Supplementary data

Magnetic and Electrochemical Properties of Lantern-Type Dinuclear Ru(II,III) Complexes with Axial Chloride Ions or Water Molecules

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Table S1. Selected bond distances (Å) and angles (°) of $^{n}Bu_4N[Ru_2(O_2CC_3H_7)_4Cl_2]$ (**2**).

Ru1-Ru2	2.3094(3)	Ru3-O10	2.0311(18)
Ru3-Ru3	2.3046(4)	Ru3-O11	2.0355(17)
Ru4-Ru4	2.3034(4)	Ru3-O12	2.0283(17)
Ru1-O1	2.0313(17)	Ru4-O13	2.0290(17)
Ru1-O3	2.0330(18)	Ru4-O14	2.0319(17)
Ru1-O5	2.0237(18)	Ru4-O15	2.0315(17)
Ru1-O7	2.0301(17)	Ru4-O16	2.0284(17)
Ru2-O2	2.0341(18)	Ru1-Cl1	2.5344(6)
Ru2-O4	2.0253(18)	Ru2-Cl2	2.5524(6)
Ru2-O6	2.0300(17)	Ru3-Cl3	2.5335(6)
Ru2-O8	2.0293(18)	Ru4-Cl4	2.5127(6)
Ru3-O9	2.0248(18)		
O1-Ru1-O3	88.69(7)	C5-O4-Ru2	119.65(17)
O1-Ru1-O5	178.19(7)	C9-O5-Ru1	119.42(16)
O1-Ru1-O7	90.42(7)	C9-O6-Ru2	118.25(17)
O3-Ru1-O5	91.03(7)	C13-O7-Ru1	119.34(16)
O3-Ru1-O7	177.85(7)	C13-O8-Ru2	119.14(17)
O5-Ru1-O7	89.80(7)	O9-Ru3-O10	177.77(7)
O1-Ru1-Cl1	92.90(5)	O9-Ru3-O11	90.05(7)
O3-Ru1-Cl1	90.90(5)	O9-Ru3-O12	90.44(7)
O5-Ru1-Cl1	88.89(6)	O10-Ru3-O11	88.97(7)
O7-Ru1-Cl1	91.11(5)	O10-Ru3-O12	90.48(7)
Ru2-Ru1-O1	89.42(5)	O11-Ru3-O12	178.24(7)
Ru2-Ru1-O3	89.21(5)	O9-Ru3-Cl3	88.68(5)
Ru2-Ru1-O5	88.79(5)	O10-Ru3-Cl3	93.37(5)
Ru2-Ru1-O7	88.82(5)	O11-Ru3-Cl3	93.03(5)
Ru2-Ru1-Cl1	177.672(17)	O12-Ru3-Cl3	88.67(5)
O2-Ru2-O4	89.38(7)	Ru3-Ru3-O9	88.27(5)
O2-Ru2-O6	178.24(8)	Ru3-Ru3-O10	89.73(5)
O2-Ru2-O8	90.32(7)	Ru3-Ru3-O11	89.94(5)
O4-Ru2-O6	90.17(7)	Ru3-Ru3-O12	88.39(5)
O4-Ru2-O8	177.87(7)	Ru3-Ru3-Cl3	175.74(2)
O6-Ru2-O8	90.07(7)	O13-Ru4-O14	178.32(7)
O2-Ru2-Cl2	88.54(5)	O13-Ru4-O15	88.06(7)
O4-Ru2-Cl2	91.07(5)	O13-Ru4-O16	91.02(7)
O6-Ru2-Cl2	93.17(5)	O14-Ru4-O15	91.73(7)
O8-Ru2-Cl2	91.03(5)	O14-Ru4-O16	89.14(7)
Ru1-Ru2-O2	88.80(5)	O15-Ru4-O16	177.85(7)
Ru1-Ru2-O4	88.75(5)	O13-Ru4-Cl4	91.20(5)
Ru1-Ru2-O6	89.48(5)	O14-Ru4-Cl4	90.47(5)
Ru1-Ru2-O8	89.14(5)	O15-Ru4-Cl4	91.60(5)
Ru1-Ru2-Cl2	177.340(17)	O16-Ru4-Cl4	90.35(5)
C1-O1-Ru1	118.20(17)	Ru4-Ru4-O13	89.52(5)
C1-O2-Ru2	118.88(16)	Ru4-Ru4-O14	88.81(5)

C5-O3-Ru1	118.77(17)	Ru4-Ru4-O15	89.06(5)
Ru4-Ru4-O16	88.99(5)		
Ru4-Ru4-Cl4	179.031(19)		
C17-O9-Ru3	120.08(18)		
C17-O10-Ru3	118.51(16)		
C21-O11-Ru3	118.26(16)		
C21-O12-Ru3	119.96(16)		
C25-O13-Ru4	118.46(16)		
C25-O14-Ru4	118.82(17)		
C29-O15-Ru4	119.28(17)		
C29-O16-Ru4	119.34(16)		

Table S2. Selected bond distances (Å) and angles (°) of $[Ru_2(O_2CC_3H_7)_4(H_2O)_2]BF_4$ (**3**).

