

Electronic Supporting Information

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Self-assembled metalla-bowls for selective sensing of multi-carboxylate anions

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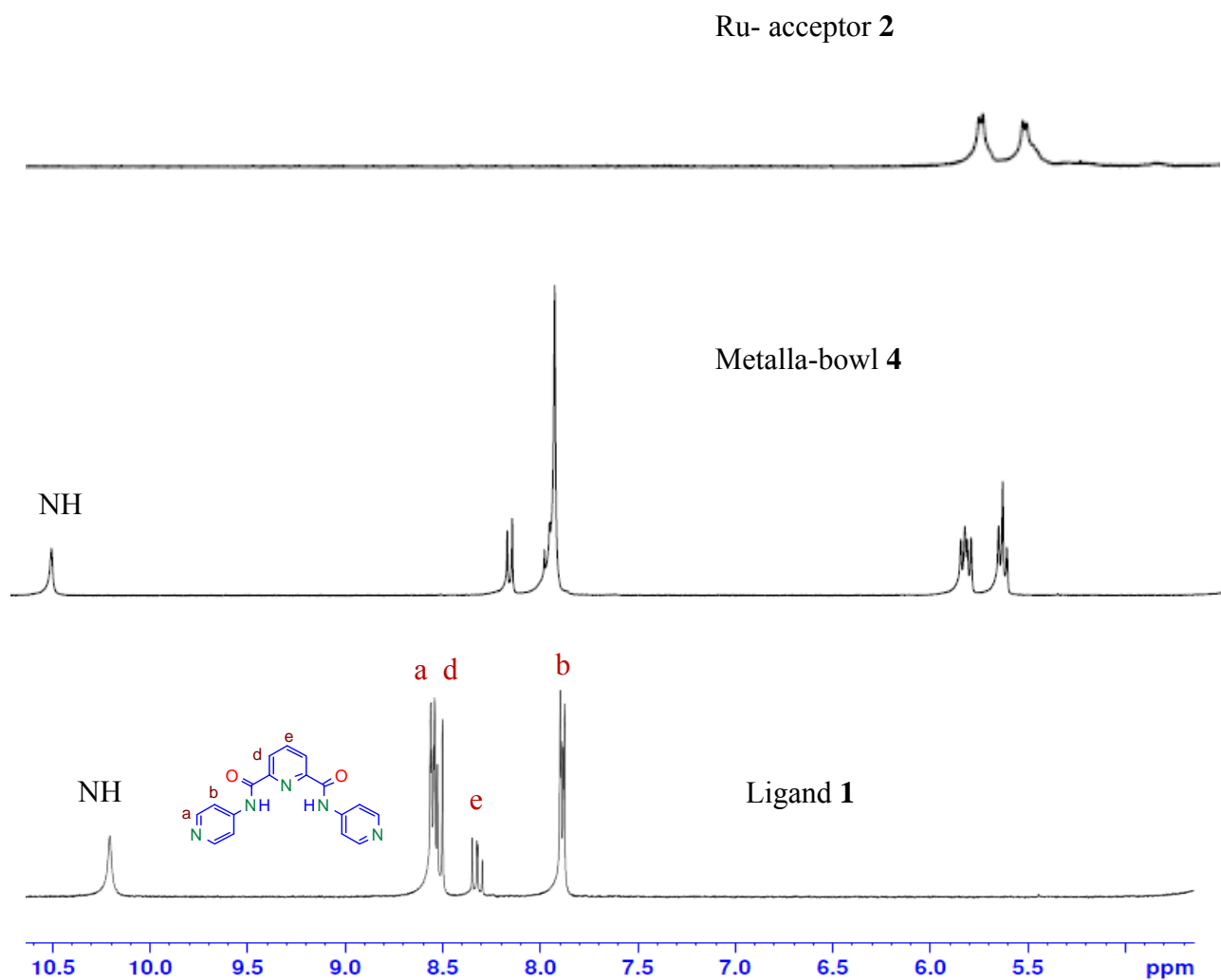


Fig. S1. Comparative NMR of metalla-bowl **4** with ligand **1** and Ru-acceptor **2** in nitromethane- d_3

