

Detailed Characterization of Dioxouranium(VI) Complexes with a Symmetrical Tetradentate N₂O₂-benzil bis(isonicotinoyl hydrazone) Ligand

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Geometry of the complex 1 in XYZ format.

Fig. S1: Mass spectrum of uranyl complex **1**

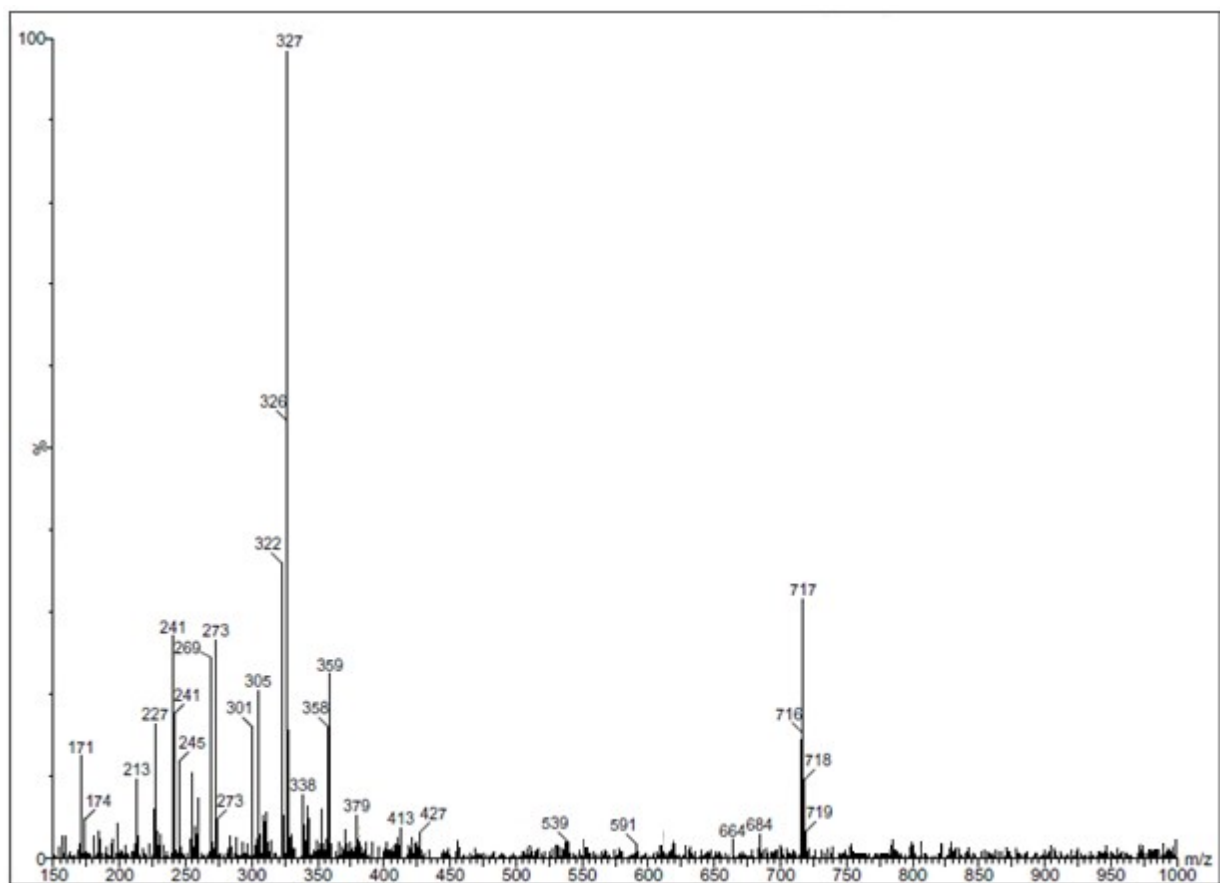


Fig. S2: Mass spectrum of uranyl complex **2**

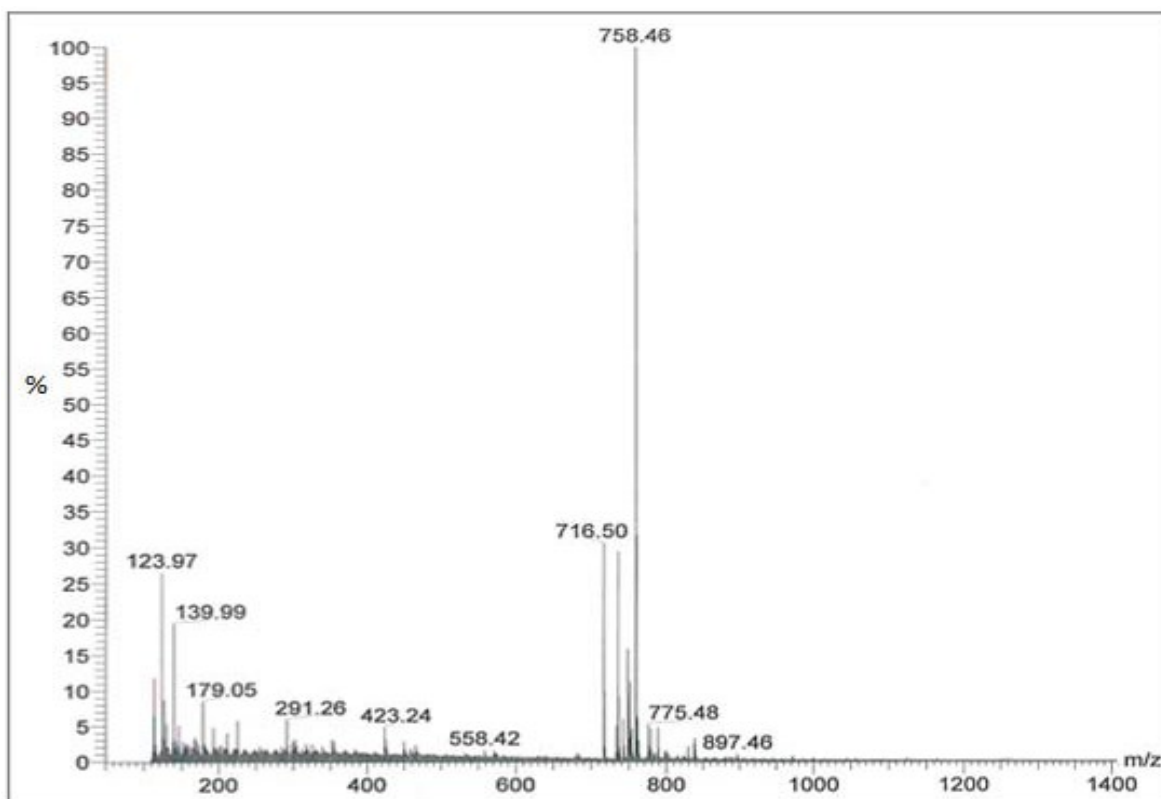


Fig. S3: Mass spectrum of uranyl complex **3**

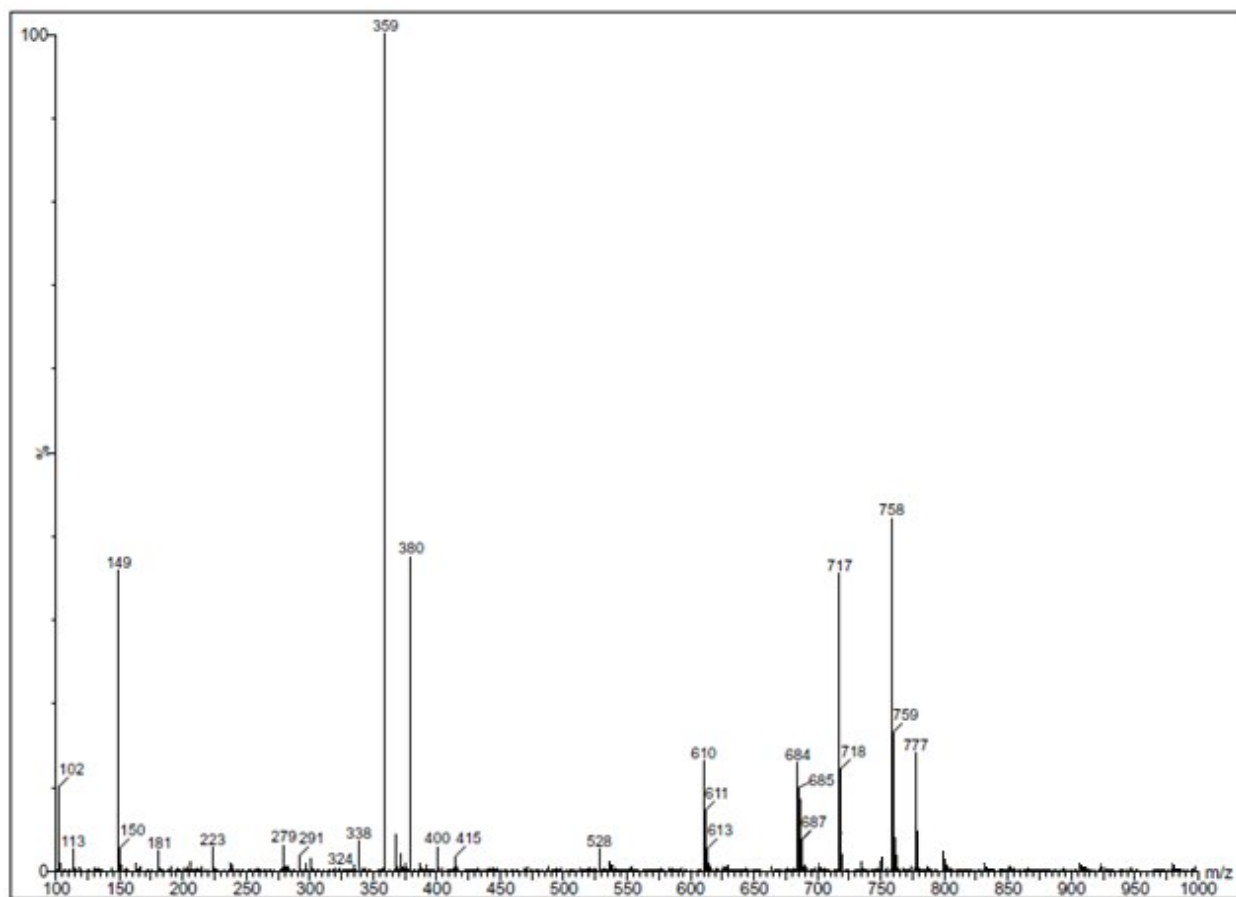