Ru1-Ru1	2.2584(7)	Ru1-O3	2.031(2)
Ru1-O1	2.005(2)	Ru1-O4	2.022(2)
Ru1-O2	2.024(2)	Ru1-O5	2.267(3)
O1-Ru1-O2	179.12(9)	O3-Ru1-O5	87.33(9)
O1-Ru1-O3	88.67(9)	O4-Ru1-O5	93.46(9)
O1-Ru1-O4	89.58(9)	O1-Ru1-Ru1	90.30(7)
O1-Ru1-O5	89.73(10)	O2-Ru1-Ru1	89.16(7)
O2-Ru1-O3	92.00(10)	O3-Ru1-Ru1	88.79(7)
O2-Ru1-O4	89.74(9)	O4-Ru1-Ru1	90.42(7)
O2-Ru1-O5	90.86(10)	O5-Ru1-Ru1	176.12(7)
O3-Ru1-O4	178.08(9)		

Table S3. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl]^-$.

Ru	9.08782654	4.79691874	7.70278373
Ru	9.76670486	6.91821729	8.22792664
O	7.25147116	5.21486458	8.65720618
O	10.96842432	4.4926036	6.80820742
O	7.9258503	7.28708807	9.14873844
O	10.50832889	6.23407995	10.0690769
O	9.02465045	7.62182633	6.40060288
O	11.61615538	6.5732278	7.29435399
O	8.37013128	5.55205695	5.87013925
O	9.86671005	4.15859291	9.55343929
C	8.52521969	6.76903481	5.61092336
C	7.0858318	6.34208318	9.18058163
C	10.37990001	5.0026162	10.32522848
C	11.80026254	5.4298169	6.78608998
C	10.91126974	4.5126041	11.65753973
C	13.13910728	5.18208145	6.11944264
C	10.50625012	7.05771608	3.38360709
C	13.20961507	3.90804782	5.28238746
C	5.78734529	6.59870498	9.91689431
C	8.11748227	7.25820679	4.23777688
C	10.2906985	3.20316477	12.13739407
C	6.88110619	6.44986917	12.20476727
C	6.00726088	7.28005281	11.26857318
C	12.33505367	3.95404798	4.03258332
C	9.27850318	7.95391072	3.5202575
C	8.80105137	3.32736865	12.44430126
H	7.76021491	6.39970883	3.66495738
H	7.28258297	7.95689295	4.35756255
H	9.54564265	8.85892622	4.07349227
H	8.93554605	8.2745698	2.52922183

H	10.91691442	6.80593995	4.36514094
H	11.29832051	7.55179888	2.81231088
H	10.26214193	6.11756941	2.87997955
H	5.27264092	5.64217303	10.03382533
H	5.16317259	7.23062533	9.2747764
H	6.47209208	8.25578327	11.1024382
H	5.03105228	7.464007	11.7331227
H	7.8805703	6.31194479	11.78310768
H	6.45231879	5.45680552	12.37188711
H	6.99643656	6.93560753	13.17869747
H	10.77068137	5.31403191	12.3897714
H	11.99502702	4.39758951	11.53460017
H	10.43892444	2.43822871	11.37093437
H	10.82890457	2.87169257	13.03404803
H	8.61283519	4.10500127	13.19327757
H	8.39784757	2.38640873	12.83057186
H	8.24135774	3.58081121	11.54134643
H	13.37763737	6.0673262	5.51971638
H	13.88453689	5.15699569	6.92286352
H	12.90777496	3.0593347	5.90185692
H	14.25562207	3.74056239	4.99645333
H	11.28130746	4.04643857	4.30168679
H	12.44850758	3.03971353	3.44244749
H	12.60258019	4.80248259	3.39212355
Cl	8.38630097	2.50569697	7.13436111

Table S4. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl]$.

Ru	9.06451375	4.7570183	7.69435261
Ru	9.76355239	6.89557871	8.21964491
O	7.2702942	5.21353944	8.63556325
O	10.92625054	4.47143256	6.82086053
O	7.97573553	7.27482195	9.10351633
O	10.48203968	6.23283549	10.00562278
O	9.04333782	7.5826043	6.44884627
O	11.55626844	6.54764007	7.32533784
O	8.3652639	5.53148883	5.89897237
O	9.83729107	4.15593028	9.52463792
C	8.51958501	6.74684207	5.6360695
C	7.1023688	6.34329071	9.15096146
C	10.3570885	4.99449469	10.29583359
C	11.76629593	5.39943418	6.802844
C	10.89119091	4.53638947	11.62558087
C	13.10751207	5.17288498	6.15995005
C	10.47746717	7.03946682	3.39613606
C	13.20704586	3.91169708	5.306418
C	5.81656185	6.63206675	9.87453515
C	8.10102152	7.26138132	4.28792552
C	10.30451151	3.21768961	12.12336732
C	6.90077206	6.43198621	12.16605849
C	6.04993352	7.29189543	11.23658648
C	12.36373603	3.96736902	4.03615027
C	9.26462165	7.94955729	3.56288306
C	8.81518183	3.30751746	12.44189943
H	7.71638369	6.41903687	3.7106766
H	7.28252095	7.97220914	4.43915875
H	9.54821721	8.85009229	4.1139776
H	8.90445372	8.27865505	2.58345196

