)	1.141(4)
N(1)-C(29)	1.474(4)	N(2)-C(33)	1.140(4)
N(2)-C(34)	1.471(4)	N(3)-C(38)	1.140(4)
N(3)-C(39)	1.471(4)	C(1)-C(6)	1.394(4)
C(1)-C(2)	1.402(4)	C(2)-C(3)	1.389(5)
C(3)-C(4)	1.383(5)	C(4)-C(5)	1.385(5)
C(5)-C(6)	1.390(5)	C(7)-C(8)	1.396(4)
C(7)-C(12)	1.397(4)	C(8)-C(9)	1.396(5)
C(9)-C(10)	1.374(6)	C(10)-C(11)	1.382(6)
C(11)-C(12)	1.398(5)	C(13)-C(14)	1.387(5)
C(13)-C(18)	1.400(4)	C(14)-C(15)	1.384(5)
C(15)-C(16)	1.385(5)	C(16)-C(17)	1.379(6)
C(17)-C(18)	1.382(5)	C(19)-C(24)	1.388(5)
C(19)-C(20)	1.400(5)	C(20)-C(21)	1.380(5)
C(21)-C(22)	1.386(7)	C(22)-C(23)	1.373(7)
C(23)-C(24)	1.400(6)	C(25)-C(26)	1.532(4)
C(29)-C(30)	1.509(6)	C(29)-C(31)	1.514(5)
C(29)-C(32)	1.516(6)	C(34)-C(37)	1.503(7)
C(34)-C(35)	1.512(6)	C(34)-C(36)	1.531(8)
C(39)-C(42)	1.519(6)	C(39)-C(41)	1.520(6)
C(39)-C(40)	1.521(5)	O(8)-C(46)	1.188(19)
C(45)-C(46)	1.56(2)	C(46)-C(47)	1.62(3)
C(27)-Ru(1)-C(33)	91.33(14)	C(27)-Ru(1)-C(28)	94.31(12)
C(33)-Ru(1)-C(28)	88.76(12)	C(27)-Ru(1)-C(38)	177.42(12)
C(33)-Ru(1)-C(38)	86.09(13)	C(28)-Ru(1)-C(38)	85.60(12)
C(27)-Ru(1)-P(2)	90.36(9)	C(33)-Ru(1)-P(2)	94.91(9)
C(28)-Ru(1)-P(2)	173.99(8)	C(38)-Ru(1)-P(2)	89.90(8)
C(27)-Ru(1)-P(1)	92.84(10)	C(33)-Ru(1)-P(1)	175.79(10)
C(28)-Ru(1)-P(1)	91.51(8)	C(38)-Ru(1)-P(1)	89.74(8)
P(2)-Ru(1)-P(1)	84.48(3)	O(3)-S(1)-O(2)	114.44(19)
O(3)-S(1)-O(4)	115.4(2)	O(2)-S(1)-O(4)	114.51(17)
O(3)-S(1)-C(43)	103.7(3)	O(2)-S(1)-C(43)	104.0(2)
O(4)-S(1)-C(43)	102.6(2)	O(7)-S(2)-O(6)	122.4(3)

O(7)-S(2)-C(44)	109.6(5)	O(6)-S(2)-C(44)	111.0(4)
O(7)-S(2)-O(5)	108.5(4)	O(6)-S(2)-O(5)	105.4(4)
C(44)-S(2)-O(5)	96.6(4)	C(1)-P(1)-C(7)	106.72(13)
C(1)-P(1)-C(25)	107.19(14)	C(7)-P(1)-C(25)	106.92(14)
C(1)-P(1)-Ru(1)	114.14(10)	C(7)-P(1)-Ru(1)	114.70(9)
C(25)-P(1)-Ru(1)	106.72(10)	C(19)-P(2)-C(13)	101.62(14)
C(19)-P(2)-C(26)	107.57(15)	C(13)-P(2)-C(26)	105.68(14)
C(19)-P(2)-Ru(1)	114.43(10)	C(13)-P(2)-Ru(1)	119.77(11)
C(26)-P(2)-Ru(1)	106.96(10)	C(28)-N(1)-C(29)	172.4(3)
C(33)-N(2)-C(34)	177.0(4)	C(38)-N(3)-C(39)	177.4(3)
C(6)-C(1)-C(2)	118.9(3)	C(6)-C(1)-P(1)	122.0(2)
C(2)-C(1)-P(1)	119.1(2)	C(3)-C(2)-C(1)	120.5(3)
C(4)-C(3)-C(2)	119.8(3)	C(3)-C(4)-C(5)	120.4(3)
C(4)-C(5)-C(6)	120.0(3)	C(5)-C(6)-C(1)	120.4(3)
C(8)-C(7)-C(12)	119.3(3)	C(8)-C(7)-P(1)	119.5(2)
C(12)-C(7)-P(1)	121.1(2)	C(9)-C(8)-C(7)	119.9(3)
C(10)-C(9)-C(8)	120.6(3)	C(9)-C(10)-C(11)	120.0(3)
C(10)-C(11)-C(12)	120.4(3)	C(7)-C(12)-C(11)	119.8(3)
C(14)-C(13)-C(18)	119.1(3)	C(14)-C(13)-P(2)	121.6(2)
C(18)-C(13)-P(2)	119.1(2)	C(15)-C(14)-C(13)	120.4(3)
C(14)-C(15)-C(16)	120.0(4)	C(17)-C(16)-C(15)	120.1(3)
C(16)-C(17)-C(18)	120.3(3)	C(17)-C(18)-C(13)	120.1(3)
C(24)-C(19)-C(20)	119.4(3)	C(24)-C(19)-P(2)	123.2(3)
C(20)-C(19)-P(2)	117.3(3)	C(21)-C(20)-C(19)	120.7(4)
C(20)-C(21)-C(22)	119.4(4)	C(23)-C(22)-C(21)	120.6(4)
C(22)-C(23)-C(24)	120.4(4)	C(19)-C(24)-C(23)	119.4(4)
C(26)-C(25)-P(1)	109.5(2)	C(25)-C(26)-P(2)	110.6(2)
O(1)-C(27)-Ru(1)	178.3(3)	N(1)-C(28)-Ru(1)	173.9(3)
N(1)-C(29)-C(30)	108.3(3)	N(1)-C(29)-C(31)	107.3(3)
C(30)-C(29)-C(31)	111.6(3)	N(1)-C(29)-C(32)	106.0(3)
C(30)-C(29)-C(32)	112.0(4)	C(31)-C(29)-C(32)	111.3(4)
N(2)-C(33)-Ru(1)	175.7(3)	N(2)-C(34)-C(37)	107.4(4)
N(2)-C(34)-C(35)	106.1(3)	C(37)-C(34)-C(35)	113.5(5)
N(2)-C(34)-C(36)	106.7(4)	C(37)-C(34)-C(36)	110.9(5)
C(35)-C(34)-C(36)	111.8(4)	N(3)-C(38)-Ru(1)	174.4(3)
N(3)-C(39)-C(42)	106.6(3)	N(3)-C(39)-C(41)	107.1(3)
C(42)-C(39)-C(41)	111.6(4)	N(3)-C(39)-C(40)	106.6(3)
C(42)-C(39)-C(40)	112.4(4)	C(41)-C(39)-C(40)	112.1(4)
F(3)-C(43)-F(2)	107.9(6)	F(3)-C(43)-F(1)	108.0(5)
F(2)-C(43)-F(1)	106.8(5)	F(3)-C(43)-S(1)	112.0(4)
F(2)-C(43)-S(1)	111.1(4)	F(1)-C(43)-S(1)	110.9(5)
F(6)-C(44)-F(4)	124.1(10)	F(6)-C(44)-F(5)	118.2(8)
F(4)-C(44)-F(5)	94.0(9)	F(6)-C(44)-S(2)	100.6(9)
F(4)-C(44)-S(2)	111.0(7)	F(5)-C(44)-S(2)	108.8(7)
O(8)-C(46)-C(45)	134.5(17)	O(8)-C(46)-C(47)	122.7(17)
C(45)-C(46)-C(47)	102.1(14)		

