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Description of Structure Determination for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (1·4THF).

A single crystal of **1** was sealed in a glass capillary. X-ray data collection was carried out by an oscillation method using a Rigaku R-AXIS IV imaging-plate system on a rotating-anode X-ray generator operated at 50 kV 100 mA. Laue group and unit-cell parameters were determined by data-processing software (*PROCESS*) attached to the R-AXIS system. Lorentz and polarization corrections were applied. The structure was solved by direct method using the SIR92 program (Altomare et al., 1994) and expanded using Fourier techniques (DIRDIF; Beurskens et al., 1992). The non-hydrogen atoms were refined anisotropically. Hydrogen atoms of tetrahydrofuran molecules, which were placed in idealized positions, were included but not refined. The refinements were carried out using full-matrix least squares techniques. All calculations were performed using the *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985, 1992) of Molecular Structure Corporation.

References

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Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Gould, R. O.; Smits, J. M. M.; Smykalla, C. (1992). *The DIRDIF Program System.* Technical Report. Crystallography Laboratory, University of Nijmegen, The Netherlands.

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Table S1. Crystal data, data collection and refinement parameters for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (**1**·4THF).

Crystal data	
Formula	$C_{56}H_{70}Cl_{16}Na_3O_{19}Ru_2$
Formula weight	1885.52
Crystal habit	column
Crystal color	deep purple
Crystal size (mm)	0.30 x 0.15 x 0.15
Indexing Images	3 oscillations, 3 minutes
Detector Position	120.00 mm
Crystal system	triclinic
Lattice parameters:	a = 20.428(7) Å
	b = 21.657(6) Å
	c = 9.443(1) Å
	α= 93.50(2)°
	β = 101.26(2)°
	γ= 108.38(2)°
	V = 3854(1) Å^3
Number of reflections for lattice parameters	80
range for lattice parameters (°)	$6.0 < 2\theta < 51.0$
Space group	$P\bar{1}$ (No. 2)
Z value	2
D_{calc}	1.625 g/cm^3
F(000)	1902.00
Radiation	Mo$K\alpha$ (λ = 0.71070 Å)
Absorption coefficient	10.26 cm^{-1}
Temperature	298 K
Data collection	
Diffractometer	Rigaku R-AXIS IV
Detector Aperture	300 mm x 300 mm
Data Images	50 exposures, 8 minutes
Oscillation Range	3°
2θ range for data collection (°)	$6.0 < 2\theta < 51.0$
hkl range, h	0, 24
k	-26, 25
l	-10, 10
Number of reflections measured	10820

Number of independent reflections	6767
R-merge	0.0331
Number of observed reflections	6767
Criterion of observation	$I > 3.00\sigma(I)$

Refinement

Treatment of hydrogen atoms	not refined
refinement	on *F*
Number of variables	865
Number of reflections used in refinement	6767
R	0.054
wR	0.067
S	2.05
Weighting scheme	$w = 1/[\sigma^2(F) + 0.00002F^2]$
$(\Delta/\sigma)_{max}$	0.21
$(\Delta\sigma)_{min}$ (e Å^{-3})	-1.02
$(\Delta\sigma)_{max}$ (e Å^{-3})	0.76

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic thermal parameters ($Å^2$) for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (**1**·4THF).

$B_{eq} = (8\pi^2/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$.

atom	x	y	z	B_{eq}
Ru(1)	0.79976(4)	0.27592(4)	0.88190(6)	2.80(2)
Ru(2)	0.68221(4)	0.21697(4)	0.82047(6)	2.77(2)
Cl(1)	0.7963(2)	0.4462(2)	0.5522(3)	7.52(9)
Cl(2)	0.7834(2)	0.5723(2)	0.7110(3)	8.37(10)
Cl(3)	0.7815(2)	0.5800(2)	1.0410(3)	8.31(10)
Cl(4)	0.7938(2)	0.4616(2)	1.2093(2)	6.85(8)
Cl(5)	0.8969(1)	0.1343(2)	0.6076(2)	7.02(7)
Cl(6)	0.9436(2)	0.0356(2)	0.8002(3)	8.24(8)
Cl(7)	0.9306(2)	0.0389(2)	1.1228(3)	7.86(8)
Cl(8)	0.8712(1)	0.1411(2)	1.2530(2)	6.60(7)
Cl(9)	0.6080(1)	0.3465(2)	0.4410(2)	6.83(7)
Cl(10)	0.5633(2)	0.4599(2)	0.5741(3)	6.54(7)
Cl(11)	0.5621(2)	0.4730(2)	0.9067(3)	6.43(7)
Cl(12)	0.5999(1)	0.3697(2)	1.0959(2)	6.03(7)
Cl(13)	0.7018(2)	0.0305(2)	0.5151(2)	6.54(8)
Cl(14)	0.7232(2)	-0.0798(2)	0.7015(3)	7.51(8)
Cl(15)	0.7109(2)	-0.0699(2)	1.0274(3)	7.84(9)
Cl(16)	0.6851(2)	0.0532(2)	1.1670(2)	6.11(8)
Na(1)	0.7298(2)	0.2953(2)	0.4824(3)	3.98(9)
Na(2)	0.7533(2)	0.2050(2)	1.2125(3)	3.98(9)
Na(3)	0.7185(2)	-0.2296(3)	0.1497(5)	7.2(1)
O(1)	0.7952(3)	0.3483(3)	1.0207(5)	3.4(1)
O(2)	0.7963(3)	0.3413(3)	0.7385(5)	3.7(1)
O(3)	0.8276(3)	0.2232(3)	1.0404(5)	3.2(1)
O(4)	0.8358(3)	0.2191(3)	0.7628(5)	3.5(1)
O(5)	0.6446(3)	0.2730(3)	0.9353(5)	3.2(1)
O(6)	0.6503(3)	0.2648(3)	0.6578(5)	3.3(1)
O(7)	0.6783(3)	0.1508(3)	0.9647(5)	3.4(1)
O(8)	0.6807(3)	0.1406(3)	0.6860(5)	3.4(1)
O(9)	0.9254(4)	0.3400(5)	0.9473(7)	7.2(2)
O(10)	0.8029(5)	-0.1536(6)	0.3453(9)	10.1(3)
O(11)	0.6270(4)	-0.1956(5)	0.2010(8)	8.3(3)
O(12)	0.6473(5)	-0.2795(5)	-0.0810(8)	10.0(3)
O(13)	0.6934(5)	-0.3232(6)	0.264(1)	11.0(3)
O(14)	0.8200(5)	-0.2132(6)	0.048(1)	11.4(4)
O(15)	0.9569(5)	0.3569(7)	0.458(1)	11.5(4)
O(16)	0.4690(5)	-0.1460(6)	-0.2186(9)	9.5(3)
O(17)	0.8145(3)	0.3204(4)	0.3173(6)	5.1(2)
O(18)	0.6553(3)	0.2425(3)	0.2267(6)	4.7(2)
O(19)	0.7557(3)	0.1954(3)	0.4719(6)	4.7(2)
C(1)	0.7930(4)	0.4002(5)	0.9532(8)	3.3(2)
C(2)	0.7939(5)	0.3974(5)	0.8039(8)	3.4(2)
C(3)	0.7922(5)	0.4508(5)	0.7317(9)	4.3(2)
C(4)	0.7887(5)	0.5081(5)	0.8074(10)	4.9(3)
C(5)	0.7860(5)	0.5106(5)	0.9487(10)	4.4(3)
C(6)	0.7920(5)	0.4583(5)	1.0272(8)	4.0(2)
C(7)	0.8551(4)	0.1809(5)	0.9896(8)	3.1(2)

C(8)	0.8584(4)	0.1777(5)	0.8393(8)	3.1(2)
C(9)	0.8872(5)	0.1334(5)	0.7880(8)	4.1(2)
C(10)	0.9086(5)	0.0895(5)	0.8698(10)	4.7(2)
C(11)	0.9048(5)	0.0923(5)	1.0193(9)	4.4(2)
C(12)	0.8771(4)	0.1369(5)	1.0717(8)	3.7(2)
C(13)	0.6259(4)	0.3171(5)	0.8602(8)	3.2(2)
C(14)	0.6275(4)	0.3120(5)	0.7063(8)	3.2(2)
C(15)	0.6062(5)	0.3553(5)	0.6230(8)	4.2(2)
C(16)	0.5859(5)	0.4054(5)	0.6825(8)	3.9(2)
C(17)	0.5841(5)	0.4097(5)	0.8280(10)	4.2(2)
C(18)	0.6039(4)	0.3659(5)	0.9157(8)	3.5(2)
C(19)	0.6870(4)	0.0983(5)	0.9092(7)	3.0(2)
C(20)	0.6891(4)	0.0917(5)	0.7595(9)	3.5(2)
C(21)	0.6979(5)	0.0355(5)	0.6956(8)	3.8(2)
C(22)	0.7078(5)	-0.0133(5)	0.7830(10)	4.6(2)
C(23)	0.7035(5)	-0.0082(5)	0.9242(9)	4.2(2)
C(24)	0.6900(5)	0.0450(5)	0.9859(8)	3.6(2)
C(25)	0.9610(7)	0.370(1)	1.086(1)	12.2(6)
C(26)	1.031(1)	0.402(2)	1.066(3)	29(1)
C(27)	1.024(2)	0.424(2)	0.935(3)	32(1)
C(28)	0.9639(7)	0.3638(9)	0.842(1)	10.6(5)
C(29)	0.840(1)	-0.166(1)	0.474(3)	19.4(9)
C(30)	0.907(1)	-0.113(1)	0.525(2)	16.1(8)
C(31)	0.9037(10)	-0.064(1)	0.432(2)	13.0(7)
C(32)	0.835(1)	-0.085(1)	0.347(2)	17.1(8)
C(33)	0.6292(10)	-0.168(1)	0.335(2)	18.6(8)
C(34)	0.567(1)	-0.149(1)	0.324(2)	22.4(8)
C(35)	0.5328(10)	-0.164(1)	0.208(2)	20.4(9)
C(36)	0.5593(9)	-0.205(1)	0.127(2)	16.6(7)
C(37)	0.611(1)	-0.2548(9)	-0.194(2)	14.8(7)
C(38)	0.598(1)	-0.296(1)	-0.321(2)	18.0(8)
C(39)	0.599(2)	-0.356(1)	-0.277(2)	25(1)
C(40)	0.633(1)	-0.3439(10)	-0.131(2)	21.6(8)
C(41)	0.6227(10)	-0.365(1)	0.246(2)	17.5(8)
C(42)	0.6198(9)	-0.4250(10)	0.295(2)	13.4(7)
C(43)	0.6898(8)	-0.4209(10)	0.354(2)	11.9(6)
C(44)	0.7342(8)	-0.3503(9)	0.357(2)	10.7(7)
C(45)	0.880(1)	-0.233(1)	0.093(2)	17.1(8)
C(46)	0.916(1)	-0.226(1)	-0.024(2)	19.4(9)
C(47)	0.888(1)	-0.189(2)	-0.124(2)	25(1)
C(48)	0.829(1)	-0.189(2)	-0.069(2)	29(1)
C(49)	0.980(1)	0.305(1)	0.470(2)	15.5(8)
C(50)	1.056(1)	0.326(1)	0.505(3)	21(1)
C(51)	1.074(1)	0.393(2)	0.538(3)	21(1)
C(52)	1.017(1)	0.415(1)	0.497(2)	18.1(10)
C(53)	0.4919(8)	-0.0809(10)	-0.141(2)	11.3(6)
C(54)	0.4946(8)	-0.034(1)	-0.254(2)	12.0(6)
C(55)	0.4884(10)	-0.076(1)	-0.388(2)	14.0(7)
C(56)	0.4909(9)	-0.1370(9)	-0.344(2)	12.4(6)
H(1)	0.9405	0.4005	1.1188	14.9933
H(2)	0.9597	0.3383	1.1519	14.9933
H(3)	1.0538	0.4378	1.1380	30.9210
H(4)	1.0552	0.3710	1.0717	30.9210
H(5)	1.0111	0.4597	0.9316	38.2352
H(6)	1.0653	0.4277	0.8977	38.2352
H(7)	0.9803	0.3316	0.8021	12.6624
H(8)	0.9358	0.3771	0.7645	12.6624
H(9)	0.8128	-0.1691	0.5432	23.2543