H	10.91149565	6.77746402	4.36596543
H	11.26061991	7.52972906	2.81260957
H	10.214948	6.10643129	2.88945864
H	5.27108745	5.69165771	9.97275537
H	5.22292831	7.29135128	9.23183615
H	6.52608726	8.26443272	11.08815449
H	5.07407121	7.48295498	11.69327582
H	7.9048443	6.28192742	11.75720339
H	6.45278494	5.44571788	12.31834887
H	7.01479489	6.90337217	13.14528622
H	10.73096217	5.34711866	12.34228552
H	11.9778458	4.45465102	11.50229675
H	10.47587016	2.44023052	11.37469344
H	10.85777691	2.92098002	13.02020608
H	8.61482289	4.08310171	13.18835416
H	8.44324008	2.36027509	12.83965593
H	8.23327276	3.53764839	11.54612718
H	13.3467204	6.07198751	5.58287586
H	13.83476661	5.14883075	6.97990956
H	12.91395612	3.0455754	5.90554454
H	14.26017966	3.76859345	5.0434779
H	11.29942993	4.0413855	4.26866939
H	12.50706671	3.06467413	3.43751858
H	12.63879067	4.82611369	3.41469466
Cl	8.37232334	2.58041894	7.15837983

Table S5. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl]^+$.

Ru	9.03944011	4.70262014	7.68529744
Ru	9.77631086	6.94583648	8.23451463
O	7.2880101	5.19508322	8.62270387
O	10.88739967	4.4472832	6.83505973
O	8.00865051	7.23581365	9.06114035
O	10.4674437	6.25450551	10.00283587
O	9.05588128	7.59347778	6.46850553
O	11.48908796	6.50570272	7.35873962
O	8.37334169	5.5392688	5.93137051
O	9.82744478	4.179222	9.50373536
C	8.52393453	6.75846428	5.65446084
C	7.10486858	6.32611044	9.13317201
C	10.34889678	5.01100941	10.29136744
C	11.73883919	5.36577422	6.81793735
C	10.8868009	4.54435783	11.60861127
C	13.08096584	5.16115994	6.19484416
C	10.46173674	7.01688365	3.39374153
C	13.20195909	3.9178759	5.31643935
C	5.83156816	6.63884969	9.84665391
C	8.09633973	7.26534169	4.31397061
C	10.3088243	3.22175422	12.10884876
C	6.91474975	6.42041347	12.14089172
C	6.07752466	7.29355138	11.21256004
C	12.37474964	3.99193352	4.03699467
C	9.26246885	7.94069351	3.57525043
C	8.8248608	3.30370919	12.45181357
H	7.6949119	6.42525105	3.74577113
H	7.28835751	7.98599394	4.47523122
H	9.55801069	8.84334771	4.11547568
H	8.88888273	8.26647037	2.60144587

H	10.90554849	6.74212488	4.35749604
H	11.24431745	7.50294328	2.80796195
H	10.1860383	6.09181112	2.88016928
H	5.26559966	5.71034513	9.93751333
H	5.25916376	7.31272522	9.19928858
H	6.55700973	8.264941	11.0690042
H	5.10125892	7.49012237	11.66198207
H	7.9225221	6.26036413	11.74157922
H	6.45471337	5.44006891	12.29207501
H	7.02814174	6.88943063	13.11992672
H	10.73635391	5.35512384	12.3270704
H	11.97297324	4.46796021	11.47181524
H	10.48144859	2.4408999	11.36393161
H	10.87639077	2.9329572	12.99750072
H	8.63268125	4.07561975	13.20310074
H	8.46838732	2.35471901	12.85672121
H	8.21872784	3.52895676	11.56990814
H	13.32293928	6.07690182	5.64580482
H	13.79184218	5.12776614	7.02994761
H	12.92439515	3.03255841	5.89473843
H	14.25936303	3.80060219	5.06524667
H	11.3040243	4.04707471	4.24882961
H	12.54049018	3.10533761	3.42241079
H	12.64797327	4.86528165	3.43710602
Cl	8.35713855	2.63907498	7.16688926

Table S6. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl_2]^{2-}$.

Ru	9.24120132	4.54687706	7.7328175
Ru	9.88720699	6.70032088	8.28222922
O	7.39702967	4.88396373	8.71539662
O	11.11041978	4.27564286	6.80101125
O	8.01773532	6.97179019	9.2134627
O	10.64642256	5.96478864	10.11435537
O	9.09030018	7.3622886	6.4474257
O	11.73171657	6.36299922	7.30032671
O	8.48153838	5.28244693	5.90089704
O	10.03860195	3.88479343	9.56735406
C	8.60679077	6.50863187	5.66280914
C	7.21096687	6.01020802	9.23897179
C	10.52175846	4.73849403	10.35215535
C	11.91753732	5.23695525	6.77624469
C	10.98653261	4.22988219	11.70742533
C	13.24442075	5.01360123	6.06682475
C	10.49988581	7.48728958	3.49050579
C	13.19956245	3.91686807	5.00577286
C	5.88426479	6.2334542	9.94875962
C	8.14215627	7.01710919	4.30743412
C	10.02788278	3.19401747	12.29538422
C	6.84974995	6.98524097	12.17755444
C	5.9293934	7.33024776	11.0097455
C	12.27973015	4.26209811	3.83761573
C	9.10079827	8.05293809	3.71942813
C	8.62879566	3.75965056	12.52433392
H	8.02429981	6.15646007	3.64291776
H	7.14911584	7.46147822	4.44581464
H	9.1631373	8.89942463	4.40821079
H	8.68679904	8.42836115	2.77342518