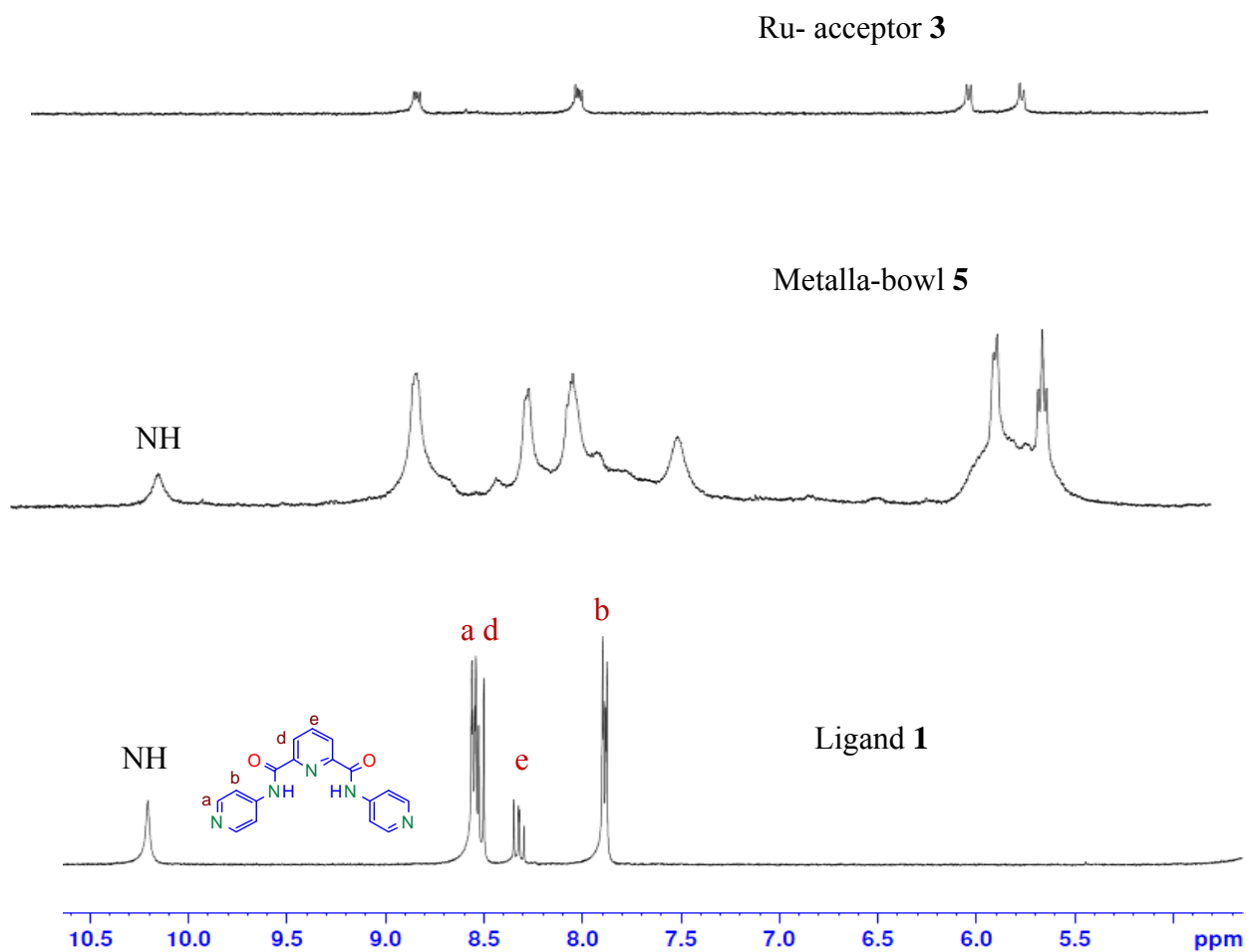


Fig. S2 Comparative NMR of metalla-bowl **5** with ligand **1** and Ru-acceptor **3** in nitromethane- d_3

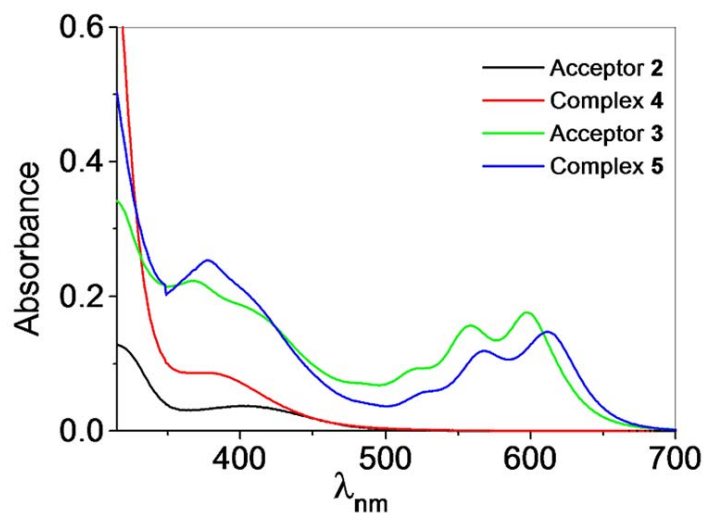


Fig. S3. Comparative absorption spectra of Ru acceptors **2**, **3** and metalla-bowls **4** and **5** in methanol.

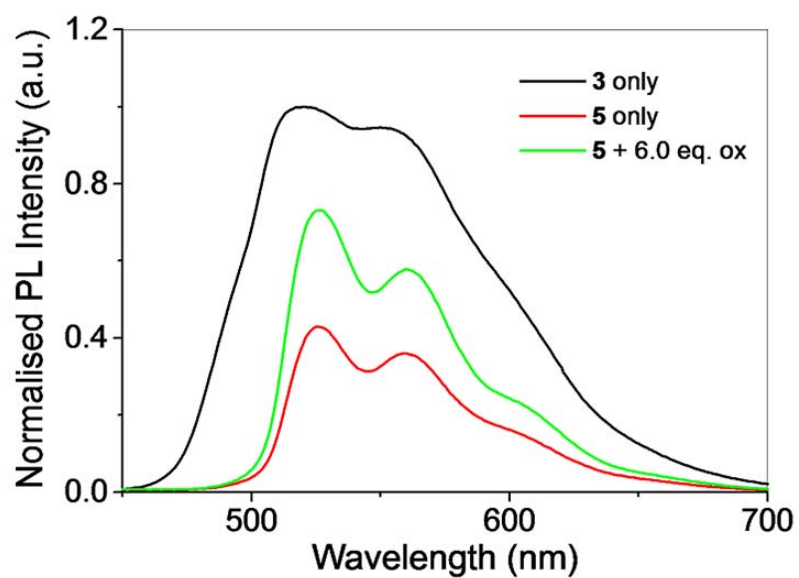


Fig. S4. Comparative emission spectra of Ru acceptor **3**, metalla-bowl **5** and after addition of 6.0 eq. of oxalate anion in **5** in methanol.

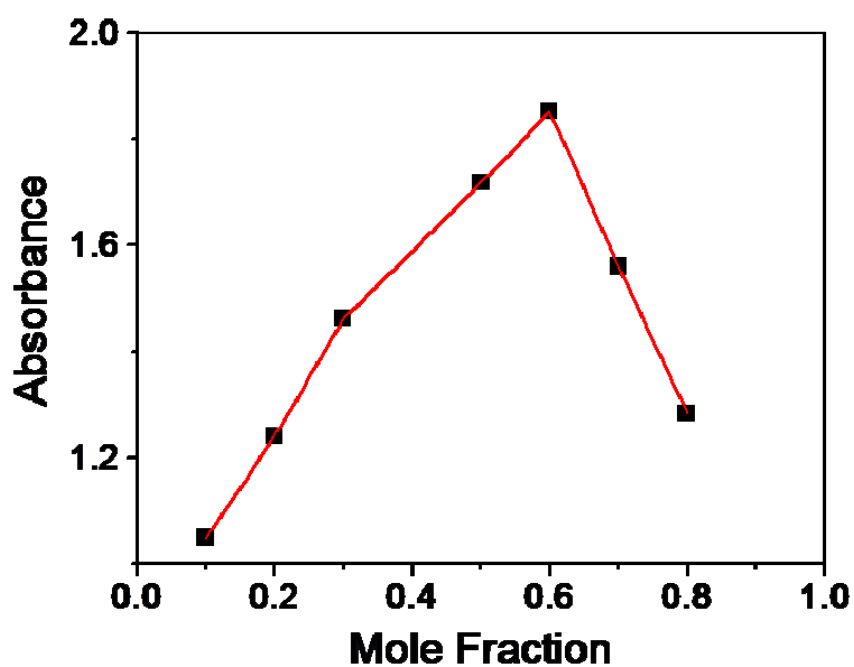


Fig. S5 Job's plot of oxalate anion titrations with **5** showing 1:1 fitting curve.