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Ru(dppe)(CO)(CNCMe_3)_3][OTf]_2$.(acetone) (**4**). The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	12(1)	18(1)	16(1)	4(1)	-2(1)	0(1)
S(1)	39(1)	30(1)	27(1)	-6(1)	-12(1)	13(1)
S(2)	100(2)	66(1)	193(3)	36(1)	-55(2)	-12(1)
P(1)	12(1)	17(1)	15(1)	1(1)	0(1)	1(1)
P(2)	15(1)	23(1)	17(1)	5(1)	0(1)	2(1)
O(1)	54(2)	25(1)	43(2)	-1(1)	-3(1)	-14(1)
O(2)	50(2)	45(2)	38(2)	-4(1)	-21(1)	18(1)
O(3)	91(3)	70(2)	34(2)	-20(2)	-10(2)	37(2)
O(4)	58(2)	30(1)	40(2)	-1(1)	-14(1)	12(1)
O(5)	195(8)	194(8)	141(6)	-56(6)	48(6)	-59(6)
O(6)	93(3)	77(3)	126(4)	25(3)	-55(3)	-19(2)
O(7)	110(4)	110(4)	68(3)	3(3)	-44(3)	23(3)
F(1)	64(2)	96(3)	161(4)	-25(3)	-59(2)	-11(2)
F(2)	68(2)	107(3)	121(3)	6(3)	39(2)	0(2)
F(3)	108(3)	48(2)	187(5)	19(2)	0(3)	-21(2)
F(4)	175(7)	420(13)	261(9)	221(10)	-160(7)	-189(8)
F(5)	173(6)	241(7)	257(8)	182(7)	-158(6)	-119(5)
F(6)	203(6)	120(4)	99(3)	-28(3)	-46(4)	45(4)
N(1)	27(1)	27(1)	22(1)	8(1)	-6(1)	-4(1)
N(2)	16(1)	47(2)	37(2)	13(1)	-1(1)	6(1)
N(3)	29(1)	23(1)	29(1)	0(1)	1(1)	5(1)
C(1)	21(1)	20(1)	18(1)	0(1)	2(1)	-1(1)
C(2)	23(2)	27(2)	22(2)	0(1)	0(1)	-1(1)
C(3)	40(2)	31(2)	22(2)	-6(1)	2(1)	-5(1)
C(4)	51(2)	29(2)	34(2)	-10(1)	7(2)	5(2)
C(5)	45(2)	31(2)	38(2)	-2(2)	-1(2)	16(2)
C(6)	30(2)	29(2)	25(2)	0(1)	-2(1)	8(1)
C(7)	12(1)	19(1)	26(2)	4(1)	-1(1)	1(1)
C(8)	26(2)	32(2)	24(2)	5(1)	-2(1)	-7(1)
C(9)	30(2)	44(2)	34(2)	18(2)	-2(1)	-9(2)
C(10)	23(2)	29(2)	56(2)	18(2)	-5(2)	-8(1)
C(11)	22(2)	24(2)	54(2)	-2(2)	-2(2)	-4(1)
C(12)	21(2)	25(2)	33(2)	-1(1)	1(1)	-1(1)
C(13)	23(2)	23(2)	22(1)	7(1)	5(1)	1(1)
C(14)	27(2)	42(2)	33(2)	17(2)	-4(1)	-7(1)
C(15)	30(2)	54(2)	44(2)	17(2)	-4(2)	-15(2)
C(16)	41(2)	34(2)	33(2)	9(2)	9(2)	-9(2)
C(17)	44(2)	28(2)	25(2)	10(1)	6(1)	1(1)
C(18)	29(2)	29(2)	23(2)	6(1)	1(1)	1(1)
C(19)	29(2)	29(2)	17(1)	3(1)	4(1)	1(1)
C(20)	31(2)	38(2)	29(2)	2(1)	6(1)	5(1)
C(21)	48(2)	48(2)	35(2)	-2(2)	16(2)	12(2)
C(22)	69(3)	60(3)	28(2)	-14(2)	17(2)	2(2)
C(23)	60(3)	73(3)	29(2)	-21(2)	1(2)	-6(2)