H	10.95002282	7.18406636	4.43938972
H	11.16182215	8.23174497	3.03507295
H	10.47393586	6.60983792	2.83490707
H	5.56727037	5.27593111	10.37426818
H	5.15071624	6.48409249	9.17273552
H	6.27491428	8.25688121	10.54428003
H	4.90986867	7.50875613	11.37899745
H	7.87988687	6.87784757	11.83058927
H	6.5506912	6.04474674	12.65476325
H	6.83553588	7.77126842	12.94012505
H	11.10448082	5.09044311	12.37203888
H	11.97952409	3.78545626	11.56889757
H	9.96554734	2.34756703	11.60655695
H	10.44188783	2.81855461	13.24136756
H	8.65474042	4.63708423	13.17995527
H	7.96686741	3.01517415	12.9797455
H	8.17864066	4.0628946	11.57546291
H	13.56162055	5.97111712	5.64144186
H	13.97772723	4.76292393	6.8430656
H	12.85370146	2.99026289	5.47104213
H	14.21921292	3.73822464	4.63693436
H	11.24947391	4.36958201	4.18419055
H	12.29416092	3.47614644	3.074968
H	12.57909863	5.20260486	3.36062387
Cl	8.54769374	2.04249653	7.09187855
Cl	10.58101355	9.20468666	8.92337932

Table S7. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl_2]^-$.

Ru	9.278052	4.513836	7.774066
Ru	10.00491	6.70099	8.30366
O	7.481762	4.846297	8.683054
O	11.119116	4.23094	6.892927
O	8.120027	6.92422	9.189181
O	10.718844	5.928107	10.096956
O	9.217445	7.271463	6.465605
O	11.803318	6.305129	7.350483
O	8.55504	5.19852	5.978383
O	10.030991	3.872712	9.568345
C	8.699779	6.426101	5.698105
C	7.289469	5.98941	9.205338
C	10.554222	4.712128	10.359926
C	11.964332	5.169697	6.835053
C	11.00005	4.197008	11.706937
C	13.257219	4.8933	6.104915
C	10.455129	7.680485	3.482296
C	13.107405	3.878259	4.973059
C	5.951027	6.222576	9.864805
C	8.19944	6.898063	4.353868
C	9.999812	3.211301	12.31405
C	6.810409	7.026026	12.119214
C	5.952751	7.345846	10.898419
C	12.180591	4.365289	3.862587
C	9.007834	8.060968	3.782109
C	8.624592	3.83385	12.537146
H	8.192971	6.037624	3.679641
H	7.152776	7.191945	4.496011
H	8.987439	8.891481	4.492098
H	8.516709	8.407741	2.865689

H	10.979013	7.387939	4.396106
H	11.000933	8.52169	3.045767
H	10.508239	6.842926	2.778871
H	5.625414	5.272731	10.298819
H	5.245235	6.443512	9.055222
H	6.314268	8.264429	10.429691
H	4.917391	7.52859	11.208961
H	7.860102	6.914231	11.838497
H	6.485595	6.097008	12.600171
H	6.752387	7.826742	12.861924
H	11.165466	5.058069	12.358795
H	11.96971	3.707678	11.560584
H	9.907268	2.347041	11.652012
H	10.406119	2.84798	13.264989
H	8.686735	4.729342	13.163922
H	7.945825	3.128062	13.024251
H	8.167456	4.120656	11.586021
H	13.649208	5.848572	5.745209
H	13.968148	4.526682	6.854947
H	12.72182	2.942089	5.383747
H	14.101973	3.668178	4.562761
H	11.166362	4.516681	4.241118
H	12.120492	3.632928	3.052699
H	12.532126	5.311187	3.436738
Cl	8.733728	2.139191	7.15729
Cl	10.441294	9.063245	8.930214

Table S8. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4Cl_2]$.

