Supporting information

Oxygen and Peroxide Bridged Uranyl(VI) Dimers Bearing Tetradentate Hybrid Ligands: Supramolecular Self-assembly and Generation Pathway

Jun Liu,[†] Xueyu Wang,[‡] Baihua Chen,[†] Lina Lv,[†,§] Qiang Li,[†] Shunzhong Luo,[†] Songdong Ding,[‡]* and Yanqiu Yang[†]*

[†] *Institute of Nuclear Physics and Chemistry, CAEP, Mianyang, Sichuan 621900, China*
[‡] *College of Chemistry, Sichuan University, Chengdu, Sichuan 610064, China*
[§] *Fundamental Science on Nuclear Wastes and Environmental Safety Laboratory, Southwest University of Science and Technology, Mianyang, Sichuan 621010, China*

*E-mail: yan.qiu.yang@163.com (Y. Y.)

*E-mail: dsd68@163.com (S. D.)

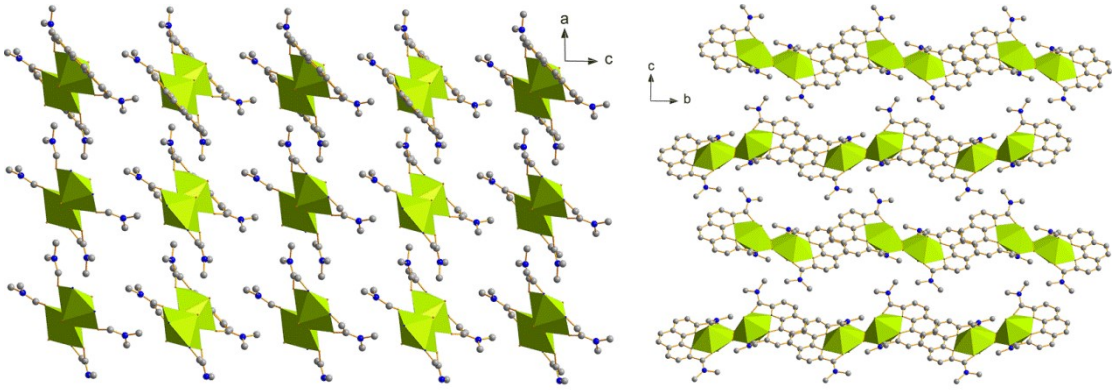

Figure S1. Packing diagrams of compound **4** viewed along the b-axis (left) and a-axis (right). Uncoordinated perchlorate and acetonitrile, and hydrogen atoms are not shown for clarity.

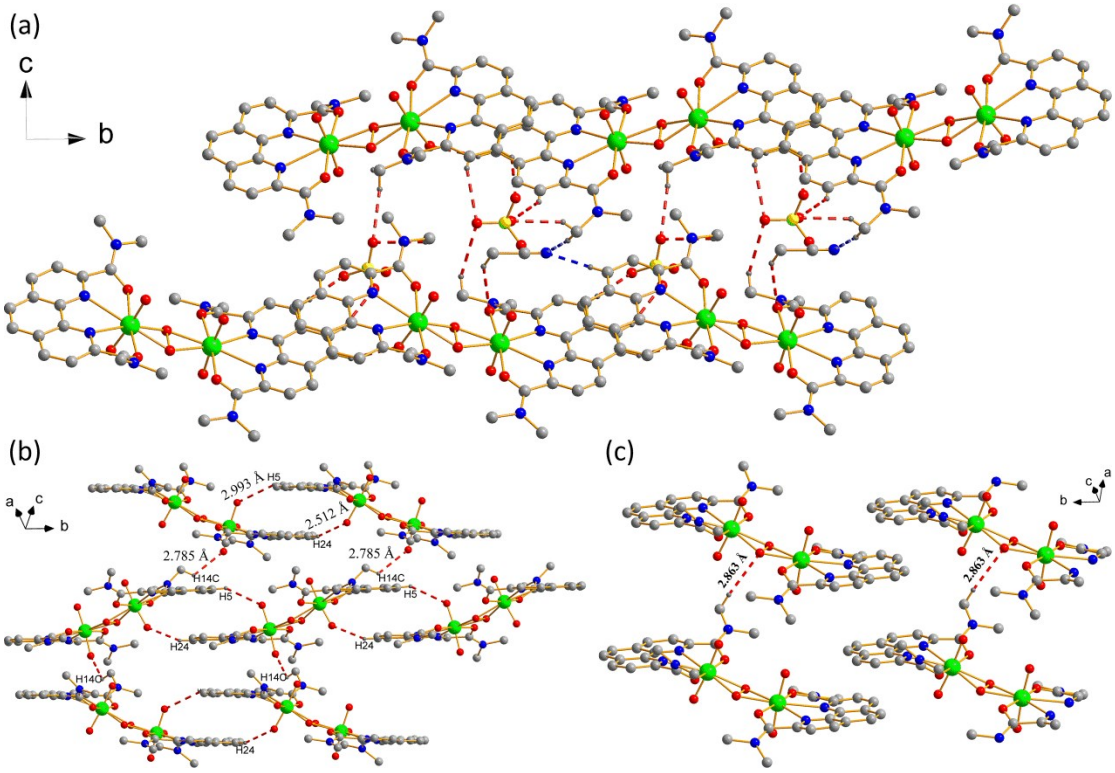

Figure S2. Hydrogen bonds in compound 4 (C-H···O, red dash line; C-H···N, blue dash line). Conditions for search of C-H···O bonds: H···O length < 2.90 Å, C-H···O angle □110°. (a) Hydrogen bonds relating uncoordinated perchlorates and acetonitriles; (b) C-H···O interations between uranyl O-atoms and the C-H donors from the neighbor ligands; (c) C17-H17C···O6 interation relating the bridging peroxide ligand in the U-O_2-U tecton. Element color: green (U), red (O), blue (N), duck gray (C), light gray (H), yellow (Cl).

