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Supporting information for article:

Li4Ru2OCl10 •10H2O: crystal structure, magnetic properties, and bonding interactions in ruthenium-oxo complexes

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Supplementary Information

Table S1. Atomic coordinates and equivalent isotropic displacement parameters of Hydogen atoms in $Li_4Ru_2OCl_{10}$ •$10H_2O$ system (U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor ($Å^2$)).

Atom	Wyck.	*x*	*y*	*z*	Occupancy	U_{eq}
H31	2i	0.513(3)	0.865(2)	0.121(2)	1	0.013
H32	2i	0.476(3)	0.032(2)	0.848(2)	1	0.013
H41	2i	0.269(3)	0.173(2)	0.309(2)	1	0.012
H42	2i	0.194(3)	0.090(2)	0.339(2)	1	0.012
H51	2i	0.789(3)	0.280(2)	0.160(2)	1	0.015
H52	2i	0.830(3)	0.378(2)	0.172(2)	1	0.015
H61	2i	0.790(3)	0.175(2)	0.415(2)	1	0.013
H62	2i	0.775(3)	0.265(2)	0.340(2)	1	0.013
H71	2i	0.233(3)	0.285(2)	0.0348(2)	1	0.015
H72	2i	0.346(3)	0.238(2)	0.0885(2)	1	0.015
H81	2i	0.414(3)	0.418(2)	0.632(2)	1	0.013
H82	2i	0.500(3)	0.517(2)	0.349(2)	1	0.013
H91	2i	0.137(3)	0.955(2)	0.175(2)	1	0.015
H92	2i	0.015(3)	0.007(2)	0.126(2)	1	0.015
H101	2i	0.147(3)	0.143(2)	0.870(2)	1	0.015
H102	2i	0.026(3)	0.171(2)	0.937(2)	1	0.015
H111	2i	0.116(3)	0.651(2)	0.424(2)	1	0.013
H112	2i	0.150(3)	0.535(2)	0.466(2)	1	0.013
H121	2i	0.029(3)	0.491(2)	0.690(2)	1	0.023
H122	2i	0.097(3)	0.449(2)	0.281(2)	1	0.023

Table S2. Anisotropic thermal displacement parameters of $Li_4Ru_2OCl_{10} \cdot 10H_2O$.

Atom	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
Ru(1)	0.00445(4)	0.00392(4)	0.00416(4)	-0.00085(3)	-0.00042(3)	-0.00135(3)
Ru(2)	0.00444(4)	0.00436(4)	0.00412(4)	-0.00111(3)	-0.00035(3)	-0.00108(3)
Cl(3)	0.00703(11)	0.00804(11)	0.00955(12)	-0.00321(9)	-0.00224(9)	-0.00172(9)
Cl(4)	0.01008(12)	0.00614(11)	0.00712(11)	-0.00197(9)	-0.00164(9)	0.00066(9)
Cl(5)	0.00767(12)	0.00881(11)	0.00876(12)	-0.00368(9)	-0.00241(9)	-0.00111(9)
Cl(6)	0.00854(12)	0.00732(11)	0.00793(11)	-0.00230(9)	-0.00063(9)	0.00165(9)
Cl(7)	0.00624(12)	0.01079(12)	0.01112(12)	-0.00316(10)	-0.00164(9)	-0.00248(9)
Cl(8)	0.00618(11)	0.00845(11)	0.01061(12)	-0.00243(9)	-0.00203(9)	-0.00158(9)
Cl(9)	0.01012(12)	0.00875(11)	0.00669(11)	-0.00128(9)	0.00057(9)	-0.00309(9)
Cl(10)	0.01006(12)	0.00666(11)	0.00714(11)	0.00269(9)	-0.00164(9)	0.00077(9)
Cl(11)	0.00997(12)	0.00768(11)	0.00792(11)	-0.00098(9)	0.00115(9)	-0.00376(9)
Cl(12)	0.00967(12)	0.00593(11)	0.00713(11)	0.000186(9)	-0.00161(9)	0.00017(9)
O(1)	0.00530(5)	0.00490(5)	0.00630(5)	-0.00200(4)	-0.00090(4)	-0.00100(4)
O(2)	0.00540(5)	0.00810(5)	0.00440(5)	-0.00360(4)	-0.00010(4)	-0.00060(4)
O(3)	0.01430(4)	0.00880(4)	0.01050(4)	-0.00380(3)	-0.00310(3)	-0.00170(3)
O(4)	0.00850(4)	0.01020(4)	0.01070(4)	-0.00040(3)	-0.00270(3)	-0.00150(3)
O(5)	0.01260(4)	0.01140(4)	0.01370(4)	-0.00130(4)	-0.00570(4)	-0.00240(4)
O(6)	0.01310(4)	0.00990(4)	0.00870(4)	-0.00380(3)	0.00010(3)	-0.00160(3)
O(7)	0.01260(5)	0.01150(4)	0.01270(4)	-0.00480(4)	-0.00010(4)	0.00010(4)
O(8)	0.01330(4)	0.01130(4)	0.00880(4)	-0.00490(3)	-0.00120(3)	-0.00050(3)
O(9)	0.01430(5)	0.01010(4)	0.01510(5)	-0.00480(4)	-0.00310(4)	-0.00090(4)
O(10)	0.00960(4)	0.01130(4)	0.01240(4)	-0.00060(3)	-0.00020(3)	0.00070(3)
O(11)	0.01440(4)	0.00840(4)	0.01060(4)	-0.00200(3)	-0.00170(4)	-0.00220(3)
O(12)	0.01460(5)	0.01200(5)	0.02390(6)	-0.00060 (4)	0.00650(4)	0.00390(4)