C(24)	35(2)	54(2)	26(2)	-8(2)	1(1)	0(2)
C(25)	16(1)	26(2)	16(1)	1(1)	-2(1)	1(1)
C(26)	18(1)	27(2)	19(1)	6(1)	-1(1)	4(1)
C(27)	22(2)	27(2)	25(2)	7(1)	-2(1)	-4(1)
C(28)	17(1)	22(1)	24(2)	2(1)	-4(1)	-2(1)
C(29)	41(2)	31(2)	22(2)	14(1)	-12(1)	-7(1)
C(30)	51(3)	70(3)	34(2)	23(2)	2(2)	-4(2)
C(31)	45(2)	58(3)	47(2)	23(2)	-25(2)	-8(2)
C(32)	100(4)	32(2)	43(2)	12(2)	-24(2)	-11(2)
C(33)	22(2)	31(2)	24(2)	8(1)	-3(1)	-1(1)
C(34)	13(2)	75(3)	48(2)	8(2)	0(2)	9(2)
C(35)	34(2)	112(5)	60(3)	-4(3)	-16(2)	27(3)
C(36)	43(3)	93(4)	98(5)	-20(4)	-11(3)	32(3)
C(37)	31(3)	137(6)	104(5)	41(4)	20(3)	-7(3)
C(38)	16(1)	24(2)	20(1)	6(1)	2(1)	5(1)
C(39)	42(2)	23(2)	35(2)	-6(1)	0(2)	4(1)
C(40)	84(3)	25(2)	43(2)	-3(2)	8(2)	-5(2)
C(41)	61(3)	41(2)	82(4)	-12(2)	22(3)	11(2)
C(42)	78(4)	47(3)	64(3)	-21(2)	-31(3)	10(2)
C(43)	56(3)	44(3)	100(4)	-5(3)	-15(3)	-5(2)
C(44)	116(8)	340(20)	118(8)	-151(11)	-46(7)	61(10)
O(8)	211(15)	44(5)	122(9)	-4(5)	11(9)	-4(7)
C(45)	61(7)	136(12)	36(5)	9(6)	-7(4)	35(7)
C(46)	96(11)	89(11)	119(13)	10(9)	30(9)	44(9)
C(47)	530(60)	129(17)	72(11)	26(11)	70(20)	180(30)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppe)(CO)(CNCMe_3)_3][OTf]_2$.(acetone) (**4**).

Atom	x	y	z	U(eq)
H(2)	3752	1641	866	29
H(3)	4260	803	205	37
H(4)	5580	120	606	46
H(5)	6404	270	1664	46
H(6)	5952	1125	2313	34
H(8)	5109	2499	840	33
H(9)	5945	3373	393	43
H(10)	6458	4168	1101	43
H(11)	6136	4104	2265	39
H(12)	5302	3235	2729	32
H(14)	554	1333	2923	41
H(15)	-607	583	3360	51
H(16)	-78	33	4321	43
H(17)	1619	221	4835	39
H(18)	2784	972	4407	32
H(20)	791	2475	3836	39
H(21)	420	3181	4688	52
H(22)	1848	3515	5394	63
H(23)	3640	3182	5223	65
H(24)	4035	2480	4355	46
H(25A)	5623	1814	3018	23
H(25B)	4927	2391	3272	23
H(26A)	4296	1547	3889	25
H(26B)	4127	1159	3207	25
H(30A)	3857	3278	-60	78
H(30B)	3052	3465	-671	78
H(30C)	3086	2776	-409	78
H(31A)	1045	2822	-239	75
H(31B)	983	3526	-448	75
H(31C)	536	3309	277	75
H(32A)	1773	4043	869	88
H(32B)	2248	4279	159	88
H(32C)	3074	4028	729	88
H(35A)	-1243	2982	1398	103
H(35B)	-2463	2861	1678	103
H(35C)	-1660	2300	1521	103
H(36A)	-957	3393	3151	117
H(36B)	-2021	3550	2701	117
H(36C)	-811	3655	2398	117
H(37A)	-1858	1907	2689	136
H(37B)	-2612	2458	2950	136
H(37C)	-1466	2311	3322	136
H(40A)	3748	4463	2174	76
H(40B)	3111	5040	2478	76
H(40C)	2462	4556	2019	76

H(41A)	1065	4332	2915	92
H(41B)	1611	4836	3396	92
H(41C)	1462	4154	3664	92
H(42A)	3453	4024	3918	94
H(42B)	3684	4714	3699	94
H(42C)	4356	4171	3349	94
H(45A)	9652	55	1929	116
H(45B)	8374	-24	1739	116
H(45C)	8729	408	2356	116
H(47A)	8324	798	399	364
H(47B)	8229	150	764	364
H(47C)	9387	369	459	364

Table 16. Crystal data and structure refinement for [Ru(dppe)(CO)(OTf)(Me_2bpy)][OTf] (7).

Identification code	k00mkw7
Empirical formula	$C_{41}H_{36}F_6N_2O_7P_2RuS_2$
Formula weight	1009.85
Temperature	170(2) K
Wavelength	0.71069 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 14.2643(2)Å α = 90°
	b = 13.7762(2)Å β = 108.1960(9)°
	c = 22.1901(4)Å γ = 90°
Volume	4143.5(1) $Å^3$
Z	4
Density (calculated)	1.619 Mg/m^3
Absorption coefficient	0.637 mm^{-1}
F(000)	2048
Crystal size	0.17 x 0.13 x 0.13 mm
Theta range for data collection	3.58 to 27.48 °.
Index ranges	0<=h<=18; -17<=k<=17; -28<=l<=27
Reflections collected	56381
Independent reflections	9467 [R(int) = 0.0468]
Reflections observed (>2σ)	8083
Max. and min. transmission	0.9247 and 0.8967
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9467 / 0 / 551
Goodness-of-fit on F^2	0.978
Final R indices [I>2σ(I)]	R_1 = 0.0332 wR_2 = 0.0934
R indices (all data)	R_1 = 0.0428 wR_2 = 0.1006
Largest diff. peak and hole	0.484 and -0.541 $e.Å^{-3}$