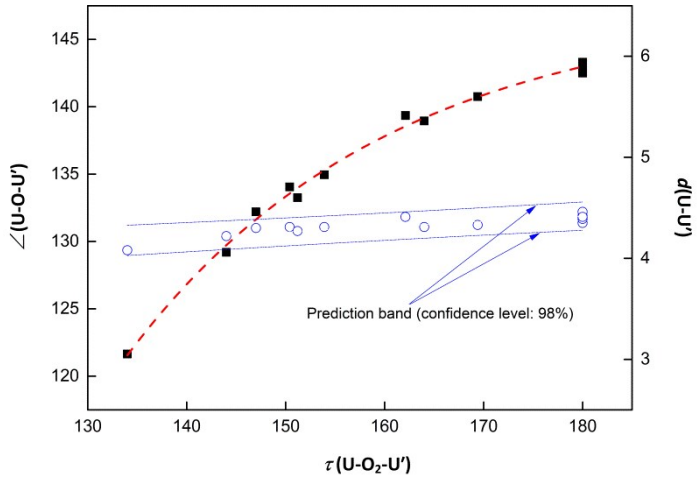

Figure S3. Relation of the (U-O-U) bond angle as well as the distance *d*(U-U′) in some U-O_2-U′ dimers with the dihedral angle *τ*(U-O_2-U′).

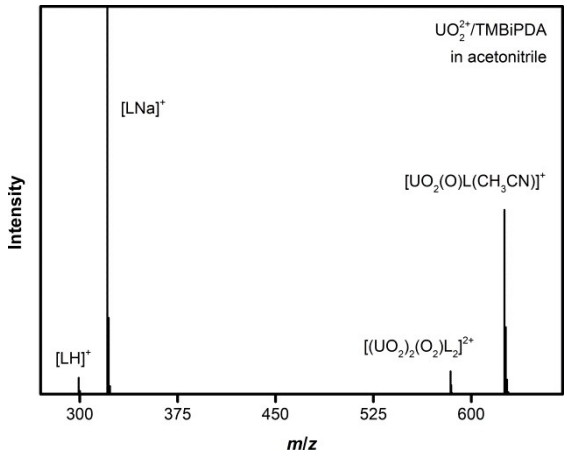

Figure S4. ESI-MS spectrum of **[**$(UO_2)_2(O_2)(TMBiPDA)_2](ClO_4)_2$ crystal (compound 2) dissolved in actonitrile.

Table S1. ESI-MS data of the U(VI)/TMBiPDA system

m/z	Abs. Inten.	Rel. Inten.	Charge	Assignment
200.0713	3328	0.15		
201.072	4778	0.21		
203.05	7722	0.34		
206.0721	5162	0.23		
206.5717	2901	0.13		
208.0579	170737	7.6	2	
208.56	38485	1.71	2	
209.054	8064	0.36	2	
210.0511	2944	0.13		
211.0461	34069	1.52	2	
211.5511	3669	0.16	2	
212.045	13226	0.59	2	
213.0372	108552	4.83		
215.0714	36288	1.61	2	
215.5668	7338	0.33	2	
216.0552	2944	0.13		
216.0834	2944	0.13	2	
216.9257	88938	3.96		
218.0566	6613	0.29		
218.9232	58808	2.62		
219.0545	3285	0.15		
219.1095	6613	0.29		
220.0431	31851	1.42	2	
220.5357	2901	0.13	2	
220.9408	2944	0.13		
221.0427	6634	0.3	2	

221.5384	3712	0.17	2
222.037	7339	0.33	2
222.0869	3669	0.16	
223.0632	286061	12.73	2
223.5655	91286	4.06	2
224.0643	13930	0.62	2
224.5602	2944	0.13	2
225.0622	5120	0.23	2
226.0969	65856	2.93	
227.0615	2901	0.13	
227.0903	2944	0.13	
228.0572	2901	0.13	
229.0406	2944	0.13	
229.0913	2944	0.13	
230.0697	37354	1.66	2
230.5779	6613	0.29	2
231.0793	2944	0.13	2
235.0477	63442	2.82	2
235.5475	5120	0.23	2
236.0464	22677	1.01	2
236.5427	8789	0.39	2
237.0532	16832	0.75	2
238.0683	82968	3.69	2
238.5697	13226	0.59	2
239.0654	6613	0.29	2
240.087	5845	0.26	
240.8907	20480	0.91	
242.129	9557	0.43	
242.2858	7339	0.33	
242.8876	13162	0.59	
244.1059	3669	0.16	
244.5272	30443	1.35	
244.8795	5120	0.23	
245.0753	6976	0.31	
247.0662	27072	1.2	
247.5615	4800	0.21	
249.1537	2944	0.13	
250.0537	4074	0.18	
251.06	3712	0.17	
251.1585	2901	0.13	
252.0389	595182	26.49	2
252.2741	2944	0.13	
252.5405	57717	2.57	2
253.0371	91873	4.09	2

254.0702	2944	0.13		
254.9249	6571	0.29		
256.1049	47936	2.13	1	
256.9208	11328	0.5		
257.1137	2944	0.13	1	
258.1195	11754	0.52	1	
258.9163	4778	0.21		
259.1579	2901	0.13		
260.9166	2901	0.13		
262.0726	37717	1.68	2	
262.5674	4416	0.2	2	
263.0689	2944	0.13	2	
269.0822	4053	0.18		
270.0406	24479	1.09	1	$[UO_2]^+$
270.1203	7317	0.33		
271.0889	2944	0.13		
271.1727	8789	0.39		
272.1365	45034	2	1	
273.1403	3712	0.17	1	
274.1373	2944	0.13	1	
274.2712	11392	0.51		
275.1361	2901	0.13	1	
276.9799	2944	0.13		
277.0903	9194	0.41		
278.9591	40662	1.81		
280.9613	15851	0.71		
282.1215	9557	0.43		
283.1273	2901	0.13		
284.0898	639774	28.47	2	$[UO_2L]^{2+}$
284.1515	5120	0.23		
284.2552	2944	0.13		
284.2944	5120	0.23	1	
284.4165	2944	0.13		
284.5916	124010	5.52	2	
285.0959	20160	0.9	2	
285.2788	4949	0.22		
285.3042	14826	0.66	1	
286.1219	8064	0.36		
286.301	4778	0.21	1	
287.101	2901	0.13		
287.1588	19138	0.85		
288.1323	84079	3.74	1	$[UO_2L(H_2O)]^+$
289.1418	12479	0.56		
292.0443	78319	3.49	2	