Ru	9.18850289	4.49654985	7.75344589
Ru	10.06387964	6.62276588	8.30339483
O	7.42065055	4.67711608	8.63400572
O	11.10567237	4.3707645	6.88515292
O	8.12244261	6.71746935	9.20907365
O	10.80529438	5.73262005	10.00818215
O	9.25934686	7.28896638	6.53866099
O	11.85185431	6.41664388	7.37246473
O	8.44439035	5.28051432	6.02590215
O	9.93420391	3.74880854	9.48609534
C	8.65233923	6.50687469	5.76189673
C	7.26111282	5.81494315	9.21523713
C	10.57210449	4.52417405	10.26775851
C	11.98506378	5.27651902	6.83348791
C	11.04683993	3.9512086	11.57205136
C	13.26967378	4.98049832	6.11031698
C	10.43570243	7.57323056	3.49537604
C	13.1355809	3.91456433	5.02444289
C	5.94644878	6.03178771	9.90944222
C	8.13888939	7.04751947	4.45689658
C	9.92001201	3.22261276	12.31356659
C	6.77758531	7.18779161	12.03054196
C	5.8870598	7.27364363	10.79433623
C	12.22782183	4.3427112	3.87540501
C	9.05166135	8.11120485	3.84550426
C	8.72441968	4.12500208	12.60197735
H	7.99070272	6.20148057	3.78227622
H	7.14703744	7.46732547	4.66132699
H	9.14266312	8.94988538	4.54012983
H	8.56415533	8.49760452	2.94528757

H	10.97072196	7.24187474	4.38998528
H	11.04600346	8.34393785	3.01869129
H	10.37248316	6.72437252	2.80772665
H	5.72463466	5.1196496	10.47297249
H	5.19057824	6.07511982	9.11683731
H	6.15993068	8.15280681	10.20455337
H	4.84527629	7.41289631	11.10039769
H	7.83338526	7.13199283	11.75751243
H	6.53314199	6.30849857	12.63568583
H	6.64851988	8.07060293	12.66114344
H	11.45945107	4.76651155	12.1688944
H	11.85945351	3.25299465	11.34630837
H	9.60198336	2.36043876	11.72232468
H	10.33020486	2.83188544	13.24955536
H	9.01747672	5.01745431	13.16287443
H	7.96448336	3.59730841	13.18308064
H	8.24913707	4.45972891	11.67474292
H	13.65195777	5.92435478	5.71239522
H	13.98442994	4.66079825	6.87800019
H	12.75551225	2.99227841	5.4700196
H	14.13787695	3.69569267	4.64289419
H	11.20154156	4.49758232	4.21897382
H	12.19722068	3.57618463	3.09767885
H	12.57912451	5.27180264	3.41517954
Cl	9.04596143	2.36658616	6.84324541
Cl	10.17220423	8.71255944	9.21797727

Table S9. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4(H_2O)_2]$.

Ru	9.42310118	4.3264112	7.82623438
Ru	10.00585705	6.43822585	8.35404709
O	7.55651189	4.63666953	8.74491085
O	11.28830134	4.03938915	6.93216619
O	8.13123135	6.73124494	9.23455337
O	10.74001243	5.76391353	10.18396869
O	9.24787991	7.09894407	6.50443666
O	11.8733732	6.12766452	7.44150236
O	8.67667969	5.01293759	5.9767627
O	10.16767776	3.67394559	9.65901607
C	8.76575154	6.24378697	5.71197907
C	7.31928522	5.77091106	9.25577407
C	10.63397356	4.53583021	10.45511557
C	12.10220103	5.00004686	6.91547604
C	11.06235434	4.06483053	11.82252699
C	13.4246635	4.78647457	6.21943391
C	10.34715732	7.88896474	3.5706134
C	13.26726152	4.08338677	4.86953411
C	5.96727153	5.97016719	9.90068619
C	8.23637241	6.71566146	4.37723439
C	9.94114153	3.30143856	12.53561878
C	6.69625606	7.12560794	12.05543843
C	5.84895105	7.20491795	10.78917252
C	12.40627098	4.87786854	3.89228598
C	8.85635436	8.0152892	3.87041737
C	8.66490396	4.12518642	12.67827984
H	8.37311906	5.90327845	3.65794255
H	7.15336058	6.83490833	4.50076108
H	8.69010105	8.80414483	4.60925051
H	8.32284527	8.31911224	2.96365256

H	10.9090119	7.62183967	4.46949667
H	10.75449183	8.82806444	3.18624183
H	10.53615753	7.11499968	2.82005816
H	5.73136908	5.05663538	10.45593627
H	5.24052948	6.01572443	9.08100857
H	6.129933	8.09090312	10.21326754
H	4.79451395	7.3286188	11.05924072
H	7.75951444	7.06573984	11.81450477
H	6.43541094	6.24511885	12.65210991
H	6.54506276	8.00827209	12.68247431
H	11.37304748	4.93744833	12.40084607
H	11.93480189	3.41540392	11.69808112
H	9.72810826	2.38230193	11.98318187
H	10.30478716	3.00024083	13.52356307
H	8.85432322	5.07301917	13.19079864
H	7.90536511	3.58236674	13.24745633
H	8.23616762	4.35951104	11.69920339
H	13.91408271	5.75676991	6.10673038
H	14.04909884	4.18213511	6.88659641
H	12.82702331	3.09641654	5.03238355
H	14.26296149	3.92201986	4.44356359
H	11.38882559	5.00046714	4.27553058
H	12.33494736	4.37306051	2.92524447
H	12.82011776	5.87616843	3.71777711
O	8.24746926	2.32344234	7.20588169
H	7.97833876	2.47826616	6.29665024
H	7.46199951	2.41241476	7.75396687
O	10.87635272	8.68376283	8.35040297
H	11.79890796	8.52961085	8.12759447
H	10.45660509	9.05735826	7.57039655

Table S10. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4(H_2O)_2]^+$.