H(10)	0.8491	-0.2053	0.4538	23.2543
H(11)	0.9115	-0.0966	0.6228	19.0546
H(12)	0.9451	-0.1277	0.5168	19.0546
H(13)	0.9119	-0.0233	0.4871	15.6041
H(14)	0.9359	-0.0598	0.3715	15.6041
H(15)	0.8363	-0.0771	0.2502	20.3317
H(16)	0.8077	-0.0637	0.3854	20.3317
H(17)	0.6296	-0.1988	0.4018	21.6928
H(18)	0.6704	-0.1304	0.3650	21.6928
H(19)	0.5414	-0.1703	0.3917	26.8852
H(20)	0.5810	-0.1034	0.3468	26.8852
H(21)	0.4855	-0.1898	0.2138	23.9684
H(22)	0.5326	-0.1278	0.1628	23.9684
H(23)	0.5597	-0.1935	0.0333	19.8766
H(24)	0.5323	-0.2506	0.1217	19.8766
H(25)	0.5687	-0.2532	-0.1722	17.8441
H(26)	0.6406	-0.2119	-0.2024	17.8441
H(27)	0.5533	-0.3006	-0.3794	21.4738
H(28)	0.6339	-0.2804	-0.3728	21.4738
H(29)	0.5514	-0.3843	-0.2854	31.4291
H(30)	0.6223	-0.3752	-0.3317	31.4291
H(31)	0.6770	-0.3517	-0.1228	25.4477
H(32)	0.6051	-0.3704	-0.0765	25.4477
H(33)	0.5996	-0.3434	0.2972	21.2306
H(34)	0.6016	-0.3718	0.1439	21.2306
H(35)	0.5926	-0.4324	0.3664	15.9722
H(36)	0.5991	-0.4595	0.2157	15.9722
H(37)	0.6938	-0.4322	0.4504	14.2104
H(38)	0.7041	-0.4489	0.2959	14.2104
H(39)	0.7760	-0.3479	0.3246	12.8723
H(40)	0.7465	-0.3273	0.4525	12.8723
H(41)	0.9078	-0.2055	0.1810	20.3916
H(42)	0.8637	-0.2770	0.1115	20.3916
H(43)	0.9653	-0.2011	0.0200	22.4348
H(44)	0.9123	-0.2673	-0.0643	22.4348
H(45)	0.9201	-0.1486	-0.1244	29.6983
H(46)	0.8737	-0.2149	-0.2188	29.6983
H(47)	0.7890	-0.2107	-0.1438	32.9060
H(48)	0.8348	-0.1436	-0.0525	32.9060
H(49)	0.9596	0.2844	0.5452	19.1178
H(50)	0.9583	0.2781	0.3800	19.1178
H(51)	1.0680	0.3031	0.5826	24.7397
H(52)	1.0682	0.3111	0.4205	24.7397
H(53)	1.0950	0.4030	0.6392	25.0496
H(54)	1.1111	0.4111	0.4862	25.0496
H(55)	1.0250	0.4386	0.4185	20.4202
H(56)	1.0168	0.4415	0.5784	20.4202
H(57)	0.4600	-0.0774	-0.0841	13.4262
H(58)	0.5380	-0.0715	-0.0807	13.4262
H(59)	0.4563	-0.0181	-0.2616	14.2316
H(60)	0.5381	0.0010	-0.2305	14.2316
H(61)	0.4446	-0.0822	-0.4541	16.3487
H(62)	0.5264	-0.0569	-0.4324	16.3487
H(63)	0.5382	-0.1375	-0.3280	14.9080
H(64)	0.4610	-0.1721	-0.4164	14.9080

Table S3. U values for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (**1**·4THF).

atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0507(4)	0.0346(5)	0.0278(3)	0.0211(3)	0.0119(3)	0.0063(3)
Ru(2)	0.0502(4)	0.0340(5)	0.0286(3)	0.0219(3)	0.0126(3)	0.0072(3)
Cl(1)	0.190(3)	0.056(2)	0.047(1)	0.043(2)	0.036(2)	0.024(1)
Cl(2)	0.193(3)	0.049(2)	0.086(2)	0.056(2)	0.022(2)	0.027(2)
Cl(3)	0.192(3)	0.050(2)	0.092(2)	0.062(2)	0.041(2)	0.003(2)
Cl(4)	0.170(3)	0.059(2)	0.043(1)	0.049(2)	0.037(1)	0.001(1)
Cl(5)	0.130(2)	0.134(2)	0.050(1)	0.099(1)	0.035(1)	0.014(1)
Cl(6)	0.143(2)	0.119(2)	0.097(2)	0.106(1)	0.030(2)	0.006(2)
Cl(7)	0.133(2)	0.102(2)	0.106(2)	0.089(2)	0.032(2)	0.050(2)
Cl(8)	0.122(2)	0.120(2)	0.049(1)	0.083(2)	0.032(1)	0.043(1)
Cl(9)	0.139(2)	0.134(2)	0.039(1)	0.104(1)	0.035(1)	0.038(1)
Cl(10)	0.125(2)	0.078(2)	0.084(2)	0.073(1)	0.037(1)	0.042(1)
Cl(11)	0.123(2)	0.068(2)	0.075(2)	0.067(1)	0.017(1)	-0.003(1)
Cl(12)	0.125(2)	0.096(2)	0.042(1)	0.076(1)	0.032(1)	0.009(1)
Cl(13)	0.167(2)	0.057(2)	0.048(1)	0.057(2)	0.046(1)	0.009(1)
Cl(14)	0.173(3)	0.061(2)	0.083(2)	0.073(2)	0.043(2)	0.014(2)
Cl(15)	0.186(3)	0.061(2)	0.071(2)	0.068(2)	0.026(2)	0.030(1)
Cl(16)	0.139(2)	0.060(2)	0.040(1)	0.036(2)	0.027(1)	0.020(1)
Na(1)	0.069(2)	0.046(3)	0.043(2)	0.027(2)	0.019(2)	0.001(2)
Na(2)	0.068(2)	0.052(3)	0.042(2)	0.029(2)	0.022(1)	0.004(2)
Na(3)	0.090(3)	0.080(4)	0.084(3)	0.013(3)	0.001(2)	-0.003(3)
O(1)	0.068(4)	0.037(4)	0.033(3)	0.024(3)	0.019(2)	0.013(3)
O(2)	0.070(4)	0.037(4)	0.040(3)	0.023(3)	0.021(3)	0.013(3)
O(3)	0.057(3)	0.042(4)	0.033(3)	0.028(3)	0.011(2)	0.005(3)
O(4)	0.056(3)	0.059(4)	0.030(3)	0.035(3)	0.014(2)	0.010(3)
O(5)	0.063(3)	0.044(4)	0.027(3)	0.031(3)	0.014(2)	0.009(3)
O(6)	0.058(3)	0.053(4)	0.030(3)	0.037(3)	0.012(2)	0.008(3)
O(7)	0.060(4)	0.031(4)	0.042(3)	0.020(3)	0.017(3)	0.003(3)
O(8)	0.077(4)	0.040(4)	0.020(2)	0.027(3)	0.015(2)	0.012(2)
O(9)	0.072(5)	0.109(9)	0.070(4)	-0.004(5)	0.027(4)	0.002(5)
O(10)	0.107(7)	0.12(1)	0.099(6)	-0.003(7)	-0.024(5)	0.001(7)
O(11)	0.102(6)	0.128(9)	0.084(5)	0.044(6)	0.015(5)	0.006(6)
O(12)	0.188(9)	0.101(8)	0.076(5)	0.064(7)	-0.026(6)	-0.013(6)
O(13)	0.102(7)	0.111(10)	0.192(9)	0.019(7)	0.016(7)	0.064(8)
O(14)	0.128(8)	0.18(1)	0.138(8)	0.059(7)	0.037(6)	0.040(8)
O(15)	0.105(8)	0.13(1)	0.166(9)	0.017(8)	-0.009(7)	0.027(9)
O(16)	0.136(8)	0.102(10)	0.108(6)	0.011(7)	0.041(5)	0.009(6)
O(17)	0.093(5)	0.046(5)	0.055(3)	0.022(4)	0.024(3)	0.001(3)
O(18)	0.087(4)	0.068(5)	0.043(3)	0.049(3)	0.018(3)	0.006(3)
O(19)	0.098(4)	0.045(5)	0.052(3)	0.043(3)	0.020(3)	0.015(3)
C(1)	0.053(5)	0.037(7)	0.038(4)	0.016(4)	0.017(4)	0.006(4)
C(2)	0.066(6)	0.038(6)	0.030(4)	0.024(4)	0.013(4)	0.007(4)
C(3)	0.082(7)	0.034(7)	0.047(5)	0.018(5)	0.012(5)	0.014(5)
C(4)	0.101(8)	0.036(7)	0.049(5)	0.027(6)	0.005(5)	0.008(5)
C(5)	0.077(7)	0.028(7)	0.060(6)	0.018(5)	0.013(5)	-0.001(5)
C(6)	0.085(6)	0.037(7)	0.034(4)	0.024(5)	0.019(4)	0.003(4)
C(7)	0.047(5)	0.045(6)	0.034(4)	0.023(4)	0.014(3)	0.005(4)
C(8)	0.043(5)	0.053(7)	0.027(4)	0.027(4)	0.007(3)	0.003(4)
C(9)	0.069(6)	0.075(8)	0.024(4)	0.043(5)	0.010(4)	0.003(4)
C(10)	0.073(6)	0.055(7)	0.072(6)	0.048(4)	0.023(5)	0.008(5)
C(11)	0.078(6)	0.055(7)	0.055(5)	0.046(5)	0.017(4)	0.017(5)
C(12)	0.060(5)	0.061(7)	0.026(4)	0.032(5)	0.006(4)	0.015(4)
C(13)	0.057(5)	0.040(6)	0.035(4)	0.025(4)	0.020(3)	0.010(4)