293.0413	3669	0.16		
293.0468	417876	18.6	2	$[UO_2L]^{2+}$
293.0977	61866	2.75		
293.2002	2944	0.13		
293.5485	60493	2.69	2	
293.5922	20565	0.92		
294.9379	441978	19.67	1	
295.9398	24597	1.09	1	
296.9349	177154	7.88	1	
297.0903	2944	0.13		
297.1398	4395	0.2		
298.1076	5141	0.23		
298.9311	11754	0.52		
299.1007	695279	30.94		
299.148	2246950	100		LH^+
299.3051	56965	2.54		
299.4128	44475	1.98	4	
299.4714	63125	2.81		
299.5982	117824	5.24		
299.6626	49758	2.21	4	
299.9	5802	0.26	4	
300.152	475208	21.15		
300.306	2922	0.13		
300.6014	4778	0.21		
301.168	13952	0.62		
302.0615	10688	0.48		
302.1518	4416	0.2		
304.6016	4778	0.21	2	$[UO_2L(CH_3CN)]^{2+}$
305.1078	3669	0.16	2	
305.6093	2944	0.13	2	
306.1062	40683	1.81	2	
306.6136	5888	0.26	2	
307.0984	21696	0.97	2	
309.9144	7744	0.34		
310.1341	23466	1.04	2	
310.6398	5162	0.23	2	
310.9844	2944	0.13		
311.1505	18752	0.83	2	
312.1453	7360	0.33		
312.3185	2944	0.13		
312.915	18751	0.83		
313.1656	219785	9.78	1	
314.1045	132430	5.89	1	
314.1573	87886	3.91	1	

314.599	11392	0.51		
314.9099	15807	0.7		
315.1137	49531	2.2	1	
315.1682	17642	0.79	1	
316.015	2901	0.13		
316.1143	13205	0.59	1	
316.168	3712	0.17	1	
317.1451	3690	0.16		
318.1229	315492	14.04	2	L_2Ca^{2+}
318.3035	25301	1.13		
318.625	131882	5.87	2	
318.9062	140860	6.27		
319.1377	43806	1.95	2	
319.5963	2901	0.13		
320.1409	28744	1.28	1	
320.902	140287	6.24	1	
321.1304	395552	17.6	1	LNa^{+}
321.2745	2944	0.13		
321.9011	8426	0.37	1	
322.1349	95247	4.24	1	
322.8994	111746	4.97	1	
323.0976	526931	23.45	2	
323.6007	121531	5.41	2	
323.9034	2944	0.13		
324.1001	43724	1.95	2	
324.8945	8426	0.37		
325.1382	115290	5.13	2	
325.6304	61610	2.74	2	
326.119	11008	0.49	1	
326.147	28367	1.26	2	
327.1115	27925	1.24	1	$[UO_2(O)(CH_3CN)]^{+}$
327.1649	42479	1.89		
327.6102	5888	0.26		
328.1086	31788	1.41	1	
329.1594	1691422	75.28	1	$[UO_2(CH_3CN)(H_2O)]^{+}$
329.3255	22741	1.01		
329.4258	7338	0.33		
329.5077	26410	1.18	10	
329.6099	3669	0.16	10	
329.6986	19861	0.88	10	
330.1091	186695	8.31	2	
330.1613	387764	17.26	1	
330.4441	2944	0.13		
330.6092	63618	2.83	2	

331.1081	122255	5.44	2	
331.1632	63650	2.83	1	
331.609	28608	1.27	2	
332.1078	72769	3.24	2	
332.154	55392	2.47	1	
332.6039	16171	0.72	2	
332.6399	9216	0.41	3	
332.9442	3669	0.16	3	
333.1284	726363	32.33	2	
333.1891	11925	0.53		
333.2934	2944	0.13	3	
333.4768	3712	0.17		
333.629	276440	12.3	2	
333.9021	4394	0.2		
334.1205	159730	7.11	2	
334.6308	5888	0.26	2	
334.9459	3669	0.16		
335.1339	46575	2.07	2	
335.6291	2944	0.13	2	
336.3217	2944	0.13		
337.1109	60920	2.71		
338.1023	633710	28.2	2	
338.1673	3306	0.15		
338.2631	2944	0.13		
338.6044	143125	6.37	2	
339.1061	59303	2.64	2	
339.161	8832	0.39		
339.6016	5888	0.26	2	
340.1391	203848	9.07	2	
340.6326	123757	5.51	2	
341.1405	55617	2.48	2	
341.6332	7765	0.35	2	
342.1225	86448	3.85	2	
342.6184	26432	1.18	2	
343.1184	35882	1.6	2	
343.1734	202115	9	1	$[UO_2(O_2)(CH_3CN)]^+$
343.6152	3669	0.16	2	
344.1204	7744	0.34	2	
344.179	104366	4.64	1	
345.1118	395926	17.62	2	
345.1887	113641	5.06	1	$[UO_2(O)(H_2O)(CH_3CN)]^+$
345.6124	163133	7.26	2	
346.1111	250399	11.14	2	
346.1808	42219	1.88	1	