Ru	9.37772397	4.36427503	7.80511105
Ru	10.03091105	6.46866534	8.30904697
O	7.57869574	4.69344813	8.68122897
O	11.16630492	4.00144715	6.92277297
O	8.19485571	6.76663129	9.17660201
O	10.75019623	5.78562483	10.10728466
O	9.28690673	7.11432238	6.50717293
O	11.82778108	6.06696477	7.39453269
O	8.66278191	5.03936533	6.02382471
O	10.10678602	3.72597209	9.58249921
C	8.76600682	6.27525428	5.72349397
C	7.34650139	5.83809413	9.20239892
C	10.62107354	4.56339355	10.39490271
C	12.03291902	4.93749408	6.87436664
C	11.05520569	4.0657431	11.73933154
C	13.327083	4.66944973	6.16679898
C	10.28822275	7.90192101	3.50592868
C	13.12087131	4.00223351	4.80249341
C	6.00331586	6.05745376	9.83324954
C	8.21320419	6.72666602	4.40362404
C	9.91551575	3.33936421	12.46784007
C	6.72117195	7.23176597	11.98383223
C	5.8924382	7.30533849	10.70530173
C	12.26930785	4.84447147	3.85838931
C	8.81178816	8.02576437	3.86877715
C	8.67445169	4.20838047	12.64079948
H	8.33612566	5.90286458	3.69536394
H	7.13182561	6.83345521	4.553805
H	8.66818401	8.82248167	4.60338992
H	8.23890315	8.31500556	2.98335013

H	10.89852938	7.65715891	4.37985111
H	10.66783688	8.83774579	3.09026696
H	10.44801242	7.12071511	2.7566765
H	5.7565014	5.14941253	10.39230821
H	5.28563022	6.09420232	9.00491574
H	6.17986183	8.18429703	10.12195044
H	4.83689956	7.43677141	10.95954997
H	7.78927225	7.15389511	11.76665037
H	6.436474	6.36785284	12.59224477
H	6.57211859	8.12628344	12.59215656
H	11.41544464	4.9190541	12.31632853
H	11.89627398	3.38224608	11.58583823
H	9.66249235	2.42776442	11.92078557
H	10.29302503	3.02506112	13.44436572
H	8.90577549	5.14511635	13.15581373
H	7.91083876	3.688634	13.22318381
H	8.22695025	4.46154216	11.67365609
H	13.86020696	5.61720613	6.07228962
H	13.92359409	4.02135526	6.81828809
H	12.66479963	3.01948782	4.94629035
H	14.10618924	3.82845609	4.36218541
H	11.25677269	4.98531796	4.2515836
H	12.17443907	4.36504344	2.88190075
H	12.7077032	5.83412255	3.70128525
O	8.69158375	2.20645123	7.27377677
H	9.16029139	1.66059973	6.63945983
H	7.76798387	1.94774735	7.28504841
O	10.73145542	8.60054267	8.84815582
H	11.29580491	8.78077785	9.60289032
H	10.83972784	9.30108746	8.20176946

Table S11. Atomic coordinates of optimized geometry of $[Ru_2(O_2CC_3H_7)_4(H_2O)_2]^{2+}$.

Ru	9.34223549	4.30089391	7.77836887
Ru	10.03407183	6.46608692	8.29769744
O	7.58729529	4.68807169	8.65729381
O	11.12527273	3.97152381	6.92801405
O	8.23320317	6.75642341	9.12770444
O	10.7374392	5.81560267	10.07014277
O	9.31351006	7.12612907	6.53589159
O	11.77412362	6.03616861	7.41236671
O	8.67919339	5.05887123	6.0624611
O	10.08735537	3.76698374	9.5387162
C	8.78033064	6.2942962	5.73711933
C	7.35417811	5.83825368	9.17365782
C	10.61480401	4.5856262	10.36984738
C	12.00384158	4.89959581	6.88172565
C	11.059954	4.08043879	11.69527113
C	13.29881081	4.64669488	6.19419872
C	10.30141762	7.93201792	3.53132368
C	13.107656	4.00423104	4.81083605
C	6.02551426	6.0875721	9.7978453
C	8.23241941	6.74019566	4.42629923
C	9.9264404	3.34031417	12.42949721
C	6.76086172	7.22908998	11.96142633
C	5.93914476	7.33172575	10.68091375
C	12.26999281	4.86668159	3.8738079
C	8.82401724	8.04515654	3.89151731
C	8.68769626	4.20503547	12.63020668
H	8.35013986	5.91217635	3.72143816
H	7.1493381	6.83870661	4.58461194
H	8.66366066	8.84658649	4.61715581
H	8.24797621	8.31784899	3.00434481