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Ru(dppe)(CO)(OTf)(Me_2bpy)][OTf] (**7**)..U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1742(1)	5129(1)	1713(1)	17(1)
P(1)	966(1)	5358(1)	2488(1)	20(1)
P(2)	2326(1)	6668(1)	1966(1)	19(1)
N(1)	2450(1)	4899(1)	1017(1)	20(1)
N(2)	3197(1)	4644(1)	2261(1)	19(1)
S(1)	744(1)	2996(1)	1089(1)	25(1)
S(2)	6378(1)	2590(1)	486(1)	30(1)
O(1)	-145(1)	5939(1)	827(1)	33(1)
O(2)	1404(1)	3559(1)	1611(1)	27(1)
O(3)	125(1)	2337(1)	1295(1)	34(1)
O(4)	292(1)	3556(1)	531(1)	37(1)
O(5)	7351(1)	2189(2)	765(1)	42(1)
O(6)	5965(1)	3030(2)	933(1)	46(1)
O(7)	6240(2)	3130(2)	-86(1)	46(1)
F(1)	4688(2)	1738(2)	-64(1)	104(1)
F(2)	5928(2)	991(2)	-186(1)	93(1)
F(3)	5676(2)	931(2)	715(1)	97(1)
F(4)	2286(1)	2668(1)	704(1)	52(1)
F(5)	2107(1)	1648(1)	1391(1)	57(1)
F(6)	1150(1)	1579(1)	428(1)	56(1)
C(1)	1385(2)	4607(2)	3199(1)	25(1)
C(2)	1329(2)	3601(2)	3107(1)	34(1)
C(3)	1654(2)	2987(2)	3620(1)	46(1)
C(4)	2042(2)	3360(2)	4231(1)	51(1)
C(5)	2099(2)	4349(3)	4319(1)	49(1)
C(6)	1764(2)	4982(2)	3805(1)	35(1)
C(7)	-369(2)	5177(2)	2242(1)	23(1)
C(8)	-971(2)	5744(2)	2488(1)	30(1)
C(9)	-1985(2)	5574(2)	2295(1)	39(1)
C(10)	-2394(2)	4848(2)	1867(1)	38(1)
C(11)	-1798(2)	4270(2)	1629(1)	34(1)
C(12)	-794(2)	4440(2)	1817(1)	28(1)
C(13)	1129(2)	6642(2)	2725(1)	24(1)
C(14)	2157(2)	6961(2)	2728(1)	24(1)
C(15)	1734(2)	7618(2)	1403(1)	22(1)
C(16)	1718(2)	7511(2)	773(1)	27(1)
C(17)	1354(2)	8247(2)	339(1)	32(1)
C(18)	990(2)	9085(2)	524(1)	36(1)
C(19)	956(2)	9178(2)	1138(1)	36(1)
C(20)	1336(2)	8447(2)	1582(1)	27(1)
C(21)	3653(2)	6843(2)	2095(1)	22(1)
C(22)	4313(2)	6957(2)	2706(1)	27(1)
C(23)	5320(2)	7067(2)	2796(1)	34(1)

C(24)	5667(2)	7071(2)	2283(1)	36(1)
C(25)	5017(2)	6966(2)	1672(1)	34(1)
C(26)	4010(2)	6852(2)	1578(1)	26(1)
C(27)	566(2)	5620(2)	1159(1)	23(1)
C(28)	1989(2)	4955(2)	385(1)	24(1)
C(29)	2457(2)	4719(2)	-48(1)	27(1)
C(30)	3436(2)	4417(2)	153(1)	27(1)
C(31)	3951(2)	4166(2)	-325(1)	43(1)
C(32)	3904(2)	4345(2)	801(1)	26(1)
C(33)	3401(2)	4599(2)	1226(1)	20(1)
C(34)	3840(2)	4556(2)	1922(1)	20(1)
C(35)	4850(2)	4466(2)	2222(1)	24(1)
C(36)	5231(2)	4466(2)	2880(1)	24(1)
C(37)	6325(2)	4450(2)	3211(1)	34(1)
C(38)	4558(2)	4502(2)	3217(1)	26(1)
C(39)	3559(2)	4592(2)	2892(1)	24(1)
C(40)	5630(3)	1521(3)	223(2)	60(1)
C(41)	1618(2)	2182(2)	889(1)	36(1)

Table 18. Bond lengths [Å] and angles [°] for [Ru(dppe)(CO)(OTf)(Me_2bpy)][OTf] (**7**).

Ru(1)-C(27)	1.869(2)
Ru(1)-N(1)	2.126(2)
Ru(1)-N(2)	2.267(2)
Ru(1)-O(2)	2.212(2)
Ru(1)-P(2)	2.2826(6)
Ru(1)-P(1)	2.3392(5)
P(1)-C(1)	1.825(2)
P(1)-C(7)	1.827(2)
P(1)-C(13)	1.839(2)
P(2)-C(15)	1.824(2)
P(2)-C(14)	1.827(2)
P(2)-C(21)	1.839(2)
N(1)-C(28)	1.353(3)
N(1)-C(33)	1.355(3)
N(2)-C(39)	1.336(3)
N(2)-C(34)	1.361(3)
S(1)-O(4)	1.430(2)
S(1)-O(3)	1.436(2)
S(1)-O(2)	1.466(2)
S(1)-C(41)	1.831(3)
S(2)-O(7)	1.431(2)
S(2)-O(6)	1.436(2)
S(2)-O(5)	1.442(2)
S(2)-C(40)	1.805(3)
O(1)-C(27)	1.140(3)
F(1)-C(40)	1.328(4)
F(2)-C(40)	1.333(5)
F(3)-C(40)	1.346(4)
F(4)-C(41)	1.329(3)
F(5)-C(41)	1.336(3)
F(6)-C(41)	1.325(3)
C(1)-C(6)	1.382(3)
C(1)-C(2)	1.400(4)
C(2)-C(3)	1.378(4)
C(3)-C(4)	1.391(4)
C(4)-C(5)	1.376(5)
C(5)-C(6)	1.398(4)
C(7)-C(12)	1.390(3)
C(7)-C(8)	1.393(3)
C(8)-C(9)	1.395(3)
C(9)-C(10)	1.376(4)
C(10)-C(11)	1.385(4)
C(11)-C(12)	1.381(3)
C(13)-C(14)	1.528(3)
C(15)-C(20)	1.388(3)
C(15)-C(16)	1.399(3)
C(16)-C(17)	1.382(3)
C(17)-C(18)	1.380(4)