Table S3. Selected bond lengths and bond angles of the ruthenium anion in the complex $Li_4Ru_2OCl_{10}\cdot 10H_2O$.

Bond length/ (Å)		**Bond angles/ (°)**		**Bond angles/(°)**	
Ru1-Cl1	2.3406(4)	Cl3-Ru1-Cl5	175.282(16)	Cl3-Ru1-Cl2	90.627(14)
Ru1-O1	1.7838(3)	Cl2-Ru1-Cl4	173.740(16)	Cl3-Ru1-Cl1	87.222(15)
Ru1-Cl2	2.3562(4)	Cl1-Ru1-O1	177.818(15)	Cl3-Ru1-Cl4	89.354(14)
Ru1-Cl3	2.3646(5)			Cl3-Ru1-O1	91.168(10)
Ru1-Cl4	2.3633(4)	Cl5-Ru1-Cl2	89.094(13)	O1-Ru1-Cl4	92.114(13)
Ru1-Cl5	2.3608(5)	Cl5-Ru1-Cl1	88.058(13)	Cl4-Ru1-Cl1	86.397(12)
		Cl5-Ru1-Cl4	90.410(14)	Cl1-Ru1-Cl2	87.349(14)
		Cl5-Ru1-O1	93.552(14)	Cl2-Ru1-O1	94.145(11)
Ru2-Cl6	2.3358(4)	Cl8-Ru2-Cl10	175.213(16)	Cl8-Ru2-Cl7	88.547(14)
Ru2-O2	1.7808(3)	Cl7-Ru2-Cl9	175.595(15)	Cl8-Ru2-Cl6	87.173(15)
Ru2-Cl7	2.3431(4)	Cl6-Ru2-O2	177.250(15)	Cl8-Ru2-Cl9	92.053(14)
Ru2-Cl8	2.3763(5)			O2-Ru2-Cl8	90.101(10)
Ru2-Cl9	2.3922(4)	Cl10-Ru2-Cl9	89.222(13)	O2-Ru2-Cl9	91.354(13)
Ru2-Cl10	2.3490(5)	Cl10-Ru2-Cl6	88.251(13)	Cl9-Ru2-Cl6	88.399(12)
		Cl10-Ru2-Cl7	89.833(14)	Cl6-Ru2-C7	87.272(13)
		Cl10-Ru2- O2	94.485(14)	Cl7-Ru2-O2	93.009(11)