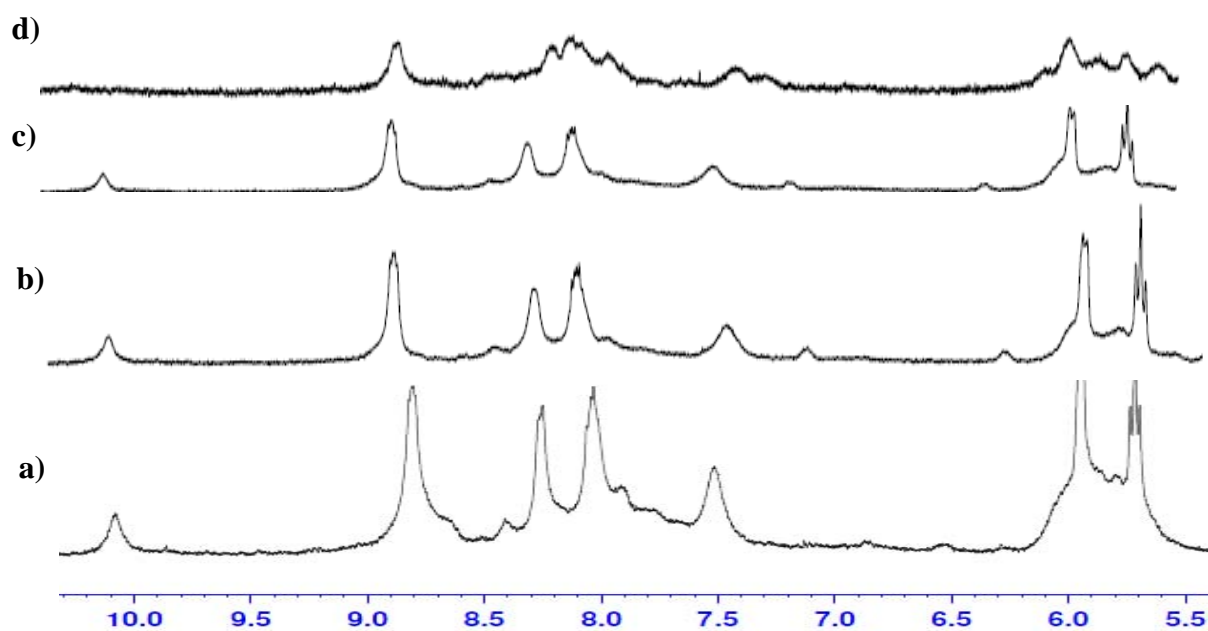


Fig. S6 ¹H NMR spectra of **5** in nitromethane-*d*₃ with increasing amounts of [Bu₄N]₂ oxalate. (a) 0, (b) 0.5, (c) 1.0, and (d) 2.2 equiv of [Bu₄N]₂ oxalate.

Table 1. Crystal data and structure refinement for **4**.

Empirical formula	C165 H89.50 F12 N12.50 O24 Ru4 S4	
Formula weight	3391.51	
Temperature	100(2) K	
Wavelength	1.00000 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 16.255(3) Å	α = 78.93(3)°
	<i>b</i> = 17.304(4) Å	β = 70.96(3)°
	<i>c</i> = 21.415(4) Å	γ = 74.07(3)°
Volume	5440.5(19) Å ³	
Z	2	
Density (calculated)	2.070 g/cm ³	
Absorption coefficient	1.849 mm ⁻¹	
F(000)	3414	
Crystal size	0.20 × 0.05 × 0.04 mm ³	
Theta range for data collection	1.92 to 30.07°	
Index ranges	-15 ≤ <i>h</i> ≤ 15, -16 ≤ <i>k</i> ≤ 17, -20 ≤ <i>l</i> ≤ 19	
Reflections collected	13204	
Independent reflections	7360 [R(int) = 0.0335]	
Completeness to theta = 30.07°	64.1 %	
Max. and min. transmission	0.9372 and 0.7347	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7360 / 0 / 1154	
Goodness-of-fit on F ²	1.865	
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.1365, <i>wR</i> ₂ = 0.3840	
R indices (all data)	<i>R</i> ₁ = 0.1450, <i>wR</i> ₂ = 0.3979	
Extinction coefficient	0.024(2)	
Largest diff. peak and hole	1.350 and -0.658 e.Å ⁻³	
Platon_squeeze_void_count_electrons	350	