346.6106	106617	4.74	2
347.1139	191643	8.53	2
347.6163	65389	2.91	2
348.0537	34403	1.53	
348.1319	666270	29.65	2
348.3127	5888	0.26	
348.4913	2944	0.13	
348.6345	254786	11.34	2
349.1367	106331	4.73	2
349.6282	4778	0.21	2
350.1472	56721	2.52	2
350.6447	3690	0.16	2
351.1411	313688	13.96	
352.1316	118538	5.28	
352.6179	10304	0.46	
353.111	184535	8.21	2
353.6148	36672	1.63	2
354.1184	59924	2.67	2
354.6076	6571	0.29	2
355.1408	195761	8.71	2
355.637	89707	3.99	2
356.1398	42175	1.88	2
356.9714	5845	0.26	
357.122	64772	2.88	2
357.1854	108619	4.83	
357.625	16149	0.72	2
358.1161	26048	1.16	2
358.1897	26174	1.16	
358.6181	4437	0.2	2
358.9624	2944	0.13	
359.1697	316051	14.07	
360.1176	369352	16.44	2
360.6176	127783	5.69	2
361.1145	224686	10	2
361.1821	61180	2.72	
361.6149	78698	3.5	2
362.1179	199382	8.87	2
362.6162	75668	3.37	2
363.136	281236	12.52	2
363.1983	456572	20.32	
363.638	95049	4.23	2
364.137	24512	1.09	2
364.1903	179894	8.01	
364.6396	3712	0.17	2

365.1432	103555	4.61		
365.645	5120	0.23		
366.097	68556	3.05		
366.1829	13719	0.61		
367.1191	108349	4.82	2	
367.6237	26773	1.19	2	
368.1206	47957	2.13	2	
368.6228	7317	0.33	2	
369.1256	30080	1.34	2	
369.6253	4395	0.2	2	
370.143	85994	3.83	2	
370.6387	54591	2.43	2	
371.1521	27157	1.21		
372.1292	30467	1.36	1	
372.951	219754	9.78		
373.1188	2944	0.13	1	
373.1837	59217	2.64		
373.9555	5866	0.26		
374.1354	6976	0.31	1	
374.1846	34296	1.53		
374.9478	104486	4.65		
375.1233	128084	5.7	2	
375.1972	117950	5.25	1	
375.6207	45077	2.01	2	
375.9422	2901	0.13		
376.1256	99862	4.44	2	
376.1893	41622	1.85	1	
376.6249	44288	1.97	2	
376.9445	6613	0.29		
377.1278	85891	3.82	2	
377.2098	70758	3.15	1	$[UO_2(O)(CH_3CN)(CH_3OH)(H_2O)]^+$
377.627	18709	0.83	2	
378.144	71199	3.17	2	
378.2085	10325	0.46	1	
378.6479	4800	0.21	2	
379.0716	77045	3.43		
379.1563	31108	1.38		
380.168	14293	0.64		
380.6496	2944	0.13		
381.1511	39541	1.76	1	
382.1435	47835	2.13	1	
382.6306	6571	0.29		
383.1279	10987	0.49	1	
384.1374	17884	0.8	1	

385.1692	34951	1.56	1	
386.1708	19498	0.87	1	
387.2028	24533	1.09		
388.1896	5888	0.26		
389.2148	198136	8.82		
390.1329	35461	1.58		
390.2216	44673	1.99		
390.6248	2944	0.13		
391.0787	2944	0.13		
391.1969	292440	13.01	1	
391.6276	3712	0.17		
391.6654	3669	0.16		
392.193	95367	4.24	1	
393.2101	176100	7.84	1	$[UO_2(O_2)(CH_3CN)(CH_3OH)(H_2O)]^+$
394.1115	3712	0.17		
394.158	3306	0.15		
394.2063	64886	2.89	1	
395.1073	3669	0.16		
395.1722	10976	0.49		
395.2255	28298	1.26	1	
396.2308	3328	0.15		
396.9171	17920	0.8	9	
397.0439	79125	3.52	9	
397.1441	23031	1.02	9	
398.0335	2944	0.13		
398.1061	40312	1.79		
398.9122	32576	1.45		
399.0393	57618	2.56	1	
399.1221	2944	0.13		
400.0496	2944	0.13	1	
400.9131	19413	0.86		
401.0351	24597	1.09	1	
401.208	6656	0.3		
402.0324	2944	0.13	1	
403.0304	2944	0.13	1	
403.2225	2944	0.13		
405.2062	19381	0.86	1	
406.1996	4800	0.21	1	
407.2125	54412	2.42	1	
408.224	3328	0.15	1	
411.04	2944	0.13		
411.0979	54936	2.44		
412.088	2944	0.13		
419.2257	34016	1.51		

421.0754	105601	4.7	1	
421.2059	90061	4.01		
421.2604	4042	0.18		
422.0761	21995	0.98	1	
422.208	14336	0.64		
423.0752	37397	1.66	1	
423.224	91160	4.06	1	
424.0717	4394	0.2	1	
424.225	6634	0.3	1	
425.2217	2944	0.13	1	
427.0582	3712	0.17		
429.0449	5888	0.26		
433.1651	79061	3.52	2	$[UO_2L_2]^{2+}$
433.6628	16895	0.75	2	
435.2221	8107	0.36	1	
436.2005	2944	0.13	1	
437.0549	317773	14.14	1	
437.2231	4747	0.21	1	
438.0577	51242	2.28	1	
439.0544	119596	5.32	1	
440.0558	5504	0.24		
440.1705	5888	0.26		
441.0691	2944	0.13		
443.0604	3712	0.17		
448.1683	184333	8.2	2	$[UO_2L_2(CH_3OH)]^{2+}$
448.6693	58602	2.61	2	
449.1613	10709	0.48	2	
449.2233	2944	0.13		
451.084	76251	3.39		
452.033	85244	3.79	1	
453.0326	8448	0.38	1	
453.0657	24597	1.09		
454.0288	8853	0.39	1	
454.0823	4437	0.2		
455.0241	35947	1.6	1	
455.1744	8832	0.39		
455.6737	2944	0.13		
457.0849	260805	11.61		
458.0947	3648	0.16		
459.0796	6250	0.28		
461.0202	771637	34.34	1	
461.2166	4757	0.21		
462.0235	136884	6.09	1	
463.0168	715655	31.85	1	