H	10.91915983	7.69850369	4.40468428
H	10.66933414	8.87088758	3.11476869
H	10.46912215	7.15427744	2.78113458
H	5.74825915	5.17627129	10.3377929
H	5.31869258	6.148086	8.95887076
H	6.23420214	8.21312597	10.10539635
H	4.88504943	7.47225512	10.93092434
H	7.83147318	7.13689873	11.75552193
H	6.45609346	6.3676255	12.562377
H	6.6230827	8.12019001	12.575536
H	11.42928659	4.92907682	12.27262727
H	11.89936802	3.39838515	11.51979696
H	9.67484541	2.42805397	11.88327617
H	10.32549656	3.02380272	13.39521854
H	8.92155895	5.13119856	13.16178285
H	7.93356158	3.67225369	13.21139507
H	8.22305493	4.47549674	11.67357275
H	13.8366754	5.59411103	6.13278849
H	13.87880325	3.98036179	6.8442808
H	12.6602803	3.0142033	4.92682508
H	14.10195862	3.84744114	4.38780409
H	11.24907925	5.00277738	4.2520622
H	12.1869848	4.40297124	2.8897732
H	12.71293089	5.85662608	3.73648481
O	8.65622482	2.18063438	7.2631765
H	9.17520498	1.52003544	6.79566608
H	7.79438886	1.80602422	7.46654144
O	10.69454748	8.52240695	8.79564503
H	11.15319339	8.77864659	9.60047732
H	10.60574037	9.28763191	8.22107707

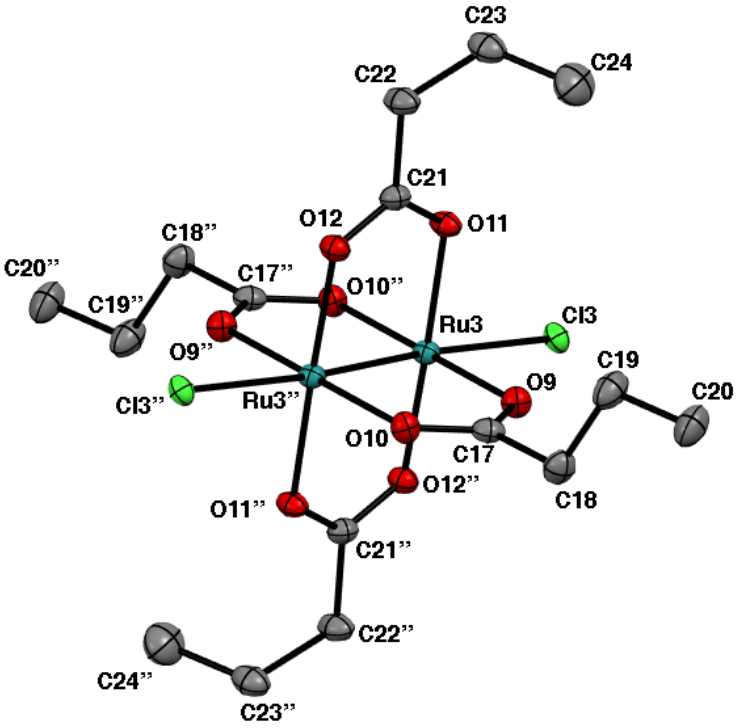

Figure S1. Structure of an anionic dinuclear unit designated as (Cl3-Ru3-Ru3″-Cl3″). Hydrogen atoms are omitted for clarity. Double primes (″) refer to the equivalent positions (-x, 1-y, -z). The thermal ellipsoids are shown at the 50% probability level.

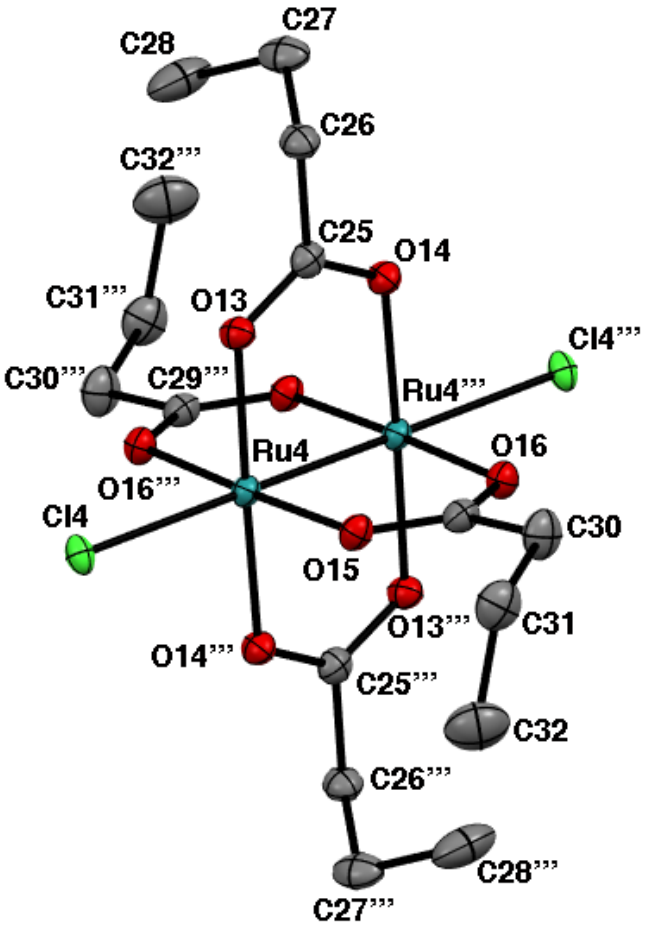

Figure S2. Structure of an anionic dinuclear unit designated as (Cl3-Ru4-Ru4′′′-Cl4′′′). Hydrogen atoms are omitted for clarity. Triple primes (′′′) refer to the equivalent positions (-x, 2-y, 1-z). The thermal ellipsoids are shown at the 50% probability level.