C(18)-C(19)	1.385(4)
C(19)-C(20)	1.393(4)
C(21)-C(26)	1.393(3)
C(21)-C(22)	1.396(3)
C(22)-C(23)	1.395(3)
C(23)-C(24)	1.376(4)
C(24)-C(25)	1.391(4)
C(25)-C(26)	1.395(3)
C(28)-C(29)	1.370(3)
C(29)-C(30)	1.390(3)
C(30)-C(32)	1.388(3)
C(30)-C(31)	1.506(3)
C(32)-C(33)	1.395(3)
C(33)-C(34)	1.474(3)
C(34)-C(35)	1.391(3)
C(35)-C(36)	1.390(3)
C(36)-C(38)	1.390(3)
C(36)-C(37)	1.503(3)
C(38)-C(39)	1.387(3)
C(27)-Ru(1)-N(1)	96.25(8)
C(27)-Ru(1)-N(2)	171.96(8)
N(1)-Ru(1)-N(2)	76.73(7)
C(27)-Ru(1)-O(2)	99.48(8)
N(1)-Ru(1)-O(2)	85.26(6)
N(2)-Ru(1)-O(2)	84.00(6)
C(27)-Ru(1)-P(2)	90.50(7)
N(1)-Ru(1)-P(2)	95.60(5)
N(2)-Ru(1)-P(2)	86.35(5)
O(2)-Ru(1)-P(2)	169.85(5)
C(27)-Ru(1)-P(1)	84.33(7)
N(1)-Ru(1)-P(1)	179.11(5)
N(2)-Ru(1)-P(1)	102.74(5)
O(2)-Ru(1)-P(1)	93.98(4)
P(2)-Ru(1)-P(1)	85.17(2)
C(1)-P(1)-C(7)	102.1(1)
C(1)-P(1)-C(13)	119.7(1)
C(7)-P(1)-C(13)	104.1(1)
C(1)-P(1)-Ru(1)	117.21(7)
C(7)-P(1)-Ru(1)	116.73(8)
C(13)-P(1)-Ru(1)	107.10(7)
C(15)-P(2)-C(14)	118.0(1)
C(15)-P(2)-C(21)	104.3(1)
C(14)-P(2)-C(21)	115.7(1)
C(15)-P(2)-Ru(1)	116.30(7)
C(14)-P(2)-Ru(1)	106.81(7)
C(21)-P(2)-Ru(1)	116.07(7)
C(28)-N(1)-C(33)	118.8(2)
C(28)-N(1)-Ru(1)	124.1(1)
C(33)-N(1)-Ru(1)	116.8(1)
C(39)-N(2)-C(34)	117.9(2)
C(39)-N(2)-Ru(1)	126.6(1)

C(34)-N(2)-Ru(1)	114.3(1)
O(4)-S(1)-O(3)	117.4(1)
O(4)-S(1)-O(2)	114.8(1)
O(3)-S(1)-O(2)	113.0(1)
O(4)-S(1)-C(41)	106.1(1)
O(3)-S(1)-C(41)	103.9(1)
O(2)-S(1)-C(41)	101.4(1)
O(7)-S(2)-O(6)	125.9(1)
O(7)-S(2)-O(5)	115.3(1)
O(6)-S(2)-O(5)	114.4(1)
O(7)-S(2)-C(40)	104.6(1)
O(6)-S(2)-C(40)	104.9(2)
O(5)-S(2)-C(40)	103.7(2)
S(1)-O(2)-Ru(1)	131.6(1)
C(6)-C(1)-C(2)	120.0(2)
C(6)-C(1)-P(1)	124.5(2)
C(2)-C(1)-P(1)	127.6(2)
C(3)-C(2)-C(1)	119.9(2)
C(2)-C(3)-C(4)	120.4(3)
C(5)-C(4)-C(3)	119.6(3)
C(4)-C(5)-C(6)	120.7(3)
C(1)-C(6)-C(5)	119.4(3)
C(12)-C(7)-C(8)	119.0(2)
C(12)-C(7)-P(1)	119.7(2)
C(8)-C(7)-P(1)	121.3(2)
C(7)-C(8)-C(9)	119.5(2)
C(10)-C(9)-C(8)	120.7(2)
C(9)-C(10)-C(11)	120.2(2)
C(12)-C(11)-C(10)	119.3(2)
C(11)-C(12)-C(7)	121.4(2)
C(14)-C(13)-P(1)	108.2(2)
C(13)-C(14)-P(2)	110.7(2)
C(20)-C(15)-C(16)	119.5(2)
C(20)-C(15)-P(2)	122.5(2)
C(16)-C(15)-P(2)	117.9(2)
C(17)-C(16)-C(15)	120.3(2)
C(18)-C(17)-C(16)	120.0(2)
C(17)-C(18)-C(19)	120.2(2)
C(18)-C(19)-C(20)	120.2(2)
C(15)-C(20)-C(19)	119.7(2)
C(26)-C(21)-C(22)	119.3(2)
C(26)-C(21)-P(2)	120.7(2)
C(22)-C(21)-P(2)	121.1(2)
C(23)-C(22)-C(21)	120.2(2)
C(24)-C(23)-C(22)	120.2(2)
C(23)-C(24)-C(25)	120.3(2)
C(24)-C(25)-C(26)	119.9(2)
C(25)-C(26)-C(21)	120.2(2)
O(1)-C(27)-Ru(1)	178.5(2)
N(1)-C(28)-C(29)	121.9(2)
C(28)-C(29)-C(30)	120.5(2)
C(32)-C(30)-C(29)	117.6(2)