C(14)	0.043(5)	0.062(7)	0.025(4)	0.025(4)	0.009(3)	0.008(4)
C(15)	0.082(6)	0.066(7)	0.039(4)	0.051(5)	0.030(4)	0.025(4)
C(16)	0.060(6)	0.060(7)	0.036(4)	0.031(5)	0.007(4)	0.014(4)
C(17)	0.059(6)	0.041(7)	0.068(6)	0.029(5)	0.017(4)	0.006(5)
C(18)	0.063(5)	0.049(6)	0.033(4)	0.033(4)	0.014(4)	0.003(4)
C(19)	0.056(5)	0.041(7)	0.021(4)	0.017(4)	0.014(3)	0.007(4)
C(20)	0.048(5)	0.038(7)	0.042(5)	0.012(5)	0.006(4)	0.001(4)
C(21)	0.085(6)	0.036(7)	0.029(4)	0.025(5)	0.018(4)	-0.002(4)
C(22)	0.087(7)	0.031(7)	0.060(6)	0.028(5)	0.014(5)	0.000(5)
C(23)	0.079(7)	0.035(7)	0.037(5)	0.014(5)	0.002(4)	0.015(4)
C(24)	0.073(6)	0.036(7)	0.029(4)	0.018(5)	0.013(4)	0.007(4)
C(25)	0.077(10)	0.27(3)	0.065(8)	0.01(1)	-0.010(7)	-0.03(1)
C(26)	0.09(2)	0.48(5)	0.45(4)	0.00(2)	-0.02(2)	0.24(3)
C(27)	0.32(3)	0.32(4)	0.34(3)	-0.18(3)	-0.08(3)	0.19(3)
C(28)	0.11(1)	0.17(2)	0.117(10)	0.01(1)	0.061(7)	0.03(1)
C(29)	0.22(2)	0.15(3)	0.27(2)	0.02(2)	-0.09(2)	0.03(2)
C(30)	0.21(2)	0.16(2)	0.15(1)	0.00(2)	-0.08(1)	0.00(2)
C(31)	0.21(2)	0.11(2)	0.12(1)	-0.01(2)	0.03(1)	0.01(1)
C(32)	0.19(2)	0.15(2)	0.18(2)	-0.05(2)	-0.09(1)	0.04(2)
C(33)	0.24(2)	0.43(3)	0.10(1)	0.20(2)	0.06(1)	0.02(2)
C(34)	0.22(1)	0.41(3)	0.26(2)	0.16(1)	0.11(1)	-0.10(2)
C(35)	0.17(2)	0.37(3)	0.22(2)	0.14(2)	-0.05(2)	-0.11(2)
C(36)	0.13(1)	0.23(2)	0.24(2)	0.05(1)	0.02(1)	-0.12(2)
C(37)	0.27(2)	0.10(1)	0.20(2)	0.09(1)	0.01(2)	0.04(1)
C(38)	0.31(2)	0.25(3)	0.08(1)	0.10(2)	-0.06(1)	-0.02(1)
C(39)	0.64(4)	0.21(2)	0.12(1)	0.24(2)	-0.10(2)	-0.03(2)
C(40)	0.47(3)	0.15(1)	0.19(2)	0.22(1)	-0.09(2)	-0.08(1)
C(41)	0.15(2)	0.14(2)	0.37(3)	0.03(1)	0.03(2)	0.16(2)
C(42)	0.17(2)	0.12(2)	0.21(2)	0.03(1)	0.04(1)	0.08(1)
C(43)	0.14(1)	0.19(2)	0.14(1)	0.09(1)	0.03(1)	0.03(1)
C(44)	0.11(1)	0.13(2)	0.14(1)	0.03(1)	-0.015(10)	0.01(1)
C(45)	0.21(2)	0.23(2)	0.26(2)	0.13(1)	0.06(2)	0.10(2)
C(46)	0.24(2)	0.30(3)	0.25(2)	0.10(2)	0.16(1)	0.03(2)
C(47)	0.27(3)	0.49(4)	0.29(2)	0.15(2)	0.09(2)	0.27(2)
C(48)	0.38(2)	0.69(4)	0.32(2)	0.39(2)	0.24(2)	0.30(2)
C(49)	0.19(2)	0.17(3)	0.15(2)	0.01(2)	-0.03(1)	0.01(2)
C(50)	0.19(2)	0.37(3)	0.29(3)	0.17(2)	0.01(2)	0.04(3)
C(51)	0.24(3)	0.17(3)	0.29(3)	-0.08(2)	0.05(2)	-0.02(3)
C(52)	0.31(3)	0.24(3)	0.09(1)	0.06(2)	0.00(2)	-0.01(2)
C(53)	0.13(1)	0.16(2)	0.12(1)	0.04(1)	0.004(10)	0.00(1)
C(54)	0.12(1)	0.16(2)	0.14(1)	0.03(1)	0.00(1)	-0.04(1)
C(55)	0.21(2)	0.16(2)	0.19(2)	0.10(1)	0.02(1)	0.05(1)
C(56)	0.23(2)	0.10(2)	0.15(1)	0.05(1)	0.10(1)	0.00(1)

Table S4. Bond lengths (Å) for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (**1**·4THF).

Ru(1)	Ru(2)	2.273(1)	Ru(1)	O(1)	2.017(6)
Ru(1)	O(2)	2.026(6)	Ru(1)	O(3)	2.038(5)
Ru(1)	O(4)	2.012(6)	Ru(1)	O(9)	2.434(7)
Ru(2)	O(5)	1.997(5)	Ru(2)	O(6)	2.021(5)
Ru(2)	O(7)	2.030(6)	Ru(2)	O(8)	2.011(6)
Cl(1)	C(3)	1.712(9)	Cl(2)	C(4)	1.73(1)
Cl(3)	C(5)	1.73(1)	Cl(4)	C(6)	1.708(8)
Cl(5)	C(9)	1.754(8)	Cl(6)	C(10)	1.710(10)
Cl(7)	C(11)	1.702(10)	Cl(8)	C(12)	1.739(8)
Cl(9)	C(15)	1.726(8)	Cl(10)	C(16)	1.720(9)
Cl(11)	C(17)	1.739(10)	Cl(12)	C(18)	1.718(8)
Cl(13)	C(21)	1.721(8)	Cl(14)	C(22)	1.73(1)
Cl(15)	C(23)	1.729(10)	Cl(16)	C(24)	1.735(8)
Na(1)	O(2)	2.500(5)	Na(1)	O(6)	2.515(7)
Na(1)	O(17)	2.507(8)	Na(1)	O(18)	2.566(6)
Na(1)	O(19)	2.384(8)	Na(2)	O(3)	2.401(7)
Na(2)	O(7)	2.516(5)	Na(2)	O(17*)	2.457(8)
Na(2)	O(18*)	2.408(9)	Na(2)	O(19*)	2.463(7)
Na(3)	O(10)	2.386(10)	Na(3)	O(11)	2.33(1)
Na(3)	O(12)	2.348(9)	Na(3)	O(13)	2.32(1)
Na(3)	O(14)	2.39(1)	O(1)	C(1)	1.33(1)
O(2)	C(2)	1.35(1)	O(3)	C(7)	1.328(10)
O(4)	C(8)	1.323(10)	O(5)	C(13)	1.330(10)
O(6)	C(14)	1.34(1)	O(7)	C(19)	1.30(1)
O(8)	C(20)	1.34(1)	O(9)	C(25)	1.38(1)
O(9)	C(28)	1.41(1)	O(10)	C(29)	1.39(2)
O(10)	C(32)	1.42(2)	O(11)	C(33)	1.35(2)
O(11)	C(36)	1.37(2)	O(12)	C(37)	1.41(2)
O(12)	C(40)	1.36(2)	O(13)	C(41)	1.41(2)
O(13)	C(44)	1.38(2)	O(14)	C(45)	1.42(2)
O(14)	C(48)	1.28(2)	O(15)	C(49)	1.35(3)
O(15)	C(52)	1.42(3)	O(16)	C(53)	1.44(2)
O(16)	C(56)	1.35(2)	C(1)	C(2)	1.41(1)
C(1)	C(6)	1.41(1)	C(2)	C(3)	1.38(1)
C(3)	C(4)	1.42(1)	C(4)	C(5)	1.34(1)
C(5)	C(6)	1.42(1)	C(7)	C(8)	1.433(10)
C(7)	C(12)	1.39(1)	C(8)	C(9)	1.38(1)
C(9)	C(10)	1.38(1)	C(10)	C(11)	1.43(1)
C(11)	C(12)	1.38(1)	C(13)	C(14)	1.458(10)
C(13)	C(18)	1.39(1)	C(14)	C(15)	1.38(1)
C(15)	C(16)	1.40(1)	C(16)	C(17)	1.38(1)
C(17)	C(18)	1.40(1)	C(19)	C(20)	1.42(1)
C(20)	C(21)	1.40(1)	C(21)	C(22)	1.42(1)
C(22)	C(23)	1.35(1)	C(23)	C(24)	1.39(1)
C(25)	C(26)	1.43(3)	C(26)	C(27)	1.35(3)
C(27)	C(28)	1.55(3)	C(29)	C(30)	1.44(3)
C(30)	C(31)	1.43(3)	C(31)	C(32)	1.39(2)
C(33)	C(34)	1.44(3)	C(34)	C(35)	1.14(3)
C(35)	C(36)	1.43(3)	C(37)	C(38)	1.38(2)
C(38)	C(39)	1.39(3)	C(39)	C(40)	1.39(2)
C(41)	C(42)	1.40(2)	C(42)	C(43)	1.40(2)
C(43)	C(44)	1.51(2)	C(45)	C(46)	1.44(2)
C(46)	C(47)	1.42(3)	C(47)	C(48)	1.39(3)
C(49)	C(50)	1.44(3)	C(50)	C(51)	1.37(4)
C(51)	C(52)	1.37(4)	C(53)	C(54)	1.51(2)
C(54)	C(55)	1.47(2)	C(55)	C(56)	1.43(2)

C(25)	H(1)	0.96	C(25)	H(2)	0.95
C(26)	H(3)	0.93	C(26)	H(4)	0.94
C(27)	H(5)	0.90	C(27)	H(6)	0.96
C(28)	H(7)	0.95	C(28)	H(8)	0.95
C(29)	H(9)	0.93	C(29)	H(10)	0.95
C(30)	H(11)	0.95	C(30)	H(12)	0.94
C(31)	H(13)	0.95	C(31)	H(14)	0.94
C(32)	H(15)	0.95	C(32)	H(16)	0.94
C(33)	H(17)	0.94	C(33)	H(18)	0.95
C(34)	H(19)	0.95	C(34)	H(20)	0.94
C(35)	H(21)	0.96	C(35)	H(22)	0.92
C(36)	H(23)	0.93	C(36)	H(24)	0.96
C(37)	H(25)	0.94	C(37)	H(26)	0.95
C(38)	H(27)	0.94	C(38)	H(28)	0.95
C(39)	H(29)	0.96	C(39)	H(30)	0.92
C(40)	H(31)	0.96	C(40)	H(32)	0.92
C(41)	H(33)	0.93	C(41)	H(34)	0.95
C(42)	H(35)	0.95	C(42)	H(36)	0.95
C(43)	H(37)	0.95	C(43)	H(38)	0.94
C(44)	H(39)	0.95	C(44)	H(40)	0.95
C(45)	H(41)	0.95	C(45)	H(42)	0.95
C(46)	H(43)	0.96	C(46)	H(44)	0.93
C(47)	H(45)	0.92	C(47)	H(46)	0.97
C(48)	H(47)	0.94	C(48)	H(48)	0.94
C(49)	H(49)	0.96	C(49)	H(50)	0.94
C(50)	H(51)	0.94	C(50)	H(52)	0.95
C(51)	H(53)	0.95	C(51)	H(54)	0.98
C(52)	H(55)	0.94	C(52)	H(56)	0.94
C(53)	H(57)	0.94	C(53)	H(58)	0.95
C(54)	H(59)	0.94	C(54)	H(60)	0.94
C(55)	H(61)	0.95	C(55)	H(62)	0.94
C(56)	H(63)	0.95	C(56)	H(64)	0.94

Symmetry Code: (*) -x, -y, -z.