463.1749	170040	7.57	2
463.6738	61082	2.72	2
464.0204	185298	8.25	1
464.1878	10283	0.46	2
465.0159	454350	20.22	1
466.02	106832	4.75	1
467.048	321932	14.33	1
468.0578	56512	2.52	1
469.0619	89657	3.99	1
470.1807	20586	0.92	
470.6822	3712	0.17	
475.0344	129979	5.78	1
476.0388	8064	0.36	1
477.0347	109798	4.89	1
478.037	19030	0.85	1
478.1775	28587	1.27	
478.6722	9216	0.41	
479.0314	92839	4.13	1
480.0387	3648	0.16	1
481.036	13205	0.59	1
481.0819	30737	1.37	
482.0396	31552	1.4	1
485.0428	13568	0.6	
485.1276	20906	0.93	
487.031	6613	0.29	
488.0552	41803	1.86	
489.1022	2944	0.13	
491.031	332509	14.8	1
492.0312	66025	2.94	1
493.028	305033	13.58	1
494.0265	77461	3.45	1
495.0257	192148	8.55	1
496.0311	43455	1.93	1
497.0389	90329	4.02	1
498.0283	3669	0.16	
505.0468	65101	2.9	
506.0448	2901	0.13	
507.0456	58917	2.62	1
508.0482	3669	0.16	1
509.0401	28971	1.29	1
510.0663	2901	0.13	1
511.0509	10645	0.47	1
513.128	3712	0.17	
515.1453	2944	0.13	

519.0828	2944	0.13		
521.0432	34069	1.52		
523.0419	52642	2.34		
525.0452	303043	13.49	1	
526.0661	41310	1.84	1	
527.0536	177937	7.92	1	
528.0769	37656	1.68	1	
529.0677	77416	3.45	1	
530.0819	11008	0.49	1	
531.0672	5120	0.23	1	
535.0973	61752	2.75		
537.0647	4395	0.2		
539.0686	42966	1.91		
541.0869	12458	0.55		
555.087	6997	0.31		
557.0548	35999	1.6		
559.0625	5120	0.23		
566.0667	24554	1.09		
584.1746	85325	3.8	2	$[UO_2)_2(O_2)L_2]^{2+}$
584.6807	12523	0.56		
586.172	69607	3.1	1	$[UO_2)(O)L]^{+}$
587.177	11226	0.5		
599.183	252939	11.26	2	$[UO_2)_2(O_2)L_2(CH_3OH)]^{2+}$
599.6844	89760	3.99	2	
600.1788	23082	1.03	2	
603.03	201830	8.98	1	$[UO_2(OH)L]^{+}$
604.0337	40164	1.79	1	
605.0287	6055	0.27	1	
606.1894	55005	2	2	$[UO_2)_2(O)L_2(CH_3CN)(H_2O)]^{2+}$
606.6954	22552	0.82	2	
614.1865	169981	7.56	2	$[UO_2)_2(OH)_2L_2(CH_3CN)(H_2O)]^{2+}$
614.6857	51626	2.3	2	
615.1859	18730	0.83	2	
617.0818	3712	0.17		
622.1949	32961	1.03	2	$[UO_2)_2(O)L_2(CH_3OH)(CH_3CN)(H_2O)]^{2+}$
622.7007	13533	0.42	2	
629.1944	93512	4.16	2	$[UO_2)_2(O_2)L_2(CH_3OH)(CH_3CN)(H_2O)]^{2+}$
629.6931	26064	1.16	2	
630.188	4800	0.21	2	
631.1903	4416	0.2		
636.1913	2944	0.13		
644.1789	2944	0.13		
659.2223	4437	0.2		
667.1297	162366	7.23	1	

668.138	13951	0.62	1
669.1317	44858	2	1
697.1409	69914	3.11	
699.1451	6634	0.3	
711.1478	2944	0.13	
735.1872	2944	0.13	
765.1997	2944	0.13	

Table S2. ESI-MS data of the U(VI)/TMPhenDA system

m/z	Abs. Inten.	Rel. Inten.	Charge	Assignment
203.0668	5931	0.11		
203.5453	23865	0.46		
205.0468	29418	0.57		
206.0456	5184	0.1		
208.0425	82859	1.6	2	
208.5395	8490	0.16	2	
209.0401	75794	1.47	2	
209.0776	6272	0.12		
209.5443	7765	0.15	2	
210.042	32363	0.63	2	
210.5505	2944	0.06	2	
211.0641	89957	1.74	1	
211.5651	2944	0.06		
212.0702	26133	0.51	1	
212.5751	2944	0.06		
213.0714	6997	0.14	1	
214.1629	64917	1.26		
214.6612	11072	0.21		
216.5617	2944	0.06		
216.9243	72464	1.4		
218.9254	13290	0.26		
220.0591	139634	2.7	2	
220.5597	28693	0.56	2	
221.0593	23957	0.46	2	
221.574	3669	0.07		
222.1012	3712	0.07		
223.0471	39317	0.76	2	
223.086	6699	0.13		
223.173	47855	0.93		
223.5435	2944	0.06	2	
224.0491	5546	0.11	2	
224.1761	113711	2.2		
225.0439	13653	0.26		

225.16	135994	2.63		
225.536	2944	0.06		
226.1598	4821	0.09		
227.0775	21376	0.41		
228.0861	3712	0.07		
232.0401	10346	0.2	1	
233.0394	11114	0.22	1	
234.0481	5931	0.11	1	
235.0636	148849	2.88	1	
235.5614	26837	0.52		
236.0632	19541	0.38	1	
237.0678	4437	0.09	1	
239.1809	177540	3.44		
240.1763	47630	0.92		
240.89	23914	0.46		
241.0961	3669	0.07		
242.2858	11093	0.21		
242.8875	27910	0.54		
244.8837	6656	0.13		
247.049	20949	0.41	1	
248.0445	8832	0.17	1	
248.5501	2944	0.06		
248.9424	5931	0.11		
249.0466	11839	0.23	1	
250.0876	129147	2.5		
250.5659	4821	0.09		
251.0904	9621	0.19		
251.151	2987	0.06		
252.0401	15445	0.3		
252.107	5888	0.11		
254.9257	39680	0.77		
256.9212	38508	0.75		
258.9221	18005	0.35		
259.0655	3669	0.07		
260.9166	3669	0.07		
268.1138	20970	0.41		
270.0447	5162	0.1		$[UO_2]^+$
273.1654	4437	0.09		
274.0818	2965	0.06		
274.272	11840	0.23		
276.0731	2987	0.06		
278.9588	15466	0.3		
280.1069	22912	0.44	1	
280.9584	2944	0.06	8	