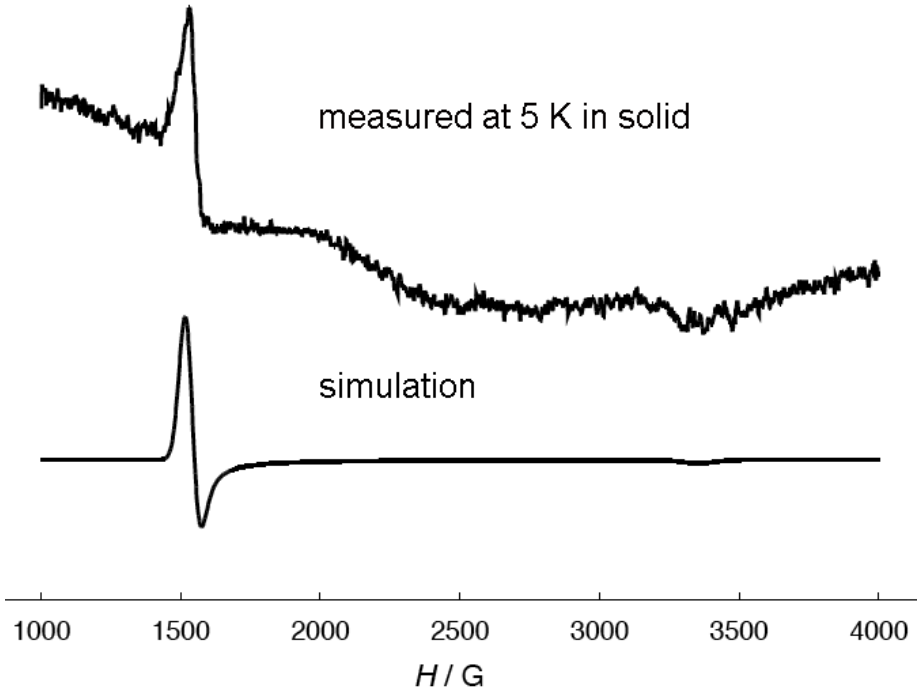

Figure S3. EPR spectra of **1**. The simulated spectrum is drawn with the parameter values with $g_z = 2.040$, $g_x = g_y = 4.390$, and W_z, = 80 G, $W_x = W_y = 30$ G.

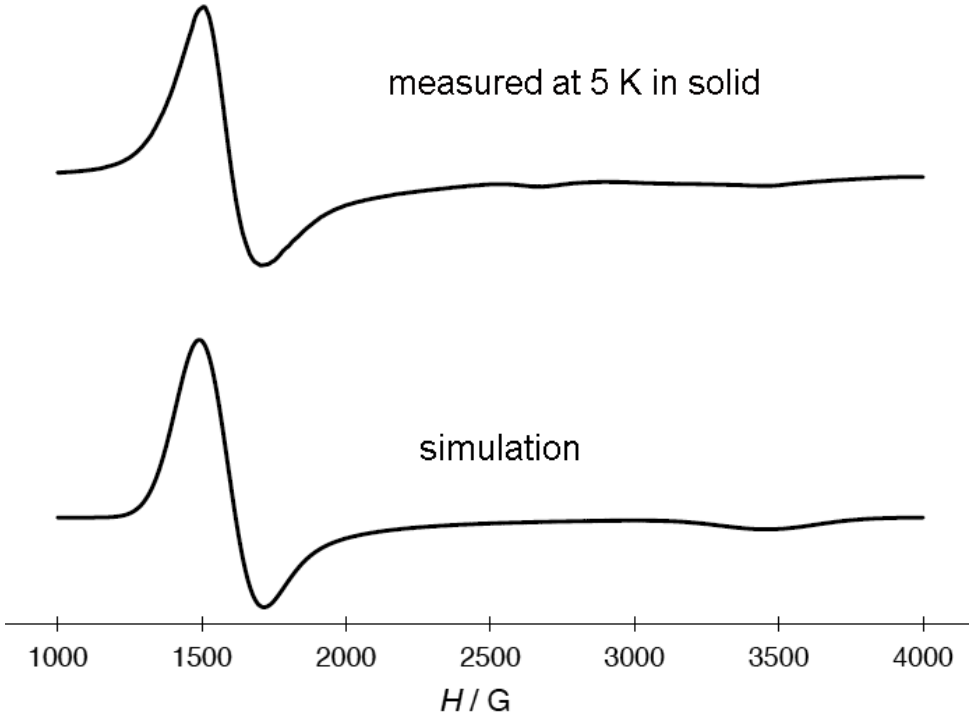

Figure S4. EPR spectra of **3**. The simulated spectrum is drawn with the parameter values with $g_z = 1.975$, $g_x = g_y = 4.335$, and $W_z = 200$ G, $W_x = W_y = 115$ G.