C(32)-C(30)-C(31)	122.1(2)
C(29)-C(30)-C(31)	120.3(2)
C(30)-C(32)-C(33)	120.0(2)
N(1)-C(33)-C(32)	121.1(2)
N(1)-C(33)-C(34)	125.0(2)
C(32)-C(33)-C(34)	123.9(2)
N(2)-C(34)-C(35)	121.3(2)
N(2)-C(34)-C(33)	126.9(2)
C(35)-C(34)-C(33)	122.8(2)
C(36)-C(35)-C(34)	120.7(2)
C(35)-C(36)-C(38)	117.1(2)
C(35)-C(36)-C(37)	121.4(2)
C(38)-C(36)-C(37)	121.5(2)
C(39)-C(38)-C(36)	119.6(2)
N(2)-C(39)-C(38)	123.2(2)
F(1)-C(40)-F(2)	106.7(3)
F(1)-C(40)-F(3)	108.1(3)
F(2)-C(40)-F(3)	106.1(3)
F(1)-C(40)-S(2)	112.2(3)
F(2)-C(40)-S(2)	112.6(3)
F(3)-C(40)-S(2)	110.8(2)
F(6)-C(41)-F(4)	108.4(2)
F(6)-C(41)-F(5)	107.7(2)
F(4)-C(41)-F(5)	107.3(2)
F(6)-C(41)-S(1)	110.7(2)
F(4)-C(41)-S(1)	111.9(2)
F(5)-C(41)-S(1)	110.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 19. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [Ru(dppe)(CO)(OTf)(Me_2bpy)][OTf] (7). The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	16(1)	20(1)	16(1)	-1(1)	6(1)	-1(1)
P(1)	19(1)	23(1)	19(1)	-2(1)	9(1)	-2(1)
P(2)	18(1)	20(1)	19(1)	-1(1)	7(1)	-1(1)
N(1)	20(1)	22(1)	18(1)	-2(1)	7(1)	0(1)
N(2)	18(1)	19(1)	22(1)	1(1)	7(1)	1(1)
S(1)	28(1)	24(1)	24(1)	-3(1)	11(1)	-5(1)
S(2)	32(1)	33(1)	24(1)	2(1)	6(1)	-1(1)
O(1)	21(1)	44(1)	30(1)	7(1)	4(1)	3(1)
O(2)	32(1)	23(1)	25(1)	-3(1)	11(1)	-3(1)
O(3)	35(1)	31(1)	40(1)	0(1)	19(1)	-8(1)
O(4)	42(1)	37(1)	27(1)	1(1)	6(1)	-8(1)
O(5)	38(1)	44(1)	38(1)	-1(1)	5(1)	10(1)
O(6)	42(1)	60(1)	38(1)	-1(1)	16(1)	8(1)
O(7)	51(1)	50(1)	37(1)	18(1)	15(1)	3(1)
F(1)	54(1)	104(2)	125(2)	7(2)	-14(1)	-36(1)
F(2)	133(2)	67(2)	60(1)	-28(1)	4(1)	-17(2)
F(3)	129(2)	68(2)	85(2)	23(1)	22(2)	-45(2)
F(4)	55(1)	43(1)	76(1)	-20(1)	48(1)	-16(1)
F(5)	60(1)	47(1)	67(1)	8(1)	26(1)	21(1)
F(6)	62(1)	48(1)	67(1)	-36(1)	32(1)	-19(1)
C(1)	22(1)	31(1)	25(1)	2(1)	12(1)	-1(1)
C(2)	45(1)	32(1)	25(1)	0(1)	13(1)	-1(1)
C(3)	65(2)	38(2)	40(2)	11(1)	22(1)	8(1)
C(4)	68(2)	56(2)	30(2)	16(1)	17(1)	11(2)
C(5)	64(2)	59(2)	21(1)	1(1)	7(1)	2(2)
C(6)	40(1)	41(2)	24(1)	-3(1)	12(1)	-4(1)
C(7)	20(1)	27(1)	23(1)	3(1)	10(1)	0(1)
C(8)	28(1)	31(1)	36(1)	0(1)	15(1)	2(1)
C(9)	26(1)	46(2)	48(2)	7(1)	18(1)	8(1)
C(10)	21(1)	54(2)	37(2)	16(1)	8(1)	-2(1)
C(11)	32(1)	41(2)	26(1)	4(1)	6(1)	-12(1)
C(12)	27(1)	32(1)	29(1)	-2(1)	12(1)	-6(1)
C(13)	26(1)	25(1)	27(1)	-4(1)	15(1)	-2(1)
C(14)	26(1)	24(1)	23(1)	-4(1)	10(1)	-3(1)
C(15)	19(1)	23(1)	25(1)	1(1)	6(1)	-1(1)
C(16)	28(1)	27(1)	24(1)	2(1)	7(1)	4(1)
C(17)	33(1)	35(1)	26(1)	4(1)	5(1)	3(1)
C(18)	34(1)	30(1)	38(1)	8(1)	2(1)	4(1)
C(19)	32(1)	28(1)	46(2)	-2(1)	9(1)	9(1)
C(20)	22(1)	29(1)	29(1)	-4(1)	8(1)	1(1)
C(21)	20(1)	19(1)	27(1)	1(1)	7(1)	-1(1)
C(22)	23(1)	26(1)	30(1)	1(1)	6(1)	1(1)
C(23)	23(1)	29(1)	42(2)	3(1)	1(1)	-1(1)
C(24)	22(1)	26(1)	62(2)	5(1)	15(1)	2(1)

C(25)	31(1)	30(1)	50(2)	3(1)	25(1)	1(1)
C(26)	26(1)	25(1)	30(1)	1(1)	11(1)	0(1)
C(27)	23(1)	27(1)	21(1)	-1(1)	10(1)	-5(1)
C(28)	23(1)	27(1)	21(1)	0(1)	7(1)	-2(1)
C(29)	27(1)	33(1)	21(1)	0(1)	9(1)	0(1)
C(30)	29(1)	31(1)	27(1)	-1(1)	17(1)	1(1)
C(31)	36(1)	68(2)	31(1)	0(1)	18(1)	10(1)
C(32)	24(1)	30(1)	27(1)	0(1)	12(1)	1(1)
C(33)	22(1)	19(1)	23(1)	0(1)	11(1)	-2(1)
C(34)	20(1)	18(1)	24(1)	0(1)	8(1)	1(1)
C(35)	21(1)	24(1)	30(1)	3(1)	11(1)	3(1)
C(36)	21(1)	20(1)	29(1)	4(1)	4(1)	2(1)
C(37)	21(1)	39(1)	36(1)	4(1)	1(1)	3(1)
C(38)	27(1)	26(1)	22(1)	1(1)	4(1)	3(1)
C(39)	24(1)	25(1)	21(1)	0(1)	7(1)	2(1)
C(40)	65(2)	53(2)	48(2)	10(2)	-1(2)	-21(2)
C(41)	38(1)	30(1)	45(2)	-12(1)	23(1)	-10(1)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Ru(dppe)(CO)(OTf)(Me_2bpy)][OTf] (7).