281.0769	4800	0.09	8	
281.0983	6656	0.13	1	
281.199	8107	0.16	8	
281.9123	3328	0.06		
282.1217	64887	1.26	1	
283.1199	8874	0.17	1	
284.2925	5930	0.11		
285.2884	2176	0.04		
287.1658	5888	0.11		
288.0743	2987	0.06		$[UO_2(H_2O)]^+$
291.0479	17280	0.33		
291.1023	11051	0.21		
294.94	151221	2.93		
295.9372	5888	0.11		
296.0919	587413	11.37	2	$[UO_2L]^{2+}$
296.25	2987	0.06		
296.594	138666	2.68	2	
296.9344	74762	1.45		
297.0942	23979	0.46	2	
297.1727	2987	0.06		
298.1199	18474	0.36		
299.1219	2987	0.06		
301.0582	27307	0.53		
302.068	8874	0.17		
302.1149	3349	0.06		
304.0727	2987	0.06		
307.0828	2987	0.06		
309.9131	3306	0.06		
310.1201	29893	0.58		
311.0958	602851	11.67		
311.5991	132933	2.57		
312.1166	93447	1.81		
312.9105	2944	0.06		
316.0915	2944	0.06		
316.6043	5162	0.1		
318.3027	5184	0.1		
318.904	71199	1.38		
320.1096	2944	0.06		
320.9016	65254	1.26	1	$[UO_2(O_2)(H_2O)]^+$
321.9093	5888	0.11	1	
322.9019	36757	0.71	1	
323.1502	5167207	100	1	LH^+
323.3116	150240	2.91		
323.4128	72797	1.41	3	

323.4899	148539	2.87		
323.6919	108334	2.1		
323.7588	5546	0.11	3	
323.9278	69707	1.35		
324.0756	2944	0.06	3	
324.1532	1109366	21.47	1	
324.3147	23957	0.46		
324.4201	9600	0.19	3	
324.4979	10730	0.21	5	
324.6884	5184	0.1	5	
324.8989	12181	0.24	5	
325.1558	136570	2.64	1	
326.1056	143523	2.78	2	
326.6055	26901	0.52	2	
327.108	67136	1.3	2	
327.6102	4800	0.09	2	
331.204	10368	0.2		
331.6112	19135	0.37		
332.1156	2944	0.06		
332.9413	30208	0.58		
333.0861	66912	1.29		
334.0912	37163	0.72		
334.1255	47640	0.92		
334.6377	6635	0.13		
334.9345	23253	0.45		
335.0976	369109	7.14	2	
335.6013	63849	1.24	2	
336.1011	15488	0.3	2	
336.5937	2987	0.06	2	
336.9372	8490	0.16		
340.1307	4437	0.09		
341.1258	13248	0.26		
342.1224	471751	9.13	1	
342.198	2987	0.06		
342.625	182698	3.54		
343.125	40455	0.78	1	
343.1657	5184	0.1		
344.1264	7787	0.15	1	
345.0531	2944	0.06		
345.132	892110	17.26	1	$[LNa]^+$
345.3002	11093	0.21		
345.4894	4074	0.08		
346.1347	197419	3.82	1	
347.1346	27989	0.54	1	

349.1377	52480	1.02		
349.6259	51911	1		
350.1044	348967	6.75	2	
350.6053	83155	1.61	2	
351.115	73235	1.42	2	
351.6108	5184	0.1	2	
352.1139	23037	0.45	2	
353.1594	2719943	52.64	1	$[UO_2(HO_2)(CH_3OH)(H_2O)]^+$
353.3295	49600	0.96	10	
353.4347	25856	0.5	10	
353.5202	64638	1.25	10	
353.6095	3349	0.06	10	
353.7266	40356	0.78	10	
353.9865	2965	0.06		
354.1066	189952	3.68	2	
354.1599	733170	14.19	1	
354.4635	2944	0.06		
354.6063	71509	1.38	2	
355.1051	145088	2.81	2	
355.1649	163034	3.16	1	$[LH(CH_3OH)]^+$
355.6079	65664	1.27	2	
356.11	113227	2.19	2	
356.1684	12202	0.24	1	
356.6069	49586	0.96	2	
357.1269	829877	16.06	2	
357.3029	4437	0.09	10	
357.4054	2987	0.06	10	
357.4858	3349	0.06	10	
357.6296	327136	6.33	2	
358.1312	113455	2.2	2	
358.2016	2987	0.06		
358.6395	11840	0.23	2	
359.1231	28373	0.55	2	
359.1799	2944	0.06		
361.1044	460723	7.5	1	$[UO_2(O_2)(CH_3CN)(H_2O)]^+$
362.1067	105843	1.72	1	
363.1058	30880	0.5	1	
364.1432	48470	0.94		
364.6291	68259	1.32	2	
365.1126	213158	4.13	2	
365.6152	11051	0.21	2	
366.1114	86644	1.68	2	
366.6126	10688	0.21	2	
367.1112	38952	0.75	2	

367.1751	3328	0.06		
367.6169	12928	0.25	2	
368.2083	180177	3.49	1	
368.6107	19583	0.38		
369.1114	423366	8.19	2	
369.2075	37250	0.72	1	
369.2943	2944	0.06		
369.6137	176867	3.42	2	
370.1108	256500	4.96	2	
370.1958	11840	0.23	1	
370.6108	129401	2.5	2	
371.1102	205190	3.97	2	
371.1811	6634	0.13		
371.6141	53226	1.03	2	
372.1316	726852	14.07	2	
372.3062	2944	0.06		
372.5001	2987	0.06		
372.6331	303355	5.87	2	
372.9528	52074	1.01		
373.0172	2987	0.06		
373.1364	116004	2.25	2	
373.6345	17685	0.34	2	
374.1331	62362	1.21	2	
374.9454	8106	0.16		
375.1415	612872	11.86	1	$[UO_2(O_2)(CH_3CN)(CH_3OH)]+?$
375.32	3349	0.06		
375.4971	2987	0.06		
376.1463	141789	2.74	1	
377.1593	8490	0.16	1	
379.0731	90303	1.75		
379.1491	6250	0.12		
379.6289	60857	1.18		
380.1231	12181	0.24		
381.122	69885	1.35	2	
381.6214	15872	0.31	2	
382.1192	6634	0.13	2	
382.6305	10346	0.2	2	
383.1699	571254	11.06	1	
383.5481	2987	0.06		
383.6144	12928	0.25		
384.1186	319504	6.18	2	
384.1712	160732	3.11	1	
384.6169	123371	2.39	2	
385.1153	281012	5.44	2	

385.1785	46251	0.9	1	
385.6155	102031	1.97	2	
386.1139	184306	3.57	2	
386.6141	43712	0.85	2	
387.1364	288614	5.59	2	
387.2281	11498	0.22		
387.6369	132806	2.57	2	
388.1379	39702	0.77	2	
388.6421	5163	0.1	2	
389.135	12202	0.24	2	
389.25	6656	0.13		
389.6612	3669	0.07		
391.1189	53438	1.03		
392.12	9621	0.19		
393.1346	67754	1.31	1	$[UO_2(O_2)(CH_3CN)(CH_3OH)(H_2O)]^+$
394.1116	6677	0.13		
394.1444	5547	0.11	1	
394.6173	10709	0.21		
395.1567	2944	0.06	1	
396.1243	22223	0.43	1	
396.2391	16918	0.33		
396.9169	4053	0.08		
397.1451	45606	0.88	1	
398.106	7381	0.14		
398.2182	36622	0.71		
398.6158	2944	0.06		
398.9119	2944	0.06		
399.1236	148607	2.88	2	
399.2368	3712	0.07		
399.6222	43349	0.84	2	
400.1165	110776	2.14	2	
400.6198	29823	0.58	2	
400.9111	2944	0.06		
401.1206	71265	1.38	2	
401.6251	7744	0.15	2	
402.1444	38229	0.74	2	
402.6464	14038	0.27	2	
403.1457	5163	0.1	2	
405.1513	94486	1.83		
406.163	23274	0.45		
407.1122	9557	0.18		
408.1165	2944	0.06		
410.1547	4437	0.09		
410.2172	3349	0.06		

411.1011	115557	2.24		
413.1805	6656	0.13		
414.6164	2944	0.06		
415.129	4821	0.09		
415.19	32283	0.62		
416.1762	2987	0.06		
417.0744	2987	0.06		
421.0405	57434	1.11		
421.1215	9194	0.18		
423.036	44458	0.86	1	
423.1135	2987	0.06		
424.0389	2944	0.06	1	
425.0404	27306	0.53	1	
439.1225	2987	0.06		
445.0766	50325	0.97	1	
446.0786	7019	0.14	1	
447.085	33821	0.65	1	
447.2991	2944	0.06		
453.0543	4074	0.08		
457.0856	108712	2.1	2	$[UO_2L_2]^{2+}$
458.0866	2987	0.06		
459.0904	6699	0.13		
461.0553	329495	6.38	1	
462.0561	67945	1.31	1	
463.0516	117778	2.28	1	
464.0549	3328	0.06		
471.0766	2987	0.06		
472.1569	6656	0.13		
475.0875	38571	0.75	1	
475.906	2944	0.06		
476.0269	16213	0.31		
476.073	8896	0.17	1	
477.0942	10325	0.2	1	
478.037	2944	0.06		
479.0291	25492	0.49		
481.0248	5909	0.11		
485.0252	186060	3.6	1	
486.0269	29460	0.57	1	
487.0177	153379	2.97	1	
487.1788	8150	0.16		
488.0422	121974	2.36	1	
488.1717	2987	0.06		
489.0159	109925	2.13	1	
490.0222	23276	0.45	1	

491.0632	251327	4.86	1	
492.0653	46053	0.89	1	
493.0621	94341	1.83	1	
505.1091	2965	0.06		
505.1629	2944	0.06		
506.0341	2944	0.06		
509.0368	15957	0.31		
511.0545	12181	0.24		
513.063	2944	0.06		
515.0299	102465	1.98		
516.0421	6634	0.13		
517.03	104185	2.02	1	
518.0324	14016	0.27	1	
519.0273	72277	1.4	1	
520.0322	4800	0.09	1	
521.0592	67862	1.31	1	
523.0681	5888	0.11		
525.0181	62910	1.22		
527.017	15872	0.31		
527.274	145626	2.82	1	
528.2819	38569	0.75	1	
529.271	59243	1.15	1	
535.1023	3712	0.07		
539.0552	43646	0.84		
545.0473	9215	0.18		
545.2765	2944	0.06		
547.0371	5888	0.11	1	
548.0388	2944	0.06	1	
549.0496	4800	0.09	1	
566.068	55874	1.08		
596.1597	2944	0.06		
603.0274	64327	1.24		
605.0244	17706	0.34		
608.1774	157963	3.06	2	$[(UO_2)_2(O_2)L_2]^{2+}$
608.6749	52139	1.01	2	
609.1754	6677	0.13	2	
611.1788	2987	0.06		
617.0602	16576	0.32		
624.1839	526176	10.18	2	$[UO_2(O_2)L_2(CH_3OH)]^{2+}$
624.685	208131	4.03	2	
625.188	16981	0.33	2	
625.662	2944	0.06		
626.1812	275298	5.35	1	$[UO_2(O)L(H_2O)]^{+}$
627.151	53683	1.04	1	

628.1865	4955	0.1	1	
638.1892	458569	8.87	2	$[UO_2(O_2)\ L_2(CH_3CN)(H_2O)]^{2+}$
638.689	208783	4.04	2	
639.1951	61688	1.19	2	
642.0197	19925	0.39		
654.1949	256558	4.97	2	$[UO_2(O_2)L(CH_3CN)(CH_3OH)(H_2O)]^{2+}$
654.6938	119556	2.32	2	
655.194	33609	0.65	2	
655.6947	6927	0.13		
668.2006	22187	0.43		
668.6878	5931	0.11		
672.0345	8853	0.17		
685.202	2987	0.06		
691.1325	198387	3.84	1	
692.1389	20950	0.41	1	
693.1309	65611	1.27	1	
707.217	45525	0.88	1	
708.2188	7786	0.15	1	
709.2217	6656	0.13	1	
721.1443	123684	2.39	1	
722.1476	6315	0.12	1	
723.1395	26111	0.51	1	
737.226	29055	0.56	1	
738.2258	6293	0.12	1	
739.2334	16152	0.31	1	
751.1502	7744	0.15		
767.2386	3712	0.07	1	
768.2194	2987	0.06	1	
769.2405	4437	0.09	1	
783.1929	6699	0.13		
785.1753	2987	0.06		
813.1871	12608	0.24		
843.2129	2987	0.06		

Table S3. ESI-MS data of dissolved compound **2** in acetonitrile

m/z	Abs. Inten.	Rel. Inten.	Charge	Assignment
200.075	1632	0.01		
208.0552	2176	0.02		
221.0073	4197	0.04		
226.0993	2240	0.02		
228.2646	25664	0.24		
241.998	3872	0.04		
242.2836	500783	4.6		

242.4297	1632	0.01		
242.5787	1632	0.01		
243.2881	90901	0.83		
244.2877	1632	0.01		
245.0775	23840	0.22		
247.2345	1632	0.01		
252.0369	24592	0.23		
259.137	1632	0.01		
261.1119	1632	0.01		
264.1194	1632	0.01		
272.1078	1632	0.01		
273.1661	1632	0.01		
277.0216	1632	0.01		
278.9607	1936	0.02		
280.9523	1632	0.01		
284.0877	2208	0.02		
285.1044	1632	0.01		
291.048	32304	0.3		
293.0086	1632	0.01		
299.1519	460169	4.22	1+	$[LH]^+$
299.3062	49329	0.45		
299.4628	1632	0.01		
299.4959	1632	0.01		
299.678	1632	0.01		
300.1555	89575	0.82	1+	
300.3159	1632	0.01		
301.2035	1632	0.01		
308.0993	4384	0.04		
310.1348	34224	0.31		
310.6336	7200	0.07		
311.1292	1632	0.01		
313.2081	6901	0.06		
313.2758	2784	0.03		
313.7162	3872	0.04		
318.12	10016	0.09		
321.1307	10895082	100	1+	$[LNa]^+$
321.2911	342454	3.14	5+	
321.3944	162819	1.49	2+	
321.4677	314755	2.89	5+	
321.5759	2176	0.02		
321.6767	248909	2.28	5+	
321.904	126333	1.16	2+	
322.1335	2142979	19.67	1+	
322.2969	65121	0.6		

322.3961	25456	0.23	2+	
322.4764	61920	0.57		
322.6725	36141	0.33		
322.7362	6127	0.06		
322.8895	9785	0.09	2+	
323.1345	224875	2.06	1+	
323.2077	1632	0.01		
323.3023	1632	0.01		
323.5862	1632	0.01		
324.1419	15488	0.14	1+	
327.1062	1632	0.01		
331.1898	2736	0.03		
337.1028	422702	3.88	1+	
338.1068	74135	0.68	1+	
339.1033	32256	0.3	1+	
344.207	29296	0.27		
345.2139	2208	0.02		
353.1956	2240	0.02		
358.2475	2240	0.02		
363.1249	10544	0.1		
365.1093	13008	0.12		
366.1122	1632	0.01		
372.236	36160	0.33		
379.2607	2208	0.02		
387.2762	1632	0.01		
413.1662	1483	0.01		
414.1701	10256	0.09		
415.1714	1632	0.01		
421.0789	2752	0.03		
431.0451	18016	0.17		
445.0653	4448	0.04		
457.0854	3056	0.03		
481.2514	2208	0.02		
523.0832	24896	0.23		
526.4131	19952	0.18		
540.4271	234868	2.16		
541.4293	96876	0.89		
542.4226	2736	0.03		
581.3123	1632	0.01		
581.4161	2176	0.02		
584.1782	640063	5.87	2+	$[(UO_2)_2(O_2)L_2]^{2+}$
584.3972	1920	0.02		
584.6792	254306	2.33	2+	
584.8928	3872	0.04		

585.1757	37760	0.35	2+	
585.2399	1632	0.01		
585.6797	2208	0.02	2+	
587.1855	2208	0.02		
600.1752	2752	0.03		
603.4601	5504	0.05		
611.4272	9360	0.09		
625.265	4176	0.04		
625.4375	5179242	47.54	1+	$[UO_2(O)L(CH_3CN)]^+$
625.5436	29984	0.28	8+	
625.664	135042	1.24	8+	
625.8084	64516	0.59	8+	
625.9059	149751	1.37	8+	
626.2002	113643	1.04		
626.2996	27444	0.25		
626.4417	1880333	17.26	1+	
626.6663	43498	0.4	9+	
626.8124	27069	0.25	9+	
626.9087	57544	0.53	9+	
627.1881	33294	0.31		
627.4464	408213	3.75	1+	
628.451	55030	0.51	1+	
641.4089	45902	0.42		
642.4246	2784	0.03		
647.4925	1632	0.01		
747.3857	1904	0.02		
803.5709	2261			
815.3832	2261			
837.5767	2261			
862.8761	2325			
866.4768	2261			
877.4939	2987			
881.8065	2261			
883.8306	640031			
884.1024	14037			
884.2797	6058			
884.3979	15979			
884.8339	382071			
885.1017	15253			
885.3895	3755			
885.8271	139057			
886.8424	28480			
899.8069	3392			
925.6311	2261			

960.8865	2261
969.6246	2261
1013.5733	2261
1015.8588	2261
1092.6927	2261
1123.8383	2261