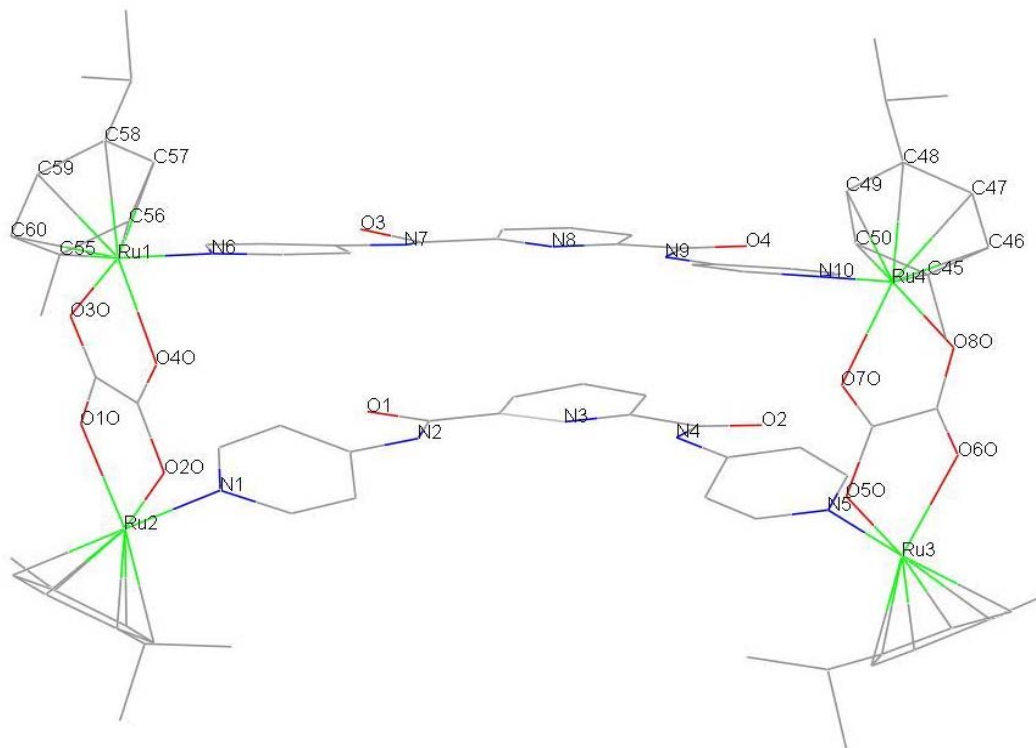


Fig. S7 Crystal structure (labeled) of metallabowl **4**.

Table 2. Bond lengths [\AA] and angles [$^\circ$] for metalla-bowl **4**.

Ru(1)-N(6)	2.061(16)
Ru(1)-C(59)	2.11(2)
Ru(1)-O(3O)	2.116(11)
Ru(1)-O(4O)	2.124(11)
Ru(1)-C(60)	2.16(3)
Ru(1)-C(56)	2.169(18)
Ru(1)-C(57)	2.20(2)
Ru(1)-C(58)	2.20(2)
Ru(1)-C(55)	2.25(2)
Ru(2)-N(1)	2.059(19)
Ru(2)-O(2O)	2.080(12)
Ru(2)-O(1O)	2.130(12)
Ru(2)-C(68)	2.141(19)
Ru(2)-C(65)	2.154(19)
Ru(2)-C(70)	2.167(17)
Ru(2)-C(66)	2.168(19)
Ru(2)-C(67)	2.176(18)
Ru(2)-C(69)	2.18(2)
Ru(3)-O(5O)	2.032(12)
Ru(3)-N(5)	2.093(17)
Ru(3)-O(6O)	2.122(13)
Ru(3)-C(39)	2.127(18)
Ru(3)-C(38)	2.128(19)
Ru(3)-C(37)	2.148(18)
Ru(3)-C(40)	2.15(2)
Ru(3)-C(35)	2.164(19)
Ru(3)-C(36)	2.24(2)
Ru(4)-N(10)	2.077(15)
Ru(4)-O(8O)	2.118(13)
Ru(4)-O(7O)	2.128(12)
Ru(4)-C(49)	2.14(2)
Ru(4)-C(50)	2.157(17)
Ru(4)-C(46)	2.16(2)
Ru(4)-C(45)	2.175(18)

Ru(4)-C(47)	2.18(2)
Ru(4)-C(48)	2.23(2)
O(1)-C(6)	1.34(2)
O(2)-C(12)	1.21(3)
O(3)-C(23)	1.29(2)
O(4)-C(29)	1.23(3)
N(1)-C(2)	1.33(3)
N(1)-C(1)	1.38(3)
N(2)-C(6)	1.30(3)
N(2)-C(5)	1.42(3)
N(3)-C(11)	1.27(2)
N(3)-C(7)	1.42(3)
N(4)-C(13)	1.36(4)
N(4)-C(12)	1.40(3)
N(5)-C(17)	1.29(3)
N(5)-C(16)	1.31(3)
N(6)-C(18)	1.33(3)
N(6)-C(19)	1.33(2)
N(7)-C(23)	1.41(3)
N(7)-C(22)	1.43(3)
N(8)-C(28)	1.30(3)
N(8)-C(24)	1.32(3)
N(9)-C(29)	1.34(3)
N(9)-C(30)	1.45(3)
N(10)-C(33)	1.30(2)
N(10)-C(34)	1.35(3)
C(1)-C(3)	1.37(3)
C(2)-C(4)	1.39(3)
C(3)-C(5)	1.43(3)
C(4)-C(5)	1.38(3)
C(6)-C(7)	1.36(3)
C(7)-C(8)	1.45(3)
C(8)-C(9)	1.37(3)
C(9)-C(10)	1.44(3)
C(10)-C(11)	1.41(3)
C(11)-C(12)	1.48(3)

C(13)-C(14)	1.30(3)
C(13)-C(15)	1.44(4)
C(14)-C(16)	1.39(3)
C(15)-C(17)	1.36(4)
C(18)-C(20)	1.33(3)
C(19)-C(21)	1.43(3)
C(20)-C(22)	1.37(3)
C(21)-C(22)	1.42(3)
C(23)-C(24)	1.47(4)
C(24)-C(25)	1.43(4)
C(25)-C(26)	1.32(3)
C(26)-C(27)	1.46(3)
C(27)-C(28)	1.33(3)
C(28)-C(29)	1.47(4)
C(30)-C(32)	1.32(3)
C(30)-C(31)	1.38(3)
C(31)-C(33)	1.40(3)
C(32)-C(34)	1.40(3)
C(35)-C(40)	1.37(3)
C(35)-C(36)	1.52(3)
C(36)-C(37)	1.38(3)
C(37)-C(38)	1.48(3)
C(37)-C(41)	1.56(3)
C(38)-C(39)	1.30(3)
C(39)-C(40)	1.30(3)
C(40)-C(42)	1.53(3)
C(42)-C(43)	1.49(3)
C(42)-C(44)	1.60(4)
C(45)-C(50)	1.40(3)
C(45)-C(46)	1.49(3)
C(45)-C(51)	1.58(3)
C(46)-C(47)	1.37(3)
C(47)-C(48)	1.35(3)
C(48)-C(49)	1.42(3)
C(48)-C(52)	1.54(3)
C(49)-C(50)	1.35(3)