Atom	x	y	z	U(eq)
H(2)	1067	3342	2692	40
H(3)	1614	2304	3557	56
H(4)	2265	2934	4583	61
H(5)	2370	4605	4735	59
H(6)	1796	5665	3870	42
H(8)	-693	6243	2786	37
H(9)	-2399	5962	2459	46
H(10)	-3087	4743	1736	45
H(11)	-2077	3762	1338	40
H(12)	-385	4044	1652	34
H(13A)	619	7043	2423	29
H(13B)	1063	6724	3153	29
H(14A)	2665	6626	3073	29
H(14B)	2233	7669	2804	29
H(16)	1958	6931	642	32
H(17)	1355	8176	-87	39
H(18)	761	9599	229	43
H(19)	674	9742	1258	43
H(20)	1322	8517	2005	32
H(22)	4076	6958	3061	32
H(23)	5766	7141	3212	41
H(24)	6353	7145	2347	44
H(25)	5259	6971	1318	41
H(26)	3566	6780	1161	32
H(28)	1322	5165	237	28
H(29)	2110	4761	-489	32
H(31A)	3497	4262	-755	65
H(31B)	4163	3486	-271	65
H(31C)	4528	4586	-260	65
H(32)	4566	4123	956	31
H(35)	5283	4404	1974	29
H(37A)	6450	4464	3671	51
H(37B)	6630	5019	3083	51
H(37C)	6608	3857	3096	51
H(38)	4781	4466	3667	31
H(39)	3111	4617	3131	28

Table 21. Crystal data and structure refinement for [{(dppe)Ru(CO)}$_2$(μ-$SCH_2CH_2CH_3)_3$][OTf] (**8**).

Identification code	k00mkw8
Empirical formula	C67 H75 F3 O6 P4 Ru2 S4
Formula weight	1487.53
Temperature	170(2) K
Wavelength	0.71069 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.65510(10)Å α = 100.9820(10)°
	b = 12.99760(10)Å β = 92.9360(10)°
	c = 21.0650(2)Å γ = 103.1430(10)°
Volume	3296.11(5) Å^3
Z	2
Density (calculated)	1.499 Mg/m^3
Absorption coefficient	0.741 mm^{-1}
F(000)	1528
Crystal size	0.25 x 0.20 x 0.10 mm
Theta range for data collection	3.54 to 27.50 °.
Index ranges	0<=h<=16; -16<=k<=16; -27<=l<=27
Reflections collected	37510
Independent reflections	14940 [R(int) = 0.0297]
Reflections observed (>2σ)	13643
Data Completeness	0.987
Max. and min. transmission	0.9296 and 0.8364
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14940 / 0 / 776
Goodness-of-fit on F^2	1.046
Final R indices [I>2σ(I)]	R_1 = 0.0308 wR_2 = 0.0758
R indices (all data)	R_1 = 0.0345 wR_2 = 0.0786
Largest diff. peak and hole	1.901 and -0.847 e.Å^{-3}

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [{(dppe)Ru(CO)}$_2$(μ-SCH$_2$CH$_2$CH$_3$)$_3$][OTf] (**8**).U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	7240(1)	3617(1)	2555(1)	16(1)
Ru(2)	7790(1)	1168(1)	2432(1)	15(1)
S(1)	8466(1)	2905(1)	3209(1)	20(1)
S(2)	7682(1)	2341(1)	1662(1)	18(1)
S(3)	3625(1)	7214(1)	2951(1)	38(1)
S(4)	6112(1)	1799(1)	2613(1)	18(1)
P(1)	6015(1)	4181(1)	1913(1)	19(1)
P(2)	6734(1)	4839(1)	3391(1)	20(1)
P(3)	7702(1)	-42(1)	3140(1)	17(1)
P(4)	6873(1)	-360(1)	1676(1)	17(1)
F(1)	1828(1)	5688(2)	2542(1)	56(1)
F(2)	2041(1)	6328(2)	3568(1)	55(1)
F(3)	2989(1)	5244(1)	3140(1)	48(1)
O(1)	9010(1)	5450(1)	2335(1)	37(1)
O(2)	10029(1)	939(1)	2122(1)	34(1)
O(3)	4090(2)	6807(2)	2377(1)	49(1)
O(4)	4343(2)	7445(2)	3543(1)	64(1)
O(5)	3010(2)	7997(2)	2882(1)	69(1)
O(6)	8908(2)	7144(2)	1405(1)	62(1)
C(1)	5852(2)	3195(2)	615(1)	32(1)
C(2)	6047(2)	3122(2)	-33(1)	42(1)
C(3)	6651(2)	4014(3)	-234(1)	49(1)
C(4)	7068(3)	4967(3)	214(2)	50(1)
C(5)	6875(2)	5050(2)	864(1)	37(1)
C(6)	6257(2)	4159(2)	1068(1)	25(1)
C(7)	4010(2)	2880(2)	2154(1)	34(1)
C(8)	2880(2)	2618(2)	2143(1)	39(1)
C(9)	2262(2)	3166(2)	1840(1)	34(1)
C(10)	2774(2)	3969(2)	1535(1)	31(1)
C(11)	3893(2)	4220(2)	1532(1)	27(1)
C(12)	4526(2)	3685(2)	1850(1)	22(1)
C(13)	6661(2)	4098(2)	4535(1)	32(1)
C(14)	6172(2)	3626(2)	5015(1)	41(1)
C(15)	5051(3)	3400(2)	5018(1)	46(1)
C(16)	4420(2)	3656(2)	4549(2)	44(1)
C(17)	4903(2)	4135(2)	4061(1)	33(1)
C(18)	6032(2)	4354(2)	4049(1)	25(1)
C(19)	7614(2)	6944(2)	4135(1)	28(1)
C(20)	8445(2)	7783(2)	4483(1)	32(1)
C(21)	9493(2)	7653(2)	4554(1)	33(1)
C(22)	9710(2)	6677(2)	4282(1)	35(1)
C(23)	8886(2)	5839(2)	3931(1)	30(1)
C(24)	7828(2)	5963(2)	3846(1)	23(1)

C(25)	7772(2)	1199(2)	4391(1)	24(1)
C(26)	7494(2)	1401(2)	5024(1)	29(1)
C(27)	6733(2)	634(2)	5244(1)	31(1)
C(28)	6257(2)	-340(2)	4827(1)	29(1)
C(29)	6530(2)	-554(2)	4194(1)	24(1)
C(30)	7297(2)	218(2)	3967(1)	19(1)
C(31)	9132(2)	-1453(2)	2992(1)	28(1)
C(32)	10132(2)	-1700(2)	3087(1)	33(1)
C(33)	10991(2)	-954(2)	3469(1)	34(1)
C(34)	10851(2)	46(2)	3758(1)	39(1)
C(35)	9859(2)	303(2)	3666(1)	32(1)
C(36)	8982(2)	-442(2)	3277(1)	21(1)
C(37)	7022(2)	-1744(2)	508(1)	33(1)
C(38)	7419(2)	-2012(2)	-86(1)	41(1)
C(39)	8204(2)	-1262(2)	-301(1)	38(1)
C(40)	8588(2)	-242(2)	78(1)	32(1)
C(41)	8199(2)	31(2)	677(1)	26(1)
C(42)	7414(2)	-717(2)	897(1)	21(1)
C(43)	4596(2)	-988(2)	1674(1)	30(1)
C(44)	3534(2)	-958(2)	1492(1)	42(1)
C(45)	3338(2)	-353(3)	1044(1)	45(1)
C(46)	4201(2)	216(2)	775(1)	37(1)
C(47)	5262(2)	198(2)	960(1)	28(1)
C(48)	5464(2)	-410(2)	1412(1)	21(1)
C(49)	8312(2)	4766(2)	2421(1)	23(1)
C(50)	9163(2)	985(2)	2241(1)	21(1)
C(51)	6808(2)	-1577(2)	2016(1)	21(1)
C(52)	6732(2)	-1320(2)	2748(1)	21(1)
C(53)	5833(2)	5530(2)	3010(1)	27(1)
C(54)	6122(2)	5591(2)	2320(1)	25(1)
C(55)	9022(2)	2905(2)	1404(1)	26(1)
C(56)	8894(2)	3245(3)	761(2)	51(1)
C(57)	9995(2)	3646(3)	516(2)	58(1)
C(58)	2572(2)	6062(2)	3054(1)	33(1)
C(59)	9915(2)	3464(2)	3103(2)	43(1)
C(60)	10754(3)	3273(3)	3523(2)	69(1)
C(61)	10776(6)	3825(4)	4155(2)	117(2)
C(62)	4812(2)	699(2)	3413(1)	32(1)
C(63)	5678(2)	1728(2)	3420(1)	24(1)
C(64)	3697(2)	723(2)	3116(2)	45(1)
C(65)	10678(3)	6795(3)	1428(2)	61(1)
C(67)	9866(2)	7456(2)	1358(1)	40(1)
C(68)	10326(3)	8567(3)	1268(2)	71(1)

Table 23. Bond lengths [Å] and angles [°] for [{(dppe)Ru(CO)}$_2$(μ-SCH$_2$CH$_2$CH$_3$)$_3$][OTf] (**8**).

Ru(1)-C(49)	1.851(2)	Ru(1)-P(1)	2.3340(5)
Ru(1)-P(2)	2.3539(5)	Ru(1)-S(2)	2.4387(5)
Ru(1)-S(1)	2.4662(5)	Ru(1)-S(4)	2.4964(5)
Ru(2)-C(50)	1.861(2)	Ru(2)-P(4)	2.3211(5)
Ru(2)-P(3)	2.3547(5)	Ru(2)-S(2)	2.4473(5)
Ru(2)-S(4)	2.4654(5)	Ru(2)-S(1)	2.4653(5)
S(1)-C(59)	1.854(2)	S(2)-C(55)	1.840(2)
S(3)-O(3)	1.435(2)	S(3)-O(5)	1.437(2)
S(3)-O(4)	1.444(2)	S(3)-C(58)	1.818(2)
S(4)-C(63)	1.826(2)	P(1)-C(6)	1.818(2)
P(1)-C(54)	1.840(2)	P(1)-C(12)	1.836(2)
P(2)-C(18)	1.821(2)	P(2)-C(24)	1.839(2)
P(2)-C(53)	1.844(2)	P(3)-C(30)	1.832(2)
P(3)-C(36)	1.835(2)	P(3)-C(52)	1.842(2)
P(4)-C(48)	1.823(2)	P(4)-C(42)	1.829(2)
P(4)-C(51)	1.843(2)	F(1)-C(58)	1.332(3)
F(2)-C(58)	1.335(3)	F(3)-C(58)	1.327(3)
O(1)-C(49)	1.151(3)	O(2)-C(50)	1.148(2)
O(6)-C(67)	1.203(3)	C(1)-C(2)	1.388(3)
C(1)-C(6)	1.395(3)	C(2)-C(3)	1.387(4)
C(3)-C(4)	1.381(5)	C(4)-C(5)	1.391(4)
C(5)-C(6)	1.396(3)	C(7)-C(12)	1.384(3)
C(7)-C(8)	1.392(3)	C(8)-C(9)	1.379(3)
C(9)-C(10)	1.383(4)	C(10)-C(11)	1.380(3)
C(11)-C(12)	1.397(3)	C(13)-C(14)	1.382(3)
C(13)-C(18)	1.400(3)	C(14)-C(15)	1.382(4)
C(15)-C(16)	1.375(4)	C(16)-C(17)	1.398(4)
C(17)-C(18)	1.394(3)	C(19)-C(20)	1.388(3)
C(19)-C(24)	1.396(3)	C(20)-C(21)	1.379(3)
C(21)-C(22)	1.382(3)	C(22)-C(23)	1.386(3)
C(23)-C(24)	1.390(3)	C(25)-C(26)	1.388(3)
C(25)-C(30)	1.396(3)	C(26)-C(27)	1.386(3)
C(27)-C(28)	1.383(3)	C(28)-C(29)	1.388(3)
C(29)-C(30)	1.401(3)	C(31)-C(32)	1.389(3)
C(31)-C(36)	1.396(3)	C(32)-C(33)	1.380(4)
C(33)-C(34)	1.380(4)	C(34)-C(35)	1.385(3)
C(35)-C(36)	1.398(3)	C(37)-C(38)	1.384(3)
C(37)-C(42)	1.393(3)	C(38)-C(39)	1.383(4)
C(39)-C(40)	1.377(4)	C(40)-C(41)	1.390(3)
C(41)-C(42)	1.388(3)	C(43)-C(48)	1.386(3)
C(43)-C(44)	1.390(3)	C(44)-C(45)	1.385(4)
C(45)-C(46)	1.384(4)	C(46)-C(47)	1.385(3)
C(47)-C(48)	1.397(3)	C(51)-C(52)	1.528(3)
C(53)-C(54)	1.529(3)	C(55)-C(56)	1.515(3)
C(56)-C(57)	1.525(4)	C(59)-C(60)	1.442(4)
C(60)-C(61)	1.382(6)	C(62)-C(63)	1.521(3)
C(62)-C(64)	1.523(3)	C(65)-C(67)	1.499(4)