Table S5. Bond angles (°) for $Na_3[Ru_2(Cl_4Cat)_4(thf)]\cdot 7THF\cdot 3H_2O$ (**1**·4THF).

Ru(2)	Ru(1)	O(1)	97.8(2)	Ru(2)	Ru(1)	O(2)	96.3(2)
Ru(2)	Ru(1)	O(3)	97.1(2)	Ru(2)	Ru(1)	O(4)	99.5(2)
Ru(2)	Ru(1)	O(9)	179.5(3)	O(1)	Ru(1)	O(2)	82.5(2)
O(1)	Ru(1)	O(3)	95.1(2)	O(1)	Ru(1)	O(4)	162.6(2)
O(1)	Ru(1)	O(9)	81.8(3)	O(2)	Ru(1)	O(3)	166.6(2)
O(2)	Ru(1)	O(4)	96.3(2)	O(2)	Ru(1)	O(9)	83.2(3)
O(3)	Ru(1)	O(4)	82.0(2)	O(3)	Ru(1)	O(9)	83.4(3)
O(4)	Ru(1)	O(9)	80.8(3)	Ru(1)	Ru(2)	O(5)	100.5(2)
Ru(1)	Ru(2)	O(6)	99.8(2)	Ru(1)	Ru(2)	O(7)	100.0(2)
Ru(1)	Ru(2)	O(8)	101.4(2)	O(5)	Ru(2)	O(6)	82.3(2)
O(5)	Ru(2)	O(7)	94.2(2)	O(5)	Ru(2)	O(8)	158.2(2)
O(6)	Ru(2)	O(7)	160.3(2)	O(6)	Ru(2)	O(8)	94.5(2)
O(7)	Ru(2)	O(8)	81.5(2)	O(2)	Na(1)	O(6)	69.0(2)
O(2)	Na(1)	O(17)	109.0(2)	O(2)	Na(1)	O(18)	176.2(2)
O(2)	Na(1)	O(19)	97.9(2)	O(6)	Na(1)	O(17)	175.5(3)
O(6)	Na(1)	O(18)	107.4(2)	O(6)	Na(1)	O(19)	95.5(3)
O(17)	Na(1)	O(18)	74.5(2)	O(17)	Na(1)	O(19)	80.7(3)
O(18)	Na(1)	O(19)	81.0(2)	O(3)	Na(2)	O(7)	71.5(2)
O(3)	Na(2)	O(17)	87.6(2)	O(3)	Na(2)	O(18)	129.4(3)
O(3)	Na(2)	O(19)	142.4(2)	O(7)	Na(2)	O(17)	132.8(3)
O(7)	Na(2)	O(18)	83.3(2)	O(7)	Na(2)	O(19)	140.0(2)
O(17)	Na(2)	O(18)	78.3(3)	O(17)	Na(2)	O(19)	80.1(2)
O(18)	Na(2)	O(19)	82.7(2)	O(10)	Na(3)	O(11)	91.7(4)
O(10)	Na(3)	O(12)	163.5(4)	O(10)	Na(3)	O(13)	99.5(4)
O(10)	Na(3)	O(14)	82.4(4)	O(11)	Na(3)	O(12)	89.6(4)
O(11)	Na(3)	O(13)	96.8(4)	O(11)	Na(3)	O(14)	150.8(5)
O(12)	Na(3)	O(13)	96.6(4)	O(12)	Na(3)	O(14)	88.4(4)
O(13)	Na(3)	O(14)	112.4(5)	Ru(1)	O(1)	C(1)	110.9(5)
Ru(1)	O(2)	Na(1)	116.7(3)	Na(1)	O(2)	C(2)	121.7(5)
Ru(1)	O(2)	C(2)	111.0(5)	Ru(1)	O(3)	Na(2)	113.6(3)
Ru(1)	O(3)	C(7)	110.6(5)	Na(2)	O(3)	C(7)	126.2(5)
Ru(1)	O(4)	C(8)	112.3(4)	Ru(1)	O(9)	C(25)	123.5(7)
Ru(1)	O(9)	C(28)	122.1(7)	Ru(2)	O(5)	C(13)	112.7(5)
Ru(2)	O(6)	Na(1)	115.9(3)	Ru(2)	O(6)	C(14)	111.8(4)
Ru(2)	O(6)	C(14)	111.8(4)	Ru(2)	O(7)	Na(2)	111.1(3)
Ru(2)	O(7)	C(19)	111.0(5)	Na(2)	O(7)	C(19)	117.9(5)
Ru(2)	O(8)	C(20)	111.4(5)	C(25)	O(9)	C(28)	112(1)
Na(3)	O(10)	C(29)	129(1)	Na(3)	O(10)	C(32)	127.2(10)
C(29)	O(10)	C(32)	102(1)	Na(3)	O(11)	C(33)	122.4(10)
Na(3)	O(11)	C(36)	133.7(10)	C(33)	O(11)	C(36)	103(1)
Na(3)	O(12)	C(37)	131(1)	Na(3)	O(12)	C(40)	123(1)
C(37)	O(12)	C(40)	105(1)	Na(3)	O(13)	C(41)	119(1)
Na(3)	O(13)	C(44)	133.8(10)	C(41)	O(13)	C(44)	106(1)
Na(3)	O(14)	C(45)	129(1)	Na(3)	O(14)	C(48)	126(1)
C(45)	O(14)	C(48)	103(1)	C(49)	O(15)	C(52)	107(1)
C(53)	O(16)	C(56)	104(1)	O(1)	C(1)	C(2)	118.7(8)
O(1)	C(1)	C(6)	122.1(7)	O(2)	C(1)	C(6)	149.8(7)
C(2)	C(1)	C(6)	119.1(9)	O(2)	C(2)	C(1)	117.0(8)
O(2)	C(2)	C(3)	123.2(7)	C(1)	C(2)	C(3)	119.9(9)
Cl(1)	C(3)	C(2)	118.2(8)	Cl(1)	C(3)	C(4)	121.7(8)
C(2)	C(3)	C(4)	120.1(8)	Cl(2)	C(4)	C(3)	118.3(7)
Cl(2)	C(4)	C(5)	121.1(9)	C(3)	C(4)	C(5)	120.5(10)
Cl(3)	C(5)	C(4)	120.7(9)	Cl(3)	C(5)	C(6)	118.7(7)
C(4)	C(5)	C(6)	120.5(10)	Cl(4)	C(6)	C(1)	118.4(7)
Cl(4)	C(6)	C(5)	121.9(7)	C(1)	C(6)	C(5)	119.7(8)
O(3)	C(7)	C(8)	118.0(8)	O(3)	C(7)	C(12)	123.7(7)

C(8)	C(7)	C(12)	118.2(8)
O(4)	C(8)	C(9)	125.6(7)
Cl(5)	C(9)	C(8)	116.9(7)
C(8)	C(9)	C(10)	124.1(8)
Cl(6)	C(10)	C(11)	119.5(8)
Cl(7)	C(11)	C(10)	119.5(8)
C(10)	C(11)	C(12)	117.7(8)
Cl(8)	C(12)	C(11)	118.8(7)
O(5)	C(13)	C(14)	116.6(8)
C(14)	C(13)	C(18)	118.1(8)
O(6)	C(14)	C(15)	125.3(7)
Cl(9)	C(15)	C(14)	116.8(7)
C(14)	C(15)	C(16)	122.2(8)
Cl(10)	C(16)	C(17)	121.2(8)
Cl(11)	C(17)	C(16)	120.0(8)
C(16)	C(17)	C(18)	120.7(9)
Cl(12)	C(18)	C(17)	121.0(7)
O(7)	C(19)	C(20)	118.6(8)
C(20)	C(19)	C(24)	117.2(9)
O(8)	C(20)	C(21)	123.5(8)
Cl(13)	C(21)	C(20)	118.5(7)
C(20)	C(21)	C(22)	119.5(8)
Cl(14)	C(22)	C(23)	121.7(8)
Cl(15)	C(23)	C(22)	120.2(8)
C(22)	C(23)	C(24)	120.5(9)
Cl(16)	C(24)	C(23)	121.5(7)
O(9)	C(25)	C(26)	101(1)
O(9)	C(25)	H(2)	110(1)
C(26)	C(25)	H(2)	112(1)
C(25)	C(26)	C(27)	107(2)
C(25)	C(26)	H(4)	108(2)
C(27)	C(26)	H(3)	108(3)
H(3)	C(26)	H(4)	111(2)
C(26)	C(27)	H(5)	115(3)
C(28)	C(27)	H(5)	110(2)
H(5)	C(27)	H(6)	112(2)
O(9)	C(28)	H(7)	111(1)
C(27)	C(28)	H(7)	113(1)
O(10)	C(29)	C(30)	110(2)
O(10)	C(29)	H(10)	107(2)
C(30)	C(29)	H(10)	108(2)
C(29)	C(30)	C(31)	104(1)
C(29)	C(30)	H(12)	111(2)
C(31)	C(30)	H(12)	110(2)
C(30)	C(31)	C(32)	106(1)
C(30)	C(31)	H(14)	111(2)
C(32)	C(31)	H(14)	109(1)
O(10)	C(32)	C(31)	110(1)
O(10)	C(32)	H(16)	108(1)
C(31)	C(32)	H(16)	110(1)
O(11)	C(33)	C(34)	107(1)
O(11)	C(33)	H(18)	109(1)
C(34)	C(33)	H(18)	109(2)
C(33)	C(34)	C(35)	109(2)
C(33)	C(34)	H(20)	109(1)
C(35)	C(34)	H(20)	109(3)
C(34)	C(35)	C(36)	109(2)
C(34)	C(35)	H(22)	110(2)