C(52)-C(53)	1.41(4)
C(52)-C(54)	1.57(3)
C(55)-C(56)	1.37(3)
C(55)-C(60)	1.42(4)
C(55)-C(61)	1.47(3)
C(56)-C(57)	1.51(3)
C(57)-C(58)	1.39(3)
C(58)-C(59)	1.35(3)
C(58)-C(62)	1.48(3)
C(59)-C(60)	1.54(3)
C(62)-C(64)	1.49(3)
C(62)-C(63)	1.67(4)
C(65)-C(66)	1.44(3)
C(65)-C(70)	1.47(3)
C(65)-C(71)	1.57(3)
C(66)-C(67)	1.27(3)
C(67)-C(68)	1.33(3)
C(68)-C(69)	1.41(3)
C(68)-C(72)	1.56(3)
C(69)-C(70)	1.43(3)
C(72)-C(73)	1.54(3)
C(72)-C(74)	1.54(3)
C(10)-O(30)	1.22(2)
C(10)-O(10)	1.31(3)
C(10)-C(20)	1.46(3)
C(20)-O(40)	1.19(2)
C(20)-O(20)	1.38(2)
C(30)-O(80)	1.17(2)
C(30)-O(60)	1.24(2)
C(30)-C(40)	1.46(3)
C(40)-O(70)	1.26(2)
C(40)-O(50)	1.38(2)
S(1F)-O(2F)	1.34(2)
S(1F)-O(3F)	1.501(18)
S(1F)-O(1F)	1.557(19)
S(1F)-C(1F)	2.14(8)

F(1F)-C(1F)	0.89(5)
F(2F)-C(1F)	1.39(4)
F(3F)-C(1F)	1.72(6)
S(2F)-O(5F)	1.364(14)
S(2F)-O(6F)	1.470(14)
S(2F)-O(4F)	1.56(2)
S(2F)-C(2F)	1.71(3)
F(4F)-C(2F)	1.33(3)
F(5F)-C(2F)	1.28(2)
F(6F)-C(2F)	1.43(3)
S(3F)-O(7F)	1.42(2)
S(3F)-O(9F)	1.435(17)
S(3F)-O(8F)	1.433(17)
S(3F)-C(3F)	1.81(3)
F(7F)-C(3F)	1.18(3)
F(8F)-C(3F)	1.46(4)
F(9F)-C(3F)	1.29(3)

N(6)-Ru(1)-C(59)	121.8(10)
N(6)-Ru(1)-O(3O)	84.0(6)
C(59)-Ru(1)-O(3O)	96.6(9)
N(6)-Ru(1)-O(4O)	83.2(5)
C(59)-Ru(1)-O(4O)	154.1(10)
O(3O)-Ru(1)-O(4O)	78.1(6)
N(6)-Ru(1)-C(60)	163.9(9)
C(59)-Ru(1)-C(60)	42.4(10)
O(3O)-Ru(1)-C(60)	94.1(10)
O(4O)-Ru(1)-C(60)	112.2(7)
N(6)-Ru(1)-C(56)	118.1(9)
C(59)-Ru(1)-C(56)	79.4(8)
O(3O)-Ru(1)-C(56)	156.2(8)
O(4O)-Ru(1)-C(56)	95.3(7)
C(60)-Ru(1)-C(56)	67.0(10)
N(6)-Ru(1)-C(57)	92.0(7)
C(59)-Ru(1)-C(57)	65.8(9)
O(3O)-Ru(1)-C(57)	156.4(7)

O(4O)-Ru(1)-C(57)	124.7(7)
C(60)-Ru(1)-C(57)	83.3(9)
C(56)-Ru(1)-C(57)	40.4(7)
N(6)-Ru(1)-C(58)	94.4(9)
C(59)-Ru(1)-C(58)	36.5(9)
O(3O)-Ru(1)-C(58)	120.2(8)
O(4O)-Ru(1)-C(58)	161.4(9)
C(60)-Ru(1)-C(58)	72.6(10)
C(56)-Ru(1)-C(58)	69.5(8)
C(57)-Ru(1)-C(58)	36.8(8)
N(6)-Ru(1)-C(55)	153.0(8)
C(59)-Ru(1)-C(55)	70.0(9)
O(3O)-Ru(1)-C(55)	120.5(7)
O(4O)-Ru(1)-C(55)	90.7(7)
C(60)-Ru(1)-C(55)	37.4(9)
C(56)-Ru(1)-C(55)	36.1(7)
C(57)-Ru(1)-C(55)	70.0(8)
C(58)-Ru(1)-C(55)	83.1(9)
N(1)-Ru(2)-O(2O)	85.1(6)
N(1)-Ru(2)-O(1O)	84.5(6)
O(2O)-Ru(2)-O(1O)	78.6(5)
N(1)-Ru(2)-C(68)	125.4(10)
O(2O)-Ru(2)-C(68)	93.3(7)
O(1O)-Ru(2)-C(68)	148.6(9)
N(1)-Ru(2)-C(65)	112.0(8)
O(2O)-Ru(2)-C(65)	162.7(7)
O(1O)-Ru(2)-C(65)	99.6(9)
C(68)-Ru(2)-C(65)	79.3(9)
N(1)-Ru(2)-C(70)	150.2(9)
O(2O)-Ru(2)-C(70)	123.0(7)
O(1O)-Ru(2)-C(70)	91.1(7)
C(68)-Ru(2)-C(70)	67.7(9)
C(65)-Ru(2)-C(70)	39.7(8)
N(1)-Ru(2)-C(66)	91.5(7)
O(2O)-Ru(2)-C(66)	148.8(8)
O(1O)-Ru(2)-C(66)	132.0(8)

C(68)-Ru(2)-C(66)	63.7(9)
C(65)-Ru(2)-C(66)	38.9(8)
C(70)-Ru(2)-C(66)	69.8(8)
N(1)-Ru(2)-C(67)	97.5(8)
O(2O)-Ru(2)-C(67)	115.7(7)
O(1O)-Ru(2)-C(67)	165.6(7)
C(68)-Ru(2)-C(67)	36.0(8)
C(65)-Ru(2)-C(67)	66.5(9)
C(70)-Ru(2)-C(67)	80.0(8)
C(66)-Ru(2)-C(67)	34.0(7)
N(1)-Ru(2)-C(69)	163.6(9)
O(2O)-Ru(2)-C(69)	94.4(6)
O(1O)-Ru(2)-C(69)	111.5(7)
C(68)-Ru(2)-C(69)	38.2(8)
C(65)-Ru(2)-C(69)	70.1(8)
C(70)-Ru(2)-C(69)	38.3(8)
C(66)-Ru(2)-C(69)	80.5(7)
C(67)-Ru(2)-C(69)	67.9(8)
O(5O)-Ru(3)-N(5)	86.3(6)
O(5O)-Ru(3)-O(6O)	78.9(5)
N(5)-Ru(3)-O(6O)	83.0(6)
O(5O)-Ru(3)-C(39)	117.1(8)
N(5)-Ru(3)-C(39)	99.9(8)
O(6O)-Ru(3)-C(39)	163.7(8)
O(5O)-Ru(3)-C(38)	151.5(8)
N(5)-Ru(3)-C(38)	91.2(7)
O(6O)-Ru(3)-C(38)	129.0(8)
C(39)-Ru(3)-C(38)	35.5(8)
O(5O)-Ru(3)-C(37)	159.3(8)
N(5)-Ru(3)-C(37)	113.2(9)
O(6O)-Ru(3)-C(37)	96.4(7)
C(39)-Ru(3)-C(37)	67.7(8)
C(38)-Ru(3)-C(37)	40.6(8)
O(5O)-Ru(3)-C(40)	92.0(7)
N(5)-Ru(3)-C(40)	125.2(10)
O(6O)-Ru(3)-C(40)	150.1(9)

C(39)-Ru(3)-C(40)	35.2(8)
C(38)-Ru(3)-C(40)	66.4(8)
C(37)-Ru(3)-C(40)	82.1(8)
O(5O)-Ru(3)-C(35)	94.2(7)
N(5)-Ru(3)-C(35)	162.3(11)
O(6O)-Ru(3)-C(35)	114.5(9)
C(39)-Ru(3)-C(35)	64.1(9)
C(38)-Ru(3)-C(35)	79.9(8)
C(37)-Ru(3)-C(35)	69.3(9)
C(40)-Ru(3)-C(35)	37.1(8)
O(5O)-Ru(3)-C(36)	122.9(7)
N(5)-Ru(3)-C(36)	148.5(8)
O(6O)-Ru(3)-C(36)	91.1(7)
C(39)-Ru(3)-C(36)	78.0(9)
C(38)-Ru(3)-C(36)	68.7(8)
C(37)-Ru(3)-C(36)	36.6(8)
C(40)-Ru(3)-C(36)	69.9(8)
C(35)-Ru(3)-C(36)	40.2(9)
N(10)-Ru(4)-O(8O)	81.4(6)
N(10)-Ru(4)-O(7O)	82.0(6)
O(8O)-Ru(4)-O(7O)	76.4(6)
N(10)-Ru(4)-C(49)	95.7(8)
O(8O)-Ru(4)-C(49)	163.2(8)
O(7O)-Ru(4)-C(49)	119.7(7)
N(10)-Ru(4)-C(50)	119.6(8)
O(8O)-Ru(4)-C(50)	155.9(8)
O(7O)-Ru(4)-C(50)	93.9(8)
C(49)-Ru(4)-C(50)	36.5(7)
N(10)-Ru(4)-C(46)	154.5(9)
O(8O)-Ru(4)-C(46)	96.5(7)
O(7O)-Ru(4)-C(46)	122.5(8)
C(49)-Ru(4)-C(46)	78.8(9)
C(50)-Ru(4)-C(46)	69.8(7)
N(10)-Ru(4)-C(45)	157.1(11)
O(8O)-Ru(4)-C(45)	119.8(9)
O(7O)-Ru(4)-C(45)	94.1(7)

C(49)-Ru(4)-C(45)	66.5(10)
C(50)-Ru(4)-C(45)	37.8(8)
C(46)-Ru(4)-C(45)	40.3(9)
N(10)-Ru(4)-C(47)	118.2(9)
O(8O)-Ru(4)-C(47)	100.9(8)
O(7O)-Ru(4)-C(47)	159.3(9)
C(49)-Ru(4)-C(47)	65.8(8)
C(50)-Ru(4)-C(47)	80.3(8)
C(46)-Ru(4)-C(47)	36.9(9)
C(45)-Ru(4)-C(47)	69.1(9)
N(10)-Ru(4)-C(48)	94.0(8)
O(8O)-Ru(4)-C(48)	125.6(8)
O(7O)-Ru(4)-C(48)	157.0(8)
C(49)-Ru(4)-C(48)	37.8(8)
C(50)-Ru(4)-C(48)	68.3(9)
C(46)-Ru(4)-C(48)	66.4(10)
C(45)-Ru(4)-C(48)	80.7(9)
C(47)-Ru(4)-C(48)	35.7(9)
C(2)-N(1)-C(1)	114.4(17)
C(2)-N(1)-Ru(2)	123.7(16)
C(1)-N(1)-Ru(2)	121.5(14)
C(6)-N(2)-C(5)	131(2)
C(11)-N(3)-C(7)	120(2)
C(13)-N(4)-C(12)	122(2)
C(17)-N(5)-C(16)	110.5(18)
C(17)-N(5)-Ru(3)	122.9(17)
C(16)-N(5)-Ru(3)	126.3(18)
C(18)-N(6)-C(19)	115.0(17)
C(18)-N(6)-Ru(1)	120.8(18)
C(19)-N(6)-Ru(1)	124.0(13)
C(23)-N(7)-C(22)	130.5(19)
C(28)-N(8)-C(24)	109(2)
C(29)-N(9)-C(30)	130(2)
C(33)-N(10)-C(34)	114.7(16)
C(33)-N(10)-Ru(4)	124.0(15)
C(34)-N(10)-Ru(4)	121.1(13)

C(3)-C(1)-N(1)	124(2)
N(1)-C(2)-C(4)	127(2)
C(1)-C(3)-C(5)	119(3)
C(5)-C(4)-C(2)	118(2)
C(4)-C(5)-N(2)	125(3)
C(4)-C(5)-C(3)	118(2)
N(2)-C(5)-C(3)	117(3)
N(2)-C(6)-O(1)	117(2)
N(2)-C(6)-C(7)	122(2)
O(1)-C(6)-C(7)	121(2)
C(6)-C(7)-N(3)	121(2)
C(6)-C(7)-C(8)	123(2)
N(3)-C(7)-C(8)	116(2)
C(9)-C(8)-C(7)	125(2)
C(8)-C(9)-C(10)	115(2)
C(11)-C(10)-C(9)	118(2)
N(3)-C(11)-C(10)	127(2)
N(3)-C(11)-C(12)	119(2)
C(10)-C(11)-C(12)	115(2)
O(2)-C(12)-N(4)	124(2)
O(2)-C(12)-C(11)	125(2)
N(4)-C(12)-C(11)	111(2)
C(14)-C(13)-N(4)	127(2)
C(14)-C(13)-C(15)	111(3)
N(4)-C(13)-C(15)	121(3)
C(13)-C(14)-C(16)	122(3)
C(17)-C(15)-C(13)	121(3)
N(5)-C(16)-C(14)	128(2)
N(5)-C(17)-C(15)	127(2)
N(6)-C(18)-C(20)	125(2)
N(6)-C(19)-C(21)	127.5(17)
C(18)-C(20)-C(22)	119(2)
C(22)-C(21)-C(19)	111(2)
C(20)-C(22)-C(21)	122(2)
C(20)-C(22)-N(7)	130(2)
C(21)-C(22)-N(7)	107(3)

O(3)-C(23)-N(7)	110(3)
O(3)-C(23)-C(24)	123(3)
N(7)-C(23)-C(24)	126.0(19)
N(8)-C(24)-C(25)	128(3)
N(8)-C(24)-C(23)	113(3)
C(25)-C(24)-C(23)	118(3)
C(26)-C(25)-C(24)	119(3)
C(25)-C(26)-C(27)	114(2)
C(28)-C(27)-C(26)	119(2)
N(8)-C(28)-C(27)	131(3)
N(8)-C(28)-C(29)	113(2)
C(27)-C(28)-C(29)	116(3)
O(4)-C(29)-N(9)	124(3)
O(4)-C(29)-C(28)	121(2)
N(9)-C(29)-C(28)	115(3)
C(32)-C(30)-C(31)	117(3)
C(32)-C(30)-N(9)	125(2)
C(31)-C(30)-N(9)	119(2)
C(30)-C(31)-C(33)	120(2)
C(30)-C(32)-C(34)	121(2)
N(10)-C(33)-C(31)	125(2)
N(10)-C(34)-C(32)	123.6(17)
C(40)-C(35)-C(36)	121.1(18)
C(40)-C(35)-Ru(3)	71.0(12)
C(36)-C(35)-Ru(3)	72.5(11)
C(37)-C(36)-C(35)	116(2)
C(37)-C(36)-Ru(3)	68.2(12)
C(35)-C(36)-Ru(3)	67.2(12)
C(36)-C(37)-C(38)	118.8(18)
C(36)-C(37)-C(41)	119(2)
C(38)-C(37)-C(41)	122(2)
C(36)-C(37)-Ru(3)	75.3(12)
C(38)-C(37)-Ru(3)	69.0(11)
C(41)-C(37)-Ru(3)	126.9(12)
C(39)-C(38)-C(37)	117.5(18)
C(39)-C(38)-Ru(3)	72.2(13)

C(37)-C(38)-Ru(3)	70.4(10)
C(40)-C(39)-C(38)	129(2)
C(40)-C(39)-Ru(3)	73.5(12)
C(38)-C(39)-Ru(3)	72.3(12)
C(39)-C(40)-C(35)	117(2)
C(39)-C(40)-C(42)	128(3)
C(35)-C(40)-C(42)	115(3)
C(39)-C(40)-Ru(3)	71.3(12)
C(35)-C(40)-Ru(3)	71.9(12)
C(42)-C(40)-Ru(3)	129.6(16)
C(43)-C(42)-C(40)	113(2)
C(43)-C(42)-C(44)	115(3)
C(40)-C(42)-C(44)	107(2)
C(50)-C(45)-C(46)	117(2)
C(50)-C(45)-C(51)	124(3)
C(46)-C(45)-C(51)	119(3)
C(50)-C(45)-Ru(4)	70.4(11)
C(46)-C(45)-Ru(4)	69.3(12)
C(51)-C(45)-Ru(4)	126.8(13)
C(47)-C(46)-C(45)	119(2)
C(47)-C(46)-Ru(4)	72.5(15)
C(45)-C(46)-Ru(4)	70.5(12)
C(48)-C(47)-C(46)	123(2)
C(48)-C(47)-Ru(4)	74.1(16)
C(46)-C(47)-Ru(4)	70.6(13)
C(47)-C(48)-C(49)	116(2)
C(47)-C(48)-C(52)	123(2)
C(49)-C(48)-C(52)	121(2)
C(47)-C(48)-Ru(4)	70.2(12)
C(49)-C(48)-Ru(4)	67.6(12)
C(52)-C(48)-Ru(4)	132.3(18)
C(50)-C(49)-C(48)	126(2)
C(50)-C(49)-Ru(4)	72.5(12)
C(48)-C(49)-Ru(4)	74.6(11)
C(49)-C(50)-C(45)	119(2)
C(49)-C(50)-Ru(4)	71.0(11)