Figure S1 XPS spectrum and its simulated peak fitting of O 1s

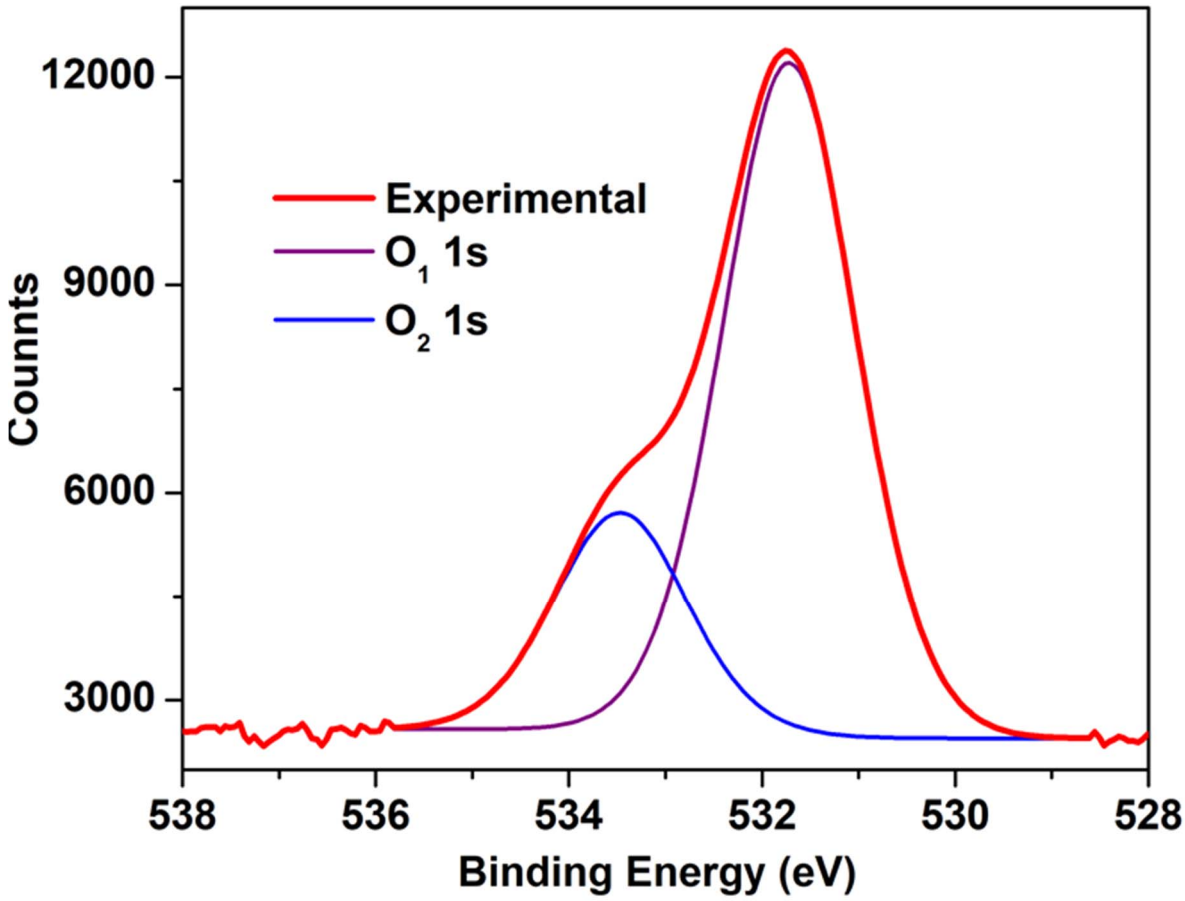

Table S4. Binding energy values for photoelectron peaks in different elements of the complex $Li_4Ru_2OCl_{10}\cdot 10H_2O$.

Photoelectron peak	Binding Energy/eV	Photoelectron peak	Binding Energy/eV
Ru 3d 3/2	284.61	O1 1s	531.72
Ru 3d 5/2	280.44	O2 1s	533.47
Ru 3d 3/2	286.00		
Ru 3d 5/2	281.83		
Ru 3p 1/2	485.13		
Ru 3p 3/2	462.91		

Figure S2. The magnetization versus magnetic field measured at temperature range of 2 K – 300 K for $Li_4Ru_2OCl_{10}\bullet 10H_2O$