O(4)	C(8)	C(7)	117.0(8)
C(7)	C(8)	C(9)	117.4(8)
Cl(5)	C(9)	C(10)	119.0(7)
Cl(6)	C(10)	C(9)	122.1(7)
C(9)	C(10)	C(11)	118.4(9)
Cl(7)	C(11)	C(12)	122.7(7)
Cl(8)	C(12)	C(7)	117.1(7)
C(7)	C(12)	C(11)	124.1(8)
O(5)	C(13)	C(18)	125.3(7)
O(6)	C(14)	C(13)	116.1(8)
C(13)	C(14)	C(15)	118.6(8)
Cl(9)	C(15)	C(16)	121.0(7)
Cl(10)	C(16)	C(15)	120.0(6)
C(15)	C(16)	C(17)	118.8(9)
Cl(11)	C(17)	C(18)	119.2(7)
Cl(12)	C(18)	C(13)	117.5(7)
C(13)	C(18)	C(17)	121.5(8)
O(7)	C(19)	C(24)	124.0(7)
O(8)	C(20)	C(19)	116.2(8)
C(19)	C(20)	C(21)	120.2(9)
Cl(13)	C(21)	C(22)	121.9(7)
Cl(14)	C(22)	C(21)	117.8(7)
C(21)	C(22)	C(23)	120.4(9)
Cl(15)	C(23)	C(24)	119.3(7)
Cl(16)	C(24)	C(19)	116.5(7)
C(19)	C(24)	C(23)	121.7(8)
O(9)	C(25)	H(1)	110(1)
C(26)	C(25)	H(1)	111(2)
H(1)	C(25)	H(2)	109(1)
C(25)	C(26)	H(3)	109(2)
C(27)	C(26)	C(28)	42(1)
C(27)	C(26)	H(4)	112(3)
C(26)	C(27)	C(28)	100(2)
C(26)	C(27)	H(6)	109(3)
C(28)	C(27)	H(6)	106(2)
O(9)	C(28)	C(27)	100(1)
O(9)	C(28)	H(8)	111(1)
C(27)	C(28)	H(8)	111(2)
O(10)	C(29)	H(9)	108(1)
C(30)	C(29)	H(9)	110(2)
H(9)	C(29)	H(10)	111(2)
C(29)	C(30)	H(11)	109(2)
C(31)	C(30)	H(11)	110(2)
H(11)	C(30)	H(12)	110(1)
C(30)	C(31)	H(13)	110(1)
C(32)	C(31)	H(13)	108(2)
H(13)	C(31)	H(14)	110(1)
O(10)	C(32)	H(15)	107(1)
C(31)	C(32)	H(15)	109(2)
H(15)	C(32)	H(16)	110(2)
O(11)	C(33)	H(17)	109(2)
C(34)	C(33)	H(17)	110(1)
H(17)	C(33)	H(18)	109(1)
C(33)	C(34)	H(19)	108(2)
C(35)	C(34)	H(19)	110(2)
H(19)	C(34)	H(20)	110(1)
C(34)	C(35)	H(21)	108(2)
C(36)	C(35)	H(21)	108(2)

C(36)	C(35)	H(22)	109(2)
O(11)	C(36)	C(35)	106(1)
O(11)	C(36)	H(24)	107(2)
C(35)	C(36)	H(24)	111(1)
O(12)	C(37)	C(38)	107(1)
O(12)	C(37)	H(26)	108(1)
C(38)	C(37)	H(26)	109(2)
C(37)	C(38)	C(39)	105(1)
C(37)	C(38)	H(28)	111(2)
C(39)	C(38)	H(28)	108(2)
C(38)	C(39)	C(40)	106(1)
C(38)	C(39)	H(30)	111(2)
C(40)	C(39)	H(30)	111(2)
O(12)	C(40)	C(39)	109(1)
O(12)	C(40)	H(32)	110(1)
C(39)	C(40)	H(32)	111(2)
O(13)	C(41)	C(42)	110(1)
O(13)	C(41)	H(34)	107(1)
C(42)	C(41)	H(34)	109(2)
C(41)	C(42)	C(43)	106(1)
C(41)	C(42)	H(36)	110(1)
C(43)	C(42)	H(36)	110(1)
C(42)	C(43)	C(44)	105(1)
C(42)	C(43)	H(38)	110(1)
C(44)	C(43)	H(38)	110(1)
O(13)	C(44)	C(43)	106(1)
O(13)	C(44)	H(40)	109(1)
C(43)	C(44)	H(40)	110(1)
O(14)	C(45)	C(46)	106(1)
O(14)	C(45)	H(42)	107(1)
C(46)	C(45)	H(42)	112(2)
C(45)	C(46)	C(47)	108(2)
C(45)	C(46)	H(44)	107(2)
C(47)	C(46)	H(44)	114(2)
C(46)	C(47)	C(48)	99(2)
C(46)	C(47)	H(46)	106(2)
C(48)	C(47)	H(46)	111(2)
O(14)	C(48)	C(47)	119(2)
O(14)	C(48)	H(48)	107(2)
C(47)	C(48)	H(48)	104(2)
O(15)	C(49)	C(50)	110(2)
O(15)	C(49)	H(50)	104(1)
C(50)	C(49)	H(50)	114(2)
C(49)	C(50)	C(51)	101(2)
C(49)	C(50)	H(52)	105(2)
C(51)	C(50)	H(52)	116(3)
C(50)	C(51)	C(52)	113(2)
C(50)	C(51)	H(54)	104(3)
C(52)	C(51)	H(54)	111(3)
O(15)	C(52)	C(51)	104(2)
O(15)	C(52)	H(56)	112(2)
C(51)	C(52)	H(56)	106(2)
O(16)	C(53)	C(54)	107(1)
O(16)	C(53)	H(58)	109(1)
C(54)	C(53)	H(58)	109(1)
C(53)	C(54)	C(55)	102(1)
C(53)	C(54)	H(60)	110(1)
C(55)	C(54)	H(60)	110(1)

H(21)	C(35)	H(22)	110(2)
O(11)	C(36)	H(23)	109(1)
C(35)	C(36)	H(23)	111(2)
H(23)	C(36)	H(24)	110(1)
O(12)	C(37)	H(25)	109(1)
C(38)	C(37)	H(25)	111(1)
H(25)	C(37)	H(26)	110(1)
C(37)	C(38)	H(27)	110(2)
C(39)	C(38)	H(27)	110(2)
H(27)	C(38)	H(28)	110(1)
C(38)	C(39)	H(29)	108(2)
C(40)	C(39)	H(29)	106(2)
H(29)	C(39)	H(30)	110(2)
O(12)	C(40)	H(31)	107(1)
C(39)	C(40)	H(31)	107(2)
H(31)	C(40)	H(32)	110(1)
O(13)	C(41)	H(33)	108(1)
C(42)	C(41)	H(33)	110(2)
H(33)	C(41)	H(34)	110(1)
C(41)	C(42)	H(35)	109(2)
C(43)	C(42)	H(35)	110(1)
H(35)	C(42)	H(36)	109(1)
C(42)	C(43)	H(37)	110(1)
C(44)	C(43)	H(37)	110(1)
H(37)	C(43)	H(38)	110(1)
O(13)	C(44)	H(39)	109(1)
C(43)	C(44)	H(39)	110(1)
H(39)	C(44)	H(40)	109(1)
O(14)	C(45)	H(41)	107(1)
C(46)	C(45)	H(41)	113(2)
H(41)	C(45)	H(42)	109(2)
C(45)	C(46)	H(43)	105(1)
C(47)	C(46)	H(43)	109(2)
H(43)	C(46)	H(44)	110(2)
C(46)	C(47)	H(45)	111(2)
C(48)	C(47)	H(45)	115(3)
H(45)	C(47)	H(46)	110(2)
O(14)	C(48)	H(47)	107(2)
C(47)	C(48)	H(47)	106(2)
H(47)	C(48)	H(48)	110(2)
O(15)	C(49)	H(49)	103(2)
C(50)	C(49)	H(49)	112(2)
H(49)	C(49)	H(50)	109(2)
C(49)	C(50)	H(51)	105(2)
C(51)	C(50)	H(51)	116(2)
H(51)	C(50)	H(52)	109(2)
C(50)	C(51)	H(53)	106(3)
C(52)	C(51)	H(53)	113(3)
H(53)	C(51)	H(54)	106(2)
O(15)	C(52)	H(55)	112(1)
C(51)	C(52)	H(55)	107(2)
H(55)	C(52)	H(56)	111(2)
O(16)	C(53)	H(57)	110(1)
C(54)	C(53)	H(57)	110(1)
H(57)	C(53)	H(58)	109(1)
C(53)	C(54)	H(59)	110(1)
C(55)	C(54)	H(59)	111(1)
H(59)	C(54)	H(60)	110(2)

C(54)	C(55)	C(56)	105(1)	C(54)	C(55)	H(61)	110(1)
C(54)	C(55)	H(62)	110(1)	C(56)	C(55)	H(61)	109(1)
C(56)	C(55)	H(62)	109(1)	H(61)	C(55)	H(62)	110(1)
O(16)	C(56)	C(55)	110(1)	O(16)	C(56)	H(63)	107(1)
O(16)	C(56)	H(64)	108(1)	C(55)	C(56)	H(63)	110(1)
C(55)	C(56)	H(64)	110(1)	H(63)	C(56)	H(64)	109(1)

Symmetry Code: (*) -x, -y, -z.

Figure S1. A view of the $[Ru_2(Cl_4Cat)_4]^{3-}$ anion including a weakly associated THF solvate molecule.

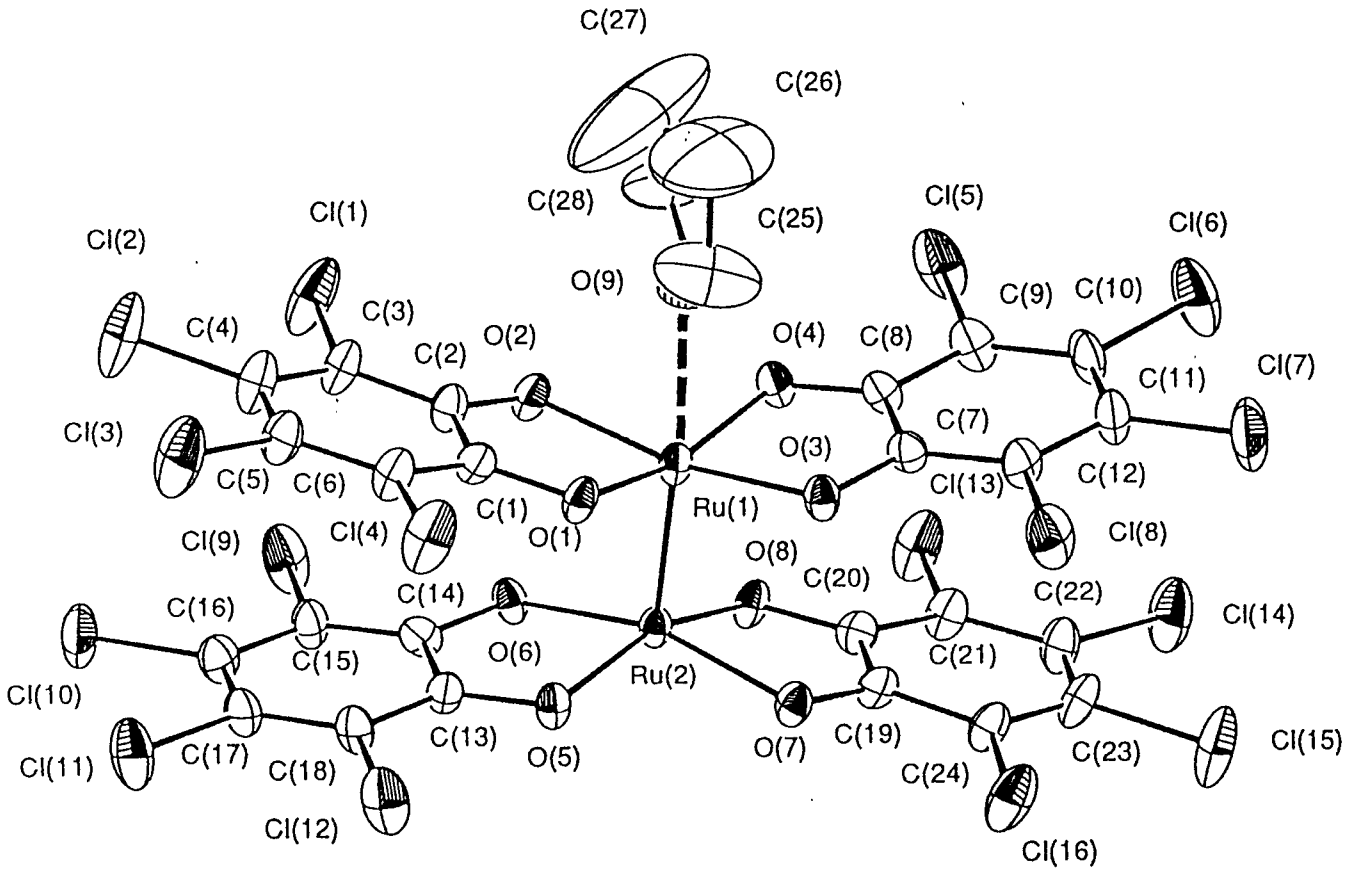


Figure S2. Chain structure of 1·4THF

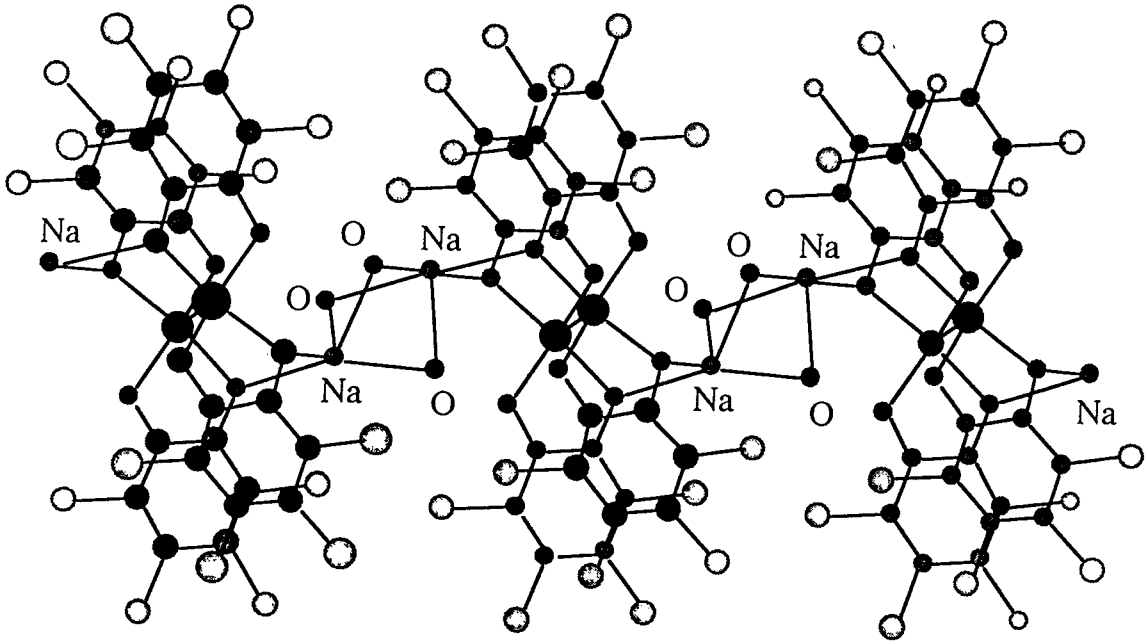
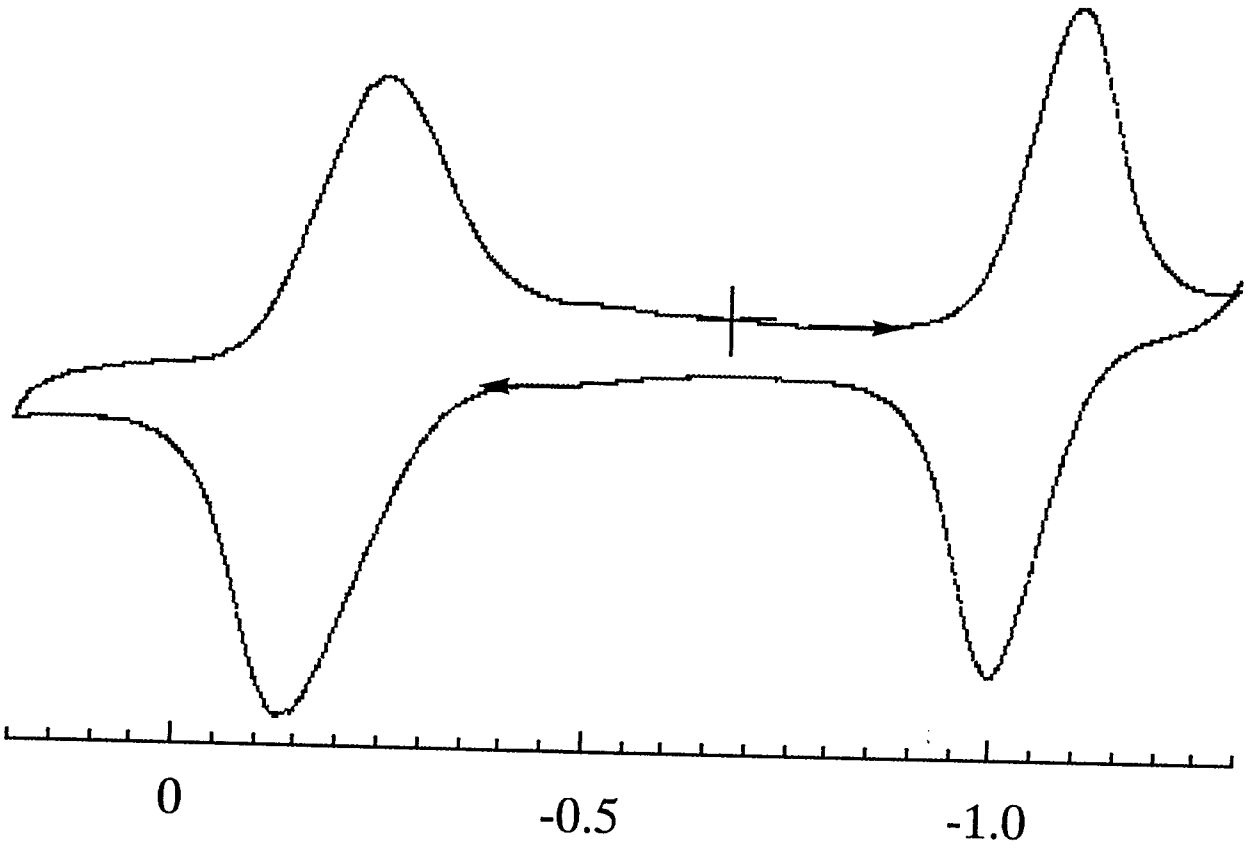


Figure S3. Cyclic voltammogram of 1 in THF.



Description of Structure Determination for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (2·2THF).

A single crystal of **2** was sealed in a glass capillary. X-ray data collection was carried out by an oscillation method using a Rigaku R-AXIS IV imaging-plate system on a rotating-anode X-ray generator operated at 50 kV 100 mA. Laue group and unit-cell parameters were determined by data-processing software (*PROCESS*) attached to the R-AXIS system. Lorentz and polarization corrections were applied. The structure was solved by heavy-atom Patterson methods using the SAPI91 program (Fan Hai-Fu, 1991) and expanded using Fourier techniques (DIRDIF; Beurskens et al., 1992). The non-hydrogen atoms were refined anisotropically. Hydrogen atoms of tetrahydrofuran molecules, which were placed in idealized positions, were included but not refined. The refinements were carried out using full-matrix least squares techniques. All calculations were performed using the *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985, 1992) of Molecular Structure Corporation.

References

Fan Hai-Fu. (1991). Structure Analysis Programs with Intelligent Control, Rigaku Corporation, Tokyo, Japan.

Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Gould, R. O.; Smits, J. M. M.; Smykalla, C. (1992). *The DIRDIF Program System*. Technical Report. Crystallography Laboratory, University of Nijmegen, The Netherlands.

Molecular Structure Corporation (1985, 1992). *TEXSAN. TEXRAY Structure Analysis Package.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Table S6. Crystal data, data collection and refinement parameters for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (**2**·2THF).

Crystal data	
Formula	$C_{40}H_{36}Cl_{16}Na_2O_{14}Ru_2$
Formula weight	1556.08
Crystal habit	column
Crystal color	deep purple
Crystal size (mm)	0.30 x 0.20 x 0.10
Indexing Images	3 oscillations, 3 minutes
Detector Position	120.00 mm
Crystal system	triclinic
Lattice parameters:	a = 12.176(3) Å
	b = 12.958(3) Å
	c = 9.3523(6) Å
	α= 93.19(1)°
	β = 102.49(1)°
	γ= 103.48(2)°
	V = 1392.2(5) Å^3
Number of reflections for lattice parameters	80
range for lattice parameters (°)	$6.0 < 2\theta < 51.2$
Space group	$P\bar{1}$ (No. 2)
Z value	1
D_{calc}	1.856 g/cm^3
F(000)	770.00
Radiation	Mo$K\alpha$ (λ = 0.71070 Å)
Absorption coefficient	13.85 cm^{-1}
Temperature	298 K
Data collection	
Diffractometer	Rigaku R-AXIS IV
Detector Aperture	300 mm x 300 mm
Data Images	28 exposures, 10 minutes
Oscillation Range	5.5°
2θ range for data collection (°)	$6 < 2\theta < 51$
hkl range, h	0, 14
k	-15, 15
l	-10, 10

Number of reflections measured	4613
Number of independent reflections	4140
R-merge	0.0339
Number of observed reflections	4140
Criterion of observation	$I > 3.00\sigma(I)$

Refinement

Treatment of hydrogen atoms	not refined
refinement	on *F*
Number of variables	335
Number of reflections used in refinement	4140
R	0.038
wR	0.046
S	1.94
Weighting scheme	$w = 1/[\sigma^2(F) + 0.00002F^2]$
$(\Delta/\sigma)_{max}$	<0.001
$(\Delta\sigma)_{min}$ (e Å^{-3})	-1.44
$(\Delta\sigma)_{max}$ (e Å^{-3})	0.50

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic thermal parameters ($Å^2$) for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (**2**·2THF).

$B_{eq} = (8\pi^2/3)(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$.

atom	x	y	z	B_{eq}
Ru(1)	0.07653(3)	0.06787(3)	0.04786(3)	2.207(6)
Cl(1)	0.2656(1)	-0.0649(1)	0.4929(1)	4.72(3)
Cl(2)	0.4437(1)	-0.1917(1)	0.4287(1)	7.36(3)
Cl(3)	0.4886(1)	-0.2071(1)	0.1117(2)	7.32(3)
Cl(4)	0.36327(9)	-0.0890(1)	-0.1327(1)	4.53(3)
Cl(5)	-0.11211(10)	0.28605(10)	0.3173(1)	4.07(2)
Cl(6)	-0.2129(1)	0.4456(1)	0.1181(2)	6.13(3)
Cl(7)	-0.1731(1)	0.4572(1)	-0.2003(2)	6.90(3)
Cl(8)	-0.0336(1)	0.3090(1)	-0.3175(1)	4.67(3)
Na(1)	0.0803(1)	0.1028(1)	0.4116(2)	3.71(4)
O(1)	0.1937(2)	0.0140(2)	-0.0342(2)	2.54(5)
O(2)	0.1477(2)	0.0155(2)	0.2294(2)	2.45(5)
O(3)	0.0438(2)	0.1666(2)	-0.1022(2)	2.49(5)
O(4)	0.0082(2)	0.1551(2)	0.1663(2)	2.48(5)
O(5)	0.2610(2)	0.2304(2)	0.1449(3)	3.74(7)
O(6)	0.2006(3)	0.2685(3)	0.5028(3)	4.74(8)
O(7)	-0.0846(2)	-0.0508(2)	0.3407(3)	3.34(6)
C(1)	0.2519(3)	-0.0366(3)	0.0676(4)	2.38(7)
C(2)	0.2295(3)	-0.0346(3)	0.2078(4)	2.43(8)
C(3)	0.2905(3)	-0.0791(3)	0.3197(4)	3.11(9)
C(4)	0.3706(4)	-0.1335(4)	0.2890(4)	3.94(10)
C(5)	0.3920(3)	-0.1379(4)	0.1510(5)	4.0(1)
C(6)	0.3345(3)	-0.0889(3)	0.0388(4)	3.08(9)
C(7)	-0.0138(3)	0.2341(3)	-0.0544(4)	2.38(8)
C(8)	-0.0327(3)	0.2278(3)	0.0871(4)	2.37(7)
C(9)	-0.0917(3)	0.2948(3)	0.1411(4)	2.68(8)
C(10)	-0.1360(4)	0.3651(3)	0.0512(4)	3.46(9)
C(11)	-0.1184(4)	0.3713(3)	-0.0887(5)	3.69(10)
C(12)	-0.0573(3)	0.3050(3)	-0.1438(4)	2.91(8)
C(13)	0.2905(4)	0.3056(4)	0.0463(5)	5.0(1)
C(14)	0.4038(4)	0.3818(4)	0.1221(6)	5.0(1)
C(15)	0.4582(4)	0.3214(5)	0.2402(6)	5.4(1)
C(16)	0.3695(4)	0.2169(4)	0.2285(5)	5.2(1)
C(17)	0.2009(5)	0.3682(4)	0.4467(5)	5.5(1)
C(18)	0.3034(6)	0.4503(5)	0.5333(6)	6.8(2)
C(19)	0.3572(5)	0.3944(5)	0.6543(6)	6.7(2)
C(20)	0.2782(5)	0.2883(5)	0.6423(6)	6.8(2)
H(1)	0.2988	0.2700	-0.0409	5.9800
H(2)	0.2324	0.3433	0.0220	5.9800
H(3)	0.4518	0.3993	0.0547	6.0119
H(4)	0.3911	0.4448	0.1643	6.0119
H(5)	0.5285	0.3101	0.2227	6.4045
H(6)	0.4731	0.3603	0.3345	6.4045
H(7)	0.3920	0.1622	0.1803	6.1370
H(8)	0.3625	0.2003	0.3244	6.1370
H(9)	0.2051	0.3624	0.3462	6.5323
H(10)	0.1321	0.3884	0.4539	6.5323

H(11)	0.3561	0.4750	0.4741	8.1322
H(12)	0.2803	0.5083	0.5731	8.1322
H(13)	0.4311	0.3878	0.6414	7.9428
H(14)	0.3662	0.4323	0.7464	7.9428
H(15)	0.3215	0.2350	0.6517	8.0960
H(16)	0.2366	0.2852	0.7170	8.0960
H(17)	-0.0581	-0.0999	0.2962	4.5440
H(18)	-0.1353	-0.0320	0.2938	4.5440

Table S8. U values for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (**2**·2THF).

atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0315(1)	0.0361(2)	0.0212(1)	0.0166(1)	0.0066(1)	0.0082(1)
Cl(1)	0.0665(7)	0.0930(9)	0.0303(5)	0.0401(6)	0.0087(4)	0.0209(5)
Cl(2)	0.1026(8)	0.139(1)	0.0656(8)	0.0908(7)	0.0065(6)	0.0386(7)
Cl(3)	0.0930(7)	0.143(1)	0.0751(9)	0.0955(6)	0.0171(6)	0.0146(7)
Cl(4)	0.0469(6)	0.0954(9)	0.0404(6)	0.0349(5)	0.0152(4)	0.0031(5)
Cl(5)	0.0607(6)	0.0658(7)	0.0373(5)	0.0278(5)	0.0192(4)	0.0027(5)
Cl(6)	0.1002(8)	0.0759(8)	0.0860(8)	0.0651(6)	0.0355(6)	0.0167(6)
Cl(7)	0.1243(10)	0.0896(8)	0.0806(8)	0.0776(6)	0.0284(7)	0.0475(6)
Cl(8)	0.0828(8)	0.0694(8)	0.0364(5)	0.0327(6)	0.0177(5)	0.0265(5)
Na(1)	0.061(1)	0.048(1)	0.0284(8)	0.0022(8)	0.0137(7)	0.0033(7)
O(1)	0.030(1)	0.044(2)	0.025(1)	0.014(1)	0.0053(9)	0.009(1)
O(2)	0.033(1)	0.041(2)	0.024(1)	0.016(1)	0.0067(9)	0.0071(10)
O(3)	0.034(1)	0.036(1)	0.028(1)	0.015(1)	0.0079(10)	0.006(1)
O(4)	0.037(1)	0.035(1)	0.026(1)	0.016(1)	0.0072(10)	0.0065(10)
O(5)	0.040(2)	0.051(2)	0.047(2)	0.007(1)	0.005(1)	0.012(1)
O(6)	0.071(2)	0.048(2)	0.044(2)	0.001(2)	-0.010(2)	0.009(1)
O(7)	0.047(2)	0.048(2)	0.034(1)	0.017(1)	0.010(1)	0.005(1)
C(1)	0.027(2)	0.035(2)	0.028(2)	0.009(2)	0.004(1)	0.004(1)
C(2)	0.025(2)	0.036(2)	0.030(2)	0.010(2)	0.002(1)	0.004(2)
C(3)	0.039(2)	0.051(3)	0.030(2)	0.018(2)	0.005(2)	0.012(2)
C(4)	0.046(2)	0.065(3)	0.042(2)	0.030(2)	-0.001(2)	0.013(2)
C(5)	0.038(2)	0.070(3)	0.052(3)	0.034(2)	0.003(2)	0.005(2)
C(6)	0.029(2)	0.056(3)	0.035(2)	0.018(2)	0.007(1)	0.003(2)
C(7)	0.030(2)	0.032(2)	0.028(2)	0.009(2)	0.004(1)	0.006(1)
C(8)	0.030(2)	0.033(2)	0.027(2)	0.010(2)	0.004(1)	0.008(1)
C(9)	0.036(2)	0.036(2)	0.031(2)	0.013(2)	0.006(1)	0.001(2)
C(10)	0.049(2)	0.040(2)	0.050(2)	0.024(2)	0.013(2)	0.007(2)
C(11)	0.051(2)	0.042(2)	0.052(2)	0.025(2)	0.004(2)	0.015(2)
C(12)	0.042(2)	0.039(2)	0.030(2)	0.012(2)	0.005(2)	0.013(2)
C(13)	0.057(3)	0.059(3)	0.067(3)	0.001(3)	0.006(2)	0.026(2)
C(14)	0.058(3)	0.056(3)	0.072(3)	0.002(3)	0.016(2)	0.011(3)
C(15)	0.051(3)	0.061(4)	0.077(3)	-0.001(3)	0.000(3)	0.000(3)
C(16)	0.048(3)	0.061(4)	0.070(3)	0.000(3)	-0.009(2)	0.014(3)
C(17)	0.072(4)	0.056(3)	0.065(3)	0.006(3)	-0.007(3)	0.018(3)
C(18)	0.093(5)	0.058(4)	0.085(4)	-0.002(3)	-0.008(3)	0.007(3)
C(19)	0.076(4)	0.075(4)	0.077(4)	0.001(3)	-0.019(3)	-0.001(3)
C(20)	0.072(4)	0.089(5)	0.064(3)	-0.003(3)	-0.028(3)	0.020(3)

Table S9. Bond lengths (Å) for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (**2**·2THF).

Ru(1)	Ru(1*)	2.2233(6)	Ru(1)	O(1)	1.998(2)
Ru(1)	O(2)	1.965(2)	Ru(1)	O(3)	1.990(2)
Ru(1)	O(4)	1.973(2)	Ru(1)	O(5)	2.647(3)
Cl(1)	C(3)	1.720(4)	Cl(2)	C(4)	1.728(4)
Cl(3)	C(5)	1.722(4)	Cl(4)	C(6)	1.715(4)
Cl(5)	C(9)	1.725(4)	Cl(6)	C(10)	1.730(4)
Cl(7)	C(11)	1.717(4)	Cl(8)	C(12)	1.712(4)
Na(1)	O(2)	2.384(3)	Na(1)	O(4)	2.464(3)
Na(1)	O(6)	2.296(4)	Na(1)	O(7)	2.418(3)
Na(1)	O(7*)	2.442(3)	O(1)	C(1)	1.354(4)
O(2)	C(2)	1.352(4)	O(3)	C(7)	1.354(4)
O(4)	C(8)	1.350(4)	O(5)	C(13)	1.418(6)
O(5)	C(16)	1.436(5)	O(6)	C(17)	1.421(6)
O(6)	C(20)	1.406(5)	C(1)	C(2)	1.396(5)
C(1)	C(6)	1.399(5)	C(2)	C(3)	1.382(5)
C(3)	C(4)	1.396(6)	C(4)	C(5)	1.371(6)
C(5)	C(6)	1.399(5)	C(7)	C(8)	1.395(5)
C(7)	C(12)	1.395(5)	C(8)	C(9)	1.386(5)
C(9)	C(10)	1.396(5)	C(10)	C(11)	1.374(6)
C(11)	C(12)	1.405(6)	C(13)	C(14)	1.499(7)
C(14)	C(15)	1.513(7)	C(15)	C(16)	1.504(7)
C(17)	C(18)	1.481(8)	C(18)	C(19)	1.492(8)
C(19)	C(20)	1.465(8)	O(7)	H(17)	0.90
O(7)	H(18)	0.77	C(13)	H(1)	0.95
C(13)	H(2)	0.94	C(14)	H(3)	0.95
C(14)	H(4)	0.95	C(15)	H(5)	0.95
C(15)	H(6)	0.95	C(16)	H(7)	0.94
C(16)	H(8)	0.95	C(17)	H(9)	0.95
C(17)	H(10)	0.95	C(18)	H(11)	0.95
C(18)	H(12)	0.95	C(19)	H(13)	0.96
C(19)	H(14)	0.94	C(20)	H(15)	0.96
C(20)	H(16)	0.94			

Symmetry Code: (*) -x, -y, -z.

Table S10. Bond angles (°) for $Na_2[Ru_2(Cl_4Cat)_4(thf)_2]\cdot 2THF\cdot 2H_2O$ (**2**·2THF).

Ru(1*)	Ru(1)	O(1)	97.85(7)	Ru(1*)	Ru(1)	O(2)	101.85(8)
Ru(1*)	Ru(1)	O(3)	97.47(7)	Ru(1*)	Ru(1)	O(4)	100.91(7)
Ru(1*)	Ru(1)	O(5)	176.39(6)	O(1)	Ru(1)	O(2)	83.69(9)
O(1)	Ru(1)	O(3)	97.34(10)	O(1)	Ru(1)	O(4)	160.92(10)
O(1)	Ru(1)	O(5)	79.97(10)	O(2)	Ru(1)	O(3)	160.3(1)
O(2)	Ru(1)	O(4)	89.04(9)	O(2)	Ru(1)	O(5)	80.83(9)
O(3)	Ru(1)	O(4)	83.72(10)	O(3)	Ru(1)	O(5)	80.03(9)
O(4)	Ru(1)	O(5)	81.47(10)	O(2)	Na(1)	O(4)	69.44(10)
O(2)	Na(1)	O(6)	112.1(1)	O(2)	Na(1)	O(7)	82.7(1)
O(2)	Na(1)	O(7*)	124.6(1)	O(4)	Na(1)	O(6)	94.5(1)
O(4)	Na(1)	O(7)	85.26(9)	O(4)	Na(1)	O(7*)	160.5(1)
O(6)	Na(1)	O(7)	164.2(2)	O(6)	Na(1)	O(7*)	91.8(1)
O(7)	Na(1)	O(7*)	83.64(10)	Ru(1)	O(1)	C(1)	109.5(2)
Ru(1)	O(2)	Na(1)	102.2(1)	Ru(1)	O(2)	C(2)	111.5(2)
Na(1)	O(2)	C(2)	144.2(2)	Ru(1)	O(3)	C(7)	110.0(2)
Ru(1)	O(4)	Na(1)	99.3(1)	Ru(1)	O(4)	C(8)	110.9(2)
Na(1)	O(4)	C(8)	147.6(2)	Ru(1)	O(5)	C(13)	118.2(2)
Ru(1)	O(5)	C(16)	122.3(3)	C(13)	O(5)	C(16)	105.7(4)
Na(1)	O(6)	C(17)	129.1(3)	Na(1)	O(6)	C(20)	122.5(3)
C(17)	O(6)	C(20)	107.9(4)	Na(1)	O(7)	Na(1*)	96.36(9)
H(17)	O(7)	H(18)	117.1(3)	O(1)	C(1)	C(2)	118.2(3)
O(1)	C(1)	C(6)	122.8(3)	C(2)	C(1)	C(6)	119.0(3)
O(2)	C(2)	C(1)	116.7(3)	O(2)	C(2)	C(3)	121.9(3)
C(1)	C(2)	C(3)	121.4(3)	Cl(1)	C(3)	C(2)	118.7(3)
Cl(1)	C(3)	C(4)	122.1(3)	C(2)	C(3)	C(4)	119.2(4)
Cl(2)	C(4)	C(3)	118.7(3)	Cl(2)	C(4)	C(5)	121.3(3)
C(3)	C(4)	C(5)	120.0(4)	Cl(3)	C(5)	C(4)	120.1(3)
Cl(3)	C(5)	C(6)	118.7(3)	C(4)	C(5)	C(6)	121.2(4)
Cl(4)	C(6)	C(1)	118.6(3)	Cl(4)	C(6)	C(5)	122.2(3)
C(1)	C(6)	C(5)	119.2(4)	O(3)	C(7)	C(8)	117.7(3)
O(3)	C(7)	C(12)	122.0(3)	C(8)	C(7)	C(12)	120.3(3)
O(4)	C(8)	C(7)	117.4(3)	O(4)	C(8)	C(9)	122.6(3)
C(7)	C(8)	C(9)	120.0(3)	Cl(5)	C(9)	C(8)	118.8(3)
Cl(5)	C(9)	C(10)	121.5(3)	C(8)	C(9)	C(10)	119.7(4)
Cl(6)	C(10)	C(9)	119.2(3)	Cl(6)	C(10)	C(11)	120.0(3)
C(9)	C(10)	C(11)	120.7(4)	Cl(7)	C(11)	C(10)	121.0(3)
Cl(7)	C(11)	C(12)	118.9(3)	C(10)	C(11)	C(12)	120.0(4)
Cl(8)	C(12)	C(7)	118.8(3)	Cl(8)	C(12)	C(11)	122.0(3)
C(7)	C(12)	C(11)	119.3(4)	O(5)	C(13)	C(14)	107.5(4)
O(5)	C(13)	H(1)	109.9(5)	O(5)	C(13)	H(2)	110.3(5)
C(14)	C(13)	H(1)	109.6(5)	C(14)	C(13)	H(2)	109.8(5)
H(1)	C(13)	H(2)	109.7(5)	C(13)	C(14)	C(15)	104.4(4)
C(13)	C(14)	H(3)	110.6(5)	C(13)	C(14)	H(4)	110.5(5)
C(15)	C(14)	H(3)	110.6(5)	C(15)	C(14)	H(4)	110.9(5)
H(3)	C(14)	H(4)	109.8(5)	C(14)	C(15)	C(16)	105.0(4)
C(14)	C(15)	H(5)	110.4(5)	C(14)	C(15)	H(6)	110.1(5)
C(16)	C(15)	H(5)	110.8(5)	C(16)	C(15)	H(6)	110.9(5)
H(5)	C(15)	H(6)	109.6(5)	O(5)	C(16)	C(15)	107.0(4)
O(5)	C(16)	H(7)	110.4(4)	O(5)	C(16)	H(8)	109.9(5)
C(15)	C(16)	H(7)	109.9(5)	C(15)	C(16)	H(8)	109.6(5)
H(7)	C(16)	H(8)	110.0(5)	O(6)	C(17)	C(18)	109.2(4)
O(6)	C(17)	H(9)	109.4(5)	O(6)	C(17)	H(10)	110.0(5)
C(18)	C(17)	H(9)	109.3(5)	C(18)	C(17)	H(10)	109.5(5)
H(9)	C(17)	H(10)	109.5(5)	C(17)	C(18)	C(19)	104.6(5)
C(17)	C(18)	H(11)	110.7(5)	C(17)	C(18)	H(12)	110.6(6)
C(19)	C(18)	H(11)	110.7(6)	C(19)	C(18)	H(12)	110.2(6)

H(11)	C(18)	H(12)	109.9(6)	C(18)	C(19)	C(20)	106.5(5)
C(18)	C(19)	H(13)	109.6(6)	C(18)	C(19)	H(14)	110.4(6)
C(20)	C(19)	H(13)	110.0(6)	C(20)	C(19)	H(14)	110.4(6)
H(13)	C(19)	H(14)	109.9(5)	O(6)	C(20)	C(19)	108.5(5)
O(6)	C(20)	H(15)	108.9(5)	O(6)	C(20)	H(16)	110.1(5)
C(19)	C(20)	H(15)	109.9(6)	C(19)	C(20)	H(16)	110.3(6)
H(14)	C(20)	H(15)	114.6(4)	H(14)	C(20)	H(16)	84.9(4)
H(15)	C(20)	H(16)	109.1(6)				

Symmetry Code: (*) -x, -y, -z.

Figure S4. A view of the $[Ru_2(Cl_4Cat)_4]^{2-}$ anion including a weakly associated THF solvate molecule.

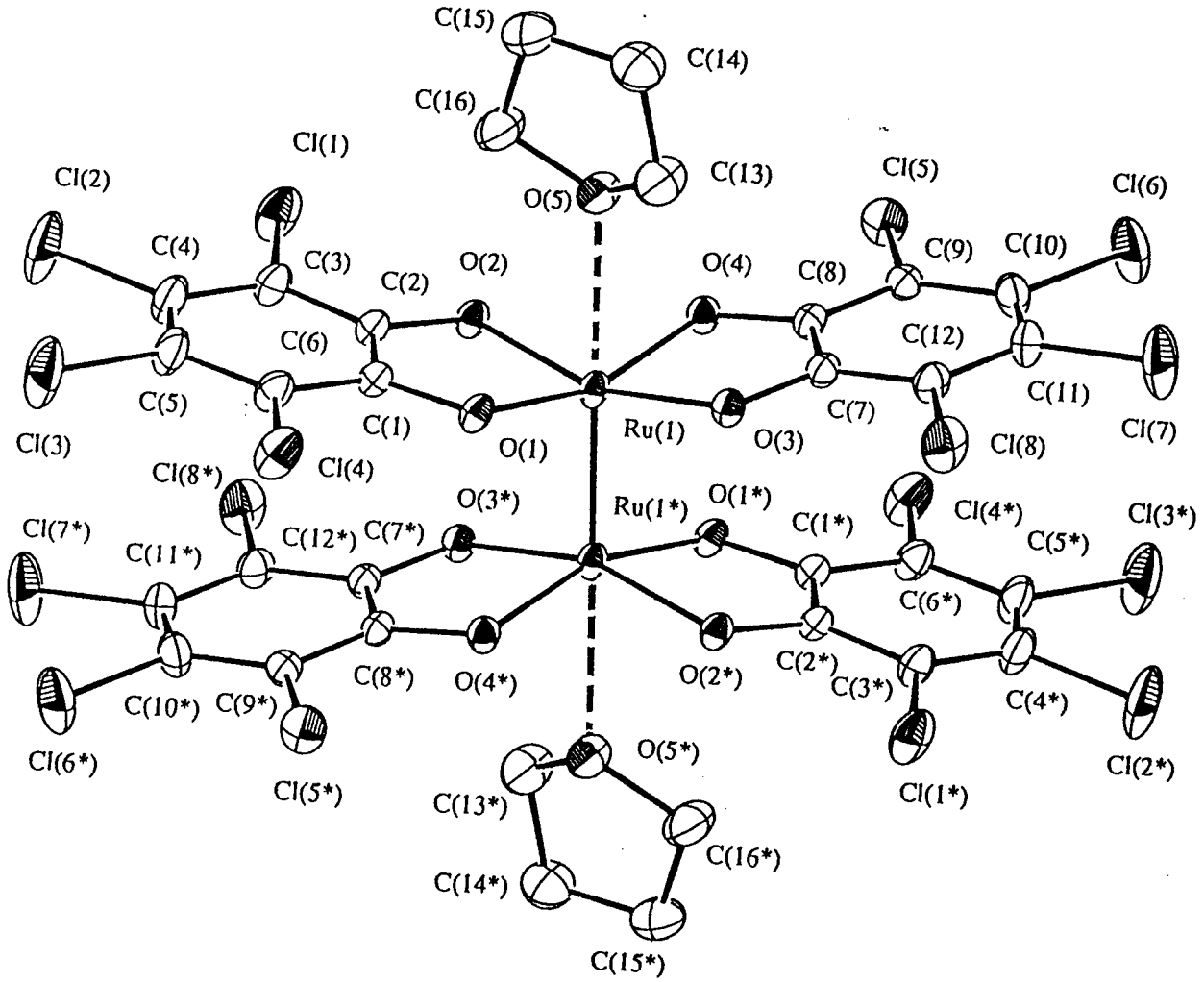


Figure S5. Chain structure of 2·2THF