C(45)-C(50)-Ru(4)	71.8(10)
C(53)-C(52)-C(48)	107(2)
C(53)-C(52)-C(54)	116(2)
C(48)-C(52)-C(54)	111(2)
C(56)-C(55)-C(60)	118(2)
C(56)-C(55)-C(61)	122(2)
C(60)-C(55)-C(61)	119(2)
C(56)-C(55)-Ru(1)	68.7(12)
C(60)-C(55)-Ru(1)	67.7(13)
C(61)-C(55)-Ru(1)	127.5(14)
C(55)-C(56)-C(57)	125(2)
C(55)-C(56)-Ru(1)	75.3(12)
C(57)-C(56)-Ru(1)	70.8(11)
C(58)-C(57)-C(56)	118(2)
C(58)-C(57)-Ru(1)	71.6(13)
C(56)-C(57)-Ru(1)	68.7(10)
C(59)-C(58)-C(57)	117(2)
C(59)-C(58)-C(62)	126(2)
C(57)-C(58)-C(62)	116(3)
C(59)-C(58)-Ru(1)	68.0(13)
C(57)-C(58)-Ru(1)	71.6(12)
C(62)-C(58)-Ru(1)	133.0(16)
C(58)-C(59)-C(60)	126(2)
C(58)-C(59)-Ru(1)	75.4(15)
C(60)-C(59)-Ru(1)	70.6(13)
C(55)-C(60)-C(59)	115(3)
C(55)-C(60)-Ru(1)	74.9(18)
C(59)-C(60)-Ru(1)	67.0(12)
C(58)-C(62)-C(64)	111.6(19)
C(58)-C(62)-C(63)	111(2)
C(64)-C(62)-C(63)	109(2)
C(66)-C(65)-C(70)	117(2)
C(66)-C(65)-C(71)	133(2)
C(70)-C(65)-C(71)	109(3)
C(66)-C(65)-Ru(2)	71.1(12)
C(70)-C(65)-Ru(2)	70.6(10)

C(71)-C(65)-Ru(2)	124.7(15)
C(67)-C(66)-C(65)	122(2)
C(67)-C(66)-Ru(2)	73.3(12)
C(65)-C(66)-Ru(2)	70.0(11)
C(66)-C(67)-C(68)	122(2)
C(66)-C(67)-Ru(2)	72.6(12)
C(68)-C(67)-Ru(2)	70.6(11)
C(67)-C(68)-C(69)	125(2)
C(67)-C(68)-C(72)	127(3)
C(69)-C(68)-C(72)	108(2)
C(67)-C(68)-Ru(2)	73.5(12)
C(69)-C(68)-Ru(2)	72.5(11)
C(72)-C(68)-Ru(2)	126.9(15)
C(68)-C(69)-C(70)	115.4(19)
C(68)-C(69)-Ru(2)	69.3(12)
C(70)-C(69)-Ru(2)	70.3(11)
C(69)-C(70)-C(65)	119(2)
C(69)-C(70)-Ru(2)	71.4(12)
C(65)-C(70)-Ru(2)	69.7(11)
C(73)-C(72)-C(74)	104.5(19)
C(73)-C(72)-C(68)	109.3(19)
C(74)-C(72)-C(68)	107.3(19)
O(30)-C(10)-O(10)	124.9(18)
O(30)-C(10)-C(20)	117(2)
O(10)-C(10)-C(20)	117(2)
O(40)-C(20)-O(20)	121(2)
O(40)-C(20)-C(10)	122(2)
O(20)-C(20)-C(10)	115.7(19)
O(80)-C(30)-O(60)	130.3(19)
O(80)-C(30)-C(40)	112(2)
O(60)-C(30)-C(40)	117(2)
O(70)-C(40)-O(50)	118(2)
O(70)-C(40)-C(30)	125(2)
O(50)-C(40)-C(30)	116.3(18)
C(10)-O(10)-Ru(2)	114.2(12)
C(20)-O(20)-Ru(2)	113.7(13)

C(1O)-O(3O)-Ru(1)	110.9(14)
C(2O)-O(4O)-Ru(1)	109.9(15)
C(4O)-O(5O)-Ru(3)	112.7(13)
C(3O)-O(6O)-Ru(3)	114.7(13)
C(4O)-O(7O)-Ru(4)	107.4(14)
C(3O)-O(8O)-Ru(4)	118.6(14)
O(2F)-S(1F)-O(3F)	119.3(12)
O(2F)-S(1F)-O(1F)	109.8(13)
O(3F)-S(1F)-O(1F)	115.4(11)
O(2F)-S(1F)-C(1F)	104.1(14)
O(3F)-S(1F)-C(1F)	115.9(13)
O(1F)-S(1F)-C(1F)	87.5(19)
F(1F)-C(1F)-F(2F)	155(7)
F(1F)-C(1F)-F(3F)	112(5)
F(2F)-C(1F)-F(3F)	83(2)
F(1F)-C(1F)-S(1F)	110(4)
F(2F)-C(1F)-S(1F)	91(4)
F(3F)-C(1F)-S(1F)	85(3)
O(5F)-S(2F)-O(6F)	116.5(9)
O(5F)-S(2F)-O(4F)	115.8(10)
O(6F)-S(2F)-O(4F)	111.2(8)
O(5F)-S(2F)-C(2F)	106.9(12)
O(6F)-S(2F)-C(2F)	104.6(12)
O(4F)-S(2F)-C(2F)	99.5(14)
F(5F)-C(2F)-F(4F)	106(2)
F(5F)-C(2F)-F(6F)	106(2)
F(4F)-C(2F)-F(6F)	107(2)
F(5F)-C(2F)-S(2F)	113(2)
F(4F)-C(2F)-S(2F)	118(2)
F(6F)-C(2F)-S(2F)	106.9(19)
O(7F)-S(3F)-O(9F)	113.1(11)
O(7F)-S(3F)-O(8F)	109.2(14)
O(9F)-S(3F)-O(8F)	119.5(13)
O(7F)-S(3F)-C(3F)	96.1(16)
O(9F)-S(3F)-C(3F)	107.0(12)
O(8F)-S(3F)-C(3F)	109.3(15)

F(7F)-C(3F)-F(9F)	115(3)
F(7F)-C(3F)-F(8F)	103(2)
F(9F)-C(3F)-F(8F)	94(3)
F(7F)-C(3F)-S(3F)	119(2)
F(9F)-C(3F)-S(3F)	116.4(18)
F(8F)-C(3F)-S(3F)	103(2)

Symmetry transformations used to generate equivalent atoms: