Table 1. Crystal data and structure refinement for [Ru(tpy)(bpy)dmso)]2+.

Empirical formula	$C_{27}H_{25}N_5ORuS\ (CF_3SO_3)_2$
Formula weight	866.79
Crystallization Solvent	Acetonitrile/Ether
Crystal Habit	Prism
Crystal size	0.16 × 0.28 × 0.31 mm
Crystal color	Red
Data Collection	
Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	293(2) K
θ range for reflections used in lattice determination	2.22 to 25.15° (4648 reflections)
Unit cell dimensions	a = 25.7825(17) Å b = 11.0774(7) Å β= 96.8620(10)° c = 23.6971(16) Å
Volume	6719.5(8) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/c
Density (calculated)	1.714 Mg/m^3
F(000)	3488
θ range for data collection	1.73 to 28.71°
Completeness to θ = 28.71°	92.0 %
Index ranges	$-32 \le h \le 32, -14 \le k \le 14, -31 \le l \le 31$
Data collection scan type	ϕ and ω scans
Reflections collected	32400
Independent reflections	7976 [Rint= 0.0541]
Absorption coefficient	0.740 mm^{-1}
Absorption correction	None
Decay correction	3.9%.

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7976 / 0 / 560
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	2.060
Final R indices [I>2s(I)]	R1 = 0.0503, *w*R2 = 0.0888
R indices (all data)	R1 = 0.0749, *w*R2 = 0.0904
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.009
Average shift/error	0.000
Largest diff. peak and hole	1.060 and -0.753 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for WAW1T. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru	1403(1)	3009(1)	3881(1)	35(1)
S(1)	1635(1)	4301(1)	4619(1)	45(1)
S(2)	3042(1)	7697(2)	3564(1)	88(1)
S(3)	-212(1)	7528(1)	3881(1)	59(1)
F(1)	2431(2)	8779(6)	4157(2)	207(3)
F(2)	2560(3)	9703(4)	3476(3)	251(3)
F(3)	2090(2)	8327(5)	3365(2)	198(3)
F(4)	-358(2)	9035(4)	4676(2)	164(2)
F(5)	-787(1)	9474(3)	3910(1)	108(1)
F(6)	9(1)	9814(3)	4007(2)	118(1)
O(1)	2076(1)	3912(3)	5028(1)	72(1)
O(2)	3436(2)	8003(5)	4015(3)	179(2)
O(3)	2865(2)	6555(4)	3725(2)	173(2)
O(4)	3112(3)	7865(8)	3043(2)	316(6)
O(5)	-226(2)	7691(3)	3291(2)	112(1)
O(6)	-649(2)	6879(3)	4009(2)	138(2)
O(7)	279(2)	7214(3)	4140(2)	129(2)
N(1)	609(1)	3352(3)	3878(1)	40(1)
N(2)	1310(1)	4365(3)	3338(1)	36(1)
N(3)	2148(1)	3122(3)	3641(1)	38(1)
N(4)	1464(1)	1408(3)	4360(1)	39(1)
N(5)	1178(1)	1693(3)	3272(1)	41(1)
C(1)	260(2)	2761(4)	4153(2)	52(1)
C(2)	-265(2)	3026(5)	4085(2)	66(1)
C(3)	-440(2)	3946(5)	3724(2)	70(2)
C(4)	-90(2)	4568(4)	3443(2)	55(1)
C(5)	434(1)	4269(3)	3521(2)	42(1)
C(6)	832(1)	4880(3)	3234(2)	39(1)
C(7)	770(2)	5863(4)	2875(2)	50(1)
C(8)	1193(2)	6250(4)	2621(2)	61(1)
C(9)	1671(2)	5708(4)	2717(2)	53(1)
C(10)	1727(1)	4741(3)	3086(2)	39(1)
C(11)	2203(1)	4027(3)	3258(2)	41(1)
C(12)	2676(2)	4227(5)	3054(2)	53(1)
C(13)	3095(2)	3515(5)	3233(2)	59(1)
C(14)	3045(2)	2602(4)	3613(2)	55(1)
C(15)	2567(2)	2425(4)	3808(2)	46(1)
C(16)	1662(2)	1269(4)	4908(2)	47(1)
C(17)	1656(2)	184(4)	5186(2)	54(1)
C(18)	1441(2)	-792(5)	4916(2)	60(1)

C(19)	1238(2)	-681(4)	4358(2)	54(1)
C(20)	1260(1)	407(3)	4082(2)	39(1)
C(21)	1091(1)	585(3)	3474(2)	40(1)
C(22)	865(2)	-314(4)	3115(2)	57(1)
C(23)	733(2)	-71(5)	2549(2)	67(1)
C(24)	845(2)	1028(5)	2346(2)	66(1)
C(25)	1065(2)	1895(4)	2711(2)	54(1)
C(26)	1795(3)	5785(5)	4411(3)	72(2)
C(27)	1105(3)	4668(9)	5005(3)	92(2)
C(28)	2514(2)	8642(6)	3648(3)	94(2)
C(29)	-330(2)	9017(5)	4138(2)	72(1)

Table 3. Selected bond lengths [Å] and angles [°] for [Ru(tpy)(bpy)dmso)]$^{2+}$.

		Distances	
Ru-N(2)	1.975(3)	Ru-S(1)	2.282(1)
Ru-N(3)	2.073(3)	S(1)-O(1)	1.467(3)
Ru-N(1)	2.079(3)	S(1)-C(26)	1.779(5)
Ru-N(5)	2.084(3)	S(1)-C(27)	1.781(6)
Ru-N(4)	2.100(3)		
		Angles	
N(2)-Ru-N(3)	79.54(12)	N(3)-Ru-S(1)	90.31(8)
N(2)-Ru-N(1)	79.36(12)	N(1)-Ru-S(1)	93.24(8)
N(3)-Ru-N(1)	158.67(12)	N(5)-Ru-S(1)	174.03(9)
N(2)-Ru-N(5)	94.44(12)	N(4)-Ru-S(1)	96.89(9)
N(3)-Ru-N(5)	92.35(11)	O(1)-S(1)-C(26)	105.5(3)
N(1)-Ru-N(5)	86.22(11)	O(1)-S(1)-C(27)	107.9(3)
N(2)-Ru-N(4)	171.80(12)	C(26)-S(1)-C(27)	98.5(4)
N(3)-Ru-N(4)	100.82(12)	O(1)-S(1)-Ru	115.70(12)
N(1)-Ru-N(4)	99.62(11)	C(26)-S(1)-Ru	114.6(2)
N(5)-Ru-N(4)	77.36(12)	C(27)-S(1)-Ru	112.9(2)
N(2)-Ru-S(1)	91.30(8)		

Table 4. Bond lengths [Å] and angles [°] for [Ru(tpy)(bpy)dmso)]$^{2+}$.

Ru-N(2)	1.975(3)	C(13)-C(14)	1.371(6)
Ru-N(3)	2.073(3)	C(14)-C(15)	1.381(6)
Ru-N(1)	2.079(3)	C(16)-C(17)	1.372(6)
Ru-N(5)	2.084(3)	C(17)-C(18)	1.342(6)
Ru-N(4)	2.100(3)	C(18)-C(19)	1.367(6)
Ru-S(1)	2.2821(10)	C(19)-C(20)	1.377(5)
S(1)-O(1)	1.467(3)	C(20)-C(21)	1.467(5)
S(1)-C(26)	1.779(5)	C(21)-C(22)	1.391(5)
S(1)-C(27)	1.781(6)	C(22)-C(23)	1.371(6)
S(2)-O(4)	1.284(4)	C(23)-C(24)	1.354(7)
S(2)-O(3)	1.413(5)	C(24)-C(25)	1.369(6)
S(2)-O(2)	1.423(5)		
S(2)-C(28)	1.748(6)	N(2)-Ru-N(3)	79.54(12)
S(3)-O(7)	1.385(3)	N(2)-Ru-N(1)	79.36(12)
S(3)-O(6)	1.399(3)	N(3)-Ru-N(1)	158.67(12)
S(3)-O(5)	1.407(3)	N(2)-Ru-N(5)	94.44(12)
S(3)-C(29)	1.797(5)	N(3)-Ru-N(5)	92.35(11)
F(1)-C(28)	1.260(6)	N(1)-Ru-N(5)	86.22(11)
F(2)-C(28)	1.254(8)	N(2)-Ru-N(4)	171.80(12)
F(3)-C(28)	1.261(6)	N(3)-Ru-N(4)	100.82(12)
F(4)-C(29)	1.287(5)	N(1)-Ru-N(4)	99.62(11)
F(5)-C(29)	1.335(5)	N(5)-Ru-N(4)	77.36(12)
F(6)-C(29)	1.306(5)	N(2)-Ru-S(1)	91.30(8)
N(1)-C(1)	1.343(5)	N(3)-Ru-S(1)	90.31(8)
N(1)-C(5)	1.364(4)	N(1)-Ru-S(1)	93.24(8)
N(2)-C(6)	1.353(4)	N(5)-Ru-S(1)	174.03(9)
N(2)-C(10)	1.356(4)	N(4)-Ru-S(1)	96.89(9)
N(3)-C(15)	1.348(5)	O(1)-S(1)-C(26)	105.5(3)
N(3)-C(11)	1.371(4)	O(1)-S(1)-C(27)	107.9(3)
N(4)-C(16)	1.346(5)	C(26)-S(1)-C(27)	98.5(4)
N(4)-C(20)	1.363(4)	O(1)-S(1)-Ru	115.70(12)
N(5)-C(25)	1.345(5)	C(26)-S(1)-Ru	114.6(2)
N(5)-C(21)	1.347(4)	C(27)-S(1)-Ru	112.9(2)
C(1)-C(2)	1.377(6)	O(4)-S(2)-O(3)	118.4(5)
C(2)-C(3)	1.371(6)	O(4)-S(2)-O(2)	121.2(5)
C(3)-C(4)	1.371(6)	O(3)-S(2)-O(2)	103.7(3)
C(4)-C(5)	1.382(5)	O(4)-S(2)-C(28)	102.9(3)
C(5)-C(6)	1.462(5)	O(3)-S(2)-C(28)	103.0(3)
C(6)-C(7)	1.379(5)	O(2)-S(2)-C(28)	105.5(3)
C(7)-C(8)	1.376(6)	O(7)-S(3)-O(6)	119.5(3)
C(8)-C(9)	1.366(6)	O(7)-S(3)-O(5)	112.7(3)
C(9)-C(10)	1.379(5)	O(6)-S(3)-O(5)	110.9(3)
C(10)-C(11)	1.475(5)	O(7)-S(3)-C(29)	105.3(2)
C(11)-C(12)	1.384(5)	O(6)-S(3)-C(29)	103.0(3)
C(12)-C(13)	1.363(6)	O(5)-S(3)-C(29)	103.5(2)

C(1)-N(1)-C(5)	118.2(3)	C(12)-C(11)-C(10)	123.9(4)
C(1)-N(1)-Ru	128.6(3)	C(13)-C(12)-C(11)	119.9(5)
C(5)-N(1)-Ru	113.0(2)	C(12)-C(13)-C(14)	119.8(4)
C(6)-N(2)-C(10)	122.9(3)	C(13)-C(14)-C(15)	118.9(4)
C(6)-N(2)-Ru	118.4(2)	N(3)-C(15)-C(14)	122.4(4)
C(10)-N(2)-Ru	118.7(2)	N(4)-C(16)-C(17)	122.6(4)
C(15)-N(3)-C(11)	118.2(3)	C(18)-C(17)-C(16)	120.2(5)
C(15)-N(3)-Ru	128.3(3)	C(17)-C(18)-C(19)	118.6(5)
C(11)-N(3)-Ru	113.5(2)	C(18)-C(19)-C(20)	120.3(4)
C(16)-N(4)-C(20)	117.0(3)	N(4)-C(20)-C(19)	121.2(4)
C(16)-N(4)-Ru	127.8(3)	N(4)-C(20)-C(21)	114.7(3)
C(20)-N(4)-Ru	115.2(2)	C(19)-C(20)-C(21)	124.1(4)
C(25)-N(5)-C(21)	118.5(3)	N(5)-C(21)-C(22)	120.7(4)
C(25)-N(5)-Ru	125.3(3)	N(5)-C(21)-C(20)	115.4(3)
C(21)-N(5)-Ru	115.8(3)	C(22)-C(21)-C(20)	123.9(4)
N(1)-C(1)-C(2)	123.1(4)	C(23)-C(22)-C(21)	119.7(5)
C(3)-C(2)-C(1)	118.5(5)	C(24)-C(23)-C(22)	119.1(5)
C(2)-C(3)-C(4)	119.4(5)	C(23)-C(24)-C(25)	119.7(5)
C(3)-C(4)-C(5)	120.3(5)	N(5)-C(25)-C(24)	122.2(5)
N(1)-C(5)-C(4)	120.5(4)	F(2)-C(28)-F(1)	103.4(6)
N(1)-C(5)-C(6)	115.7(3)	F(2)-C(28)-F(3)	101.3(7)
C(4)-C(5)-C(6)	123.8(4)	F(1)-C(28)-F(3)	107.9(6)
N(2)-C(6)-C(7)	118.7(4)	F(2)-C(28)-S(2)	114.8(6)
N(2)-C(6)-C(5)	113.2(3)	F(1)-C(28)-S(2)	113.8(5)
C(7)-C(6)-C(5)	128.0(4)	F(3)-C(28)-S(2)	114.3(5)
C(8)-C(7)-C(6)	118.5(4)	F(4)-C(29)-F(6)	110.1(5)
C(9)-C(8)-C(7)	122.4(4)	F(4)-C(29)-F(5)	104.1(5)
C(8)-C(9)-C(10)	118.1(4)	F(6)-C(29)-F(5)	103.4(5)
N(2)-C(10)-C(9)	119.3(4)	F(4)-C(29)-S(3)	112.4(4)
N(2)-C(10)-C(11)	113.1(3)	F(6)-C(29)-S(3)	113.3(4)
C(9)-C(10)-C(11)	127.7(4)	F(5)-C(29)-S(3)	112.8(3)
N(3)-C(11)-C(12)	120.8(4)		
N(3)-C(11)-C(10)	115.2(3)		

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^4$) for $[Ru(tpy)(bpy)dmso)]^{2+}$. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	351(2)	340(2)	364(2)	25(2)	40(1)	-22(2)
S(1)	521(6)	405(6)	402(6)	-7(5)	29(5)	-26(5)
S(2)	711(10)	888(12)	1074(13)	57(10)	260(9)	145(8)
S(3)	571(7)	543(7)	634(8)	87(6)	34(6)	-105(6)
F(1)	1600(40)	3490(80)	1140(40)	-660(40)	230(30)	980(40)
F(2)	3680(90)	650(30)	3290(90)	40(40)	750(60)	520(40)
F(3)	1000(30)	2390(60)	2380(50)	-1040(50)	-560(30)	640(30)
F(4)	2970(50)	1330(30)	650(20)	-160(20)	360(30)	210(30)
F(5)	880(20)	1030(30)	1320(30)	-190(20)	120(20)	158(19)
F(6)	910(20)	620(20)	2080(40)	-170(20)	510(20)	-179(18)
O(1)	820(20)	580(20)	670(20)	-62(17)	-316(17)	65(17)
O(2)	780(30)	2130(60)	2380(60)	300(50)	-130(30)	-170(30)
O(3)	2370(60)	770(30)	1940(50)	200(30)	-160(40)	40(40)
O(4)	3490(80)	4820(130)	1560(50)	1980(70)	1950(60)	3270(90)
O(5)	1910(40)	720(30)	710(30)	-30(20)	100(30)	260(30)
O(6)	1170(30)	810(30)	2290(50)	80(30)	740(30)	-370(30)
O(7)	1000(30)	770(30)	1930(40)	-100(30)	-610(30)	170(20)
N(1)	348(17)	380(20)	480(20)	14(15)	71(15)	-37(15)
N(2)	372(17)	349(18)	350(18)	-5(14)	40(14)	-56(15)
N(3)	338(16)	413(19)	387(18)	-23(16)	20(13)	-24(16)
N(4)	345(17)	393(19)	440(20)	39(16)	69(14)	2(15)
N(5)	401(18)	430(20)	420(20)	-29(16)	76(14)	-52(15)
C(1)	500(30)	440(30)	630(30)	80(20)	90(20)	-30(20)
C(2)	460(30)	630(30)	950(40)	100(30)	280(30)	-60(30)
C(3)	400(30)	720(40)	980(40)	50(30)	70(30)	-10(30)
C(4)	430(30)	500(30)	730(30)	60(30)	50(20)	0(20)
C(5)	380(20)	380(20)	480(20)	26(19)	13(18)	7(19)
C(6)	380(20)	370(20)	420(20)	20(19)	8(17)	21(19)
C(7)	500(30)	440(30)	550(30)	100(20)	0(20)	70(20)
C(8)	750(40)	490(30)	590(30)	220(30)	30(30)	0(30)
C(9)	610(30)	470(30)	530(30)	130(20)	170(20)	-60(20)
C(10)	450(20)	400(20)	320(20)	0(18)	48(18)	-59(19)
C(11)	420(20)	380(20)	430(20)	-56(19)	72(18)	-58(19)
C(12)	500(30)	550(30)	570(30)	-10(20)	200(20)	-130(20)
C(13)	410(30)	690(30)	690(30)	-80(30)	190(20)	-40(20)
C(14)	430(30)	630(30)	580(30)	-110(20)	50(20)	90(20)
C(15)	460(30)	500(30)	420(30)	-10(20)	20(20)	0(20)
C(16)	510(30)	450(30)	450(30)	50(20)	40(20)	-10(20)
C(17)	620(30)	540(30)	460(30)	110(30)	50(20)	40(20)
C(18)	680(30)	450(30)	690(40)	210(30)	200(30)	60(30)
C(19)	550(30)	390(30)	690(30)	20(30)	140(20)	-40(20)

C(20)	360(20)	360(20)	460(30)	0(20)	83(18)	-5(18)
C(21)	370(20)	370(20)	480(30)	-50(20)	96(18)	-17(18)
C(22)	680(30)	430(30)	620(30)	-40(30)	150(20)	-150(20)
C(23)	760(30)	620(40)	590(40)	-240(30)	10(30)	-170(30)
C(24)	890(40)	710(40)	360(30)	-100(30)	0(30)	-70(30)
C(25)	670(30)	540(30)	400(30)	0(20)	50(20)	-80(30)
C(26)	1140(50)	440(30)	570(40)	-40(30)	50(40)	-220(30)
C(27)	780(50)	1280(70)	760(50)	-510(50)	270(40)	-190(40)
C(28)	940(50)	990(50)	890(50)	-290(40)	170(40)	40(40)
C(29)	670(30)	840(40)	640(40)	-100(30)	70(30)	-50(30)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Ru(tpy)(bpy)dmso)]^{2+}$.

	x	y	z	Uiso
H(1)	376(12)	2220(30)	4414(14)	32(10)
H(2)	-515(14)	2540(30)	4290(15)	54(11)
H(3)	-768(14)	4080(30)	3645(15)	52(13)
H(4)	-196(14)	5200(40)	3130(16)	61(12)
H(7)	447(15)	6250(30)	2779(16)	60(12)
H(8)	1141(14)	6810(30)	2381(16)	49(12)
H(9)	1958(13)	6000(30)	2514(15)	56(12)
H(12)	2692(13)	4840(30)	2823(15)	41(12)
H(13)	3443(12)	3650(30)	3115(12)	31(9)
H(14)	3376(15)	1980(40)	3757(16)	77(13)
H(15)	2494(12)	1820(30)	4068(14)	36(10)
H(16)	1850(12)	1920(30)	5065(13)	32(10)
H(17)	1772(12)	190(30)	5520(14)	27(11)
H(18)	1410(12)	-1490(30)	5115(14)	37(10)
H(19)	1113(13)	-1370(30)	4128(15)	44(11)
H(22)	782(13)	-1010(30)	3271(15)	43(11)
H(23)	592(14)	-630(40)	2316(17)	57(13)
H(24)	795(13)	1180(30)	1994(15)	41(12)
H(25)	1146(14)	2690(30)	2581(15)	54(12)
H(26A)	1850(14)	6210(40)	4714(17)	55(13)
H(27A)	1219(17)	5200(40)	5280(20)	79(16)
H(26B)	1550(20)	6170(50)	4160(20)	120(20)
H(27B)	990(20)	3850(60)	5150(20)	130(30)
H(26C)	2042(17)	5800(40)	4180(20)	79(19)
H(27C)	800(20)	4810(50)	4790(20)	100(20)

Table 7. Torsion angles [°] for [Ru(tpy)(bpy)dmso)]$^{2+}$.

O(1)-S(1)-Ru-N(4)	42.55(17)
O(1)-S(1)-Ru-N(3)	-58.39(18)

Table 8. Hydrogen bonds for [Ru(tpy)(bpy)dmso)]$^{2+}$. [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(16)-H(16)...O(1)	0.92(3)	2.29(3)	3.117(5)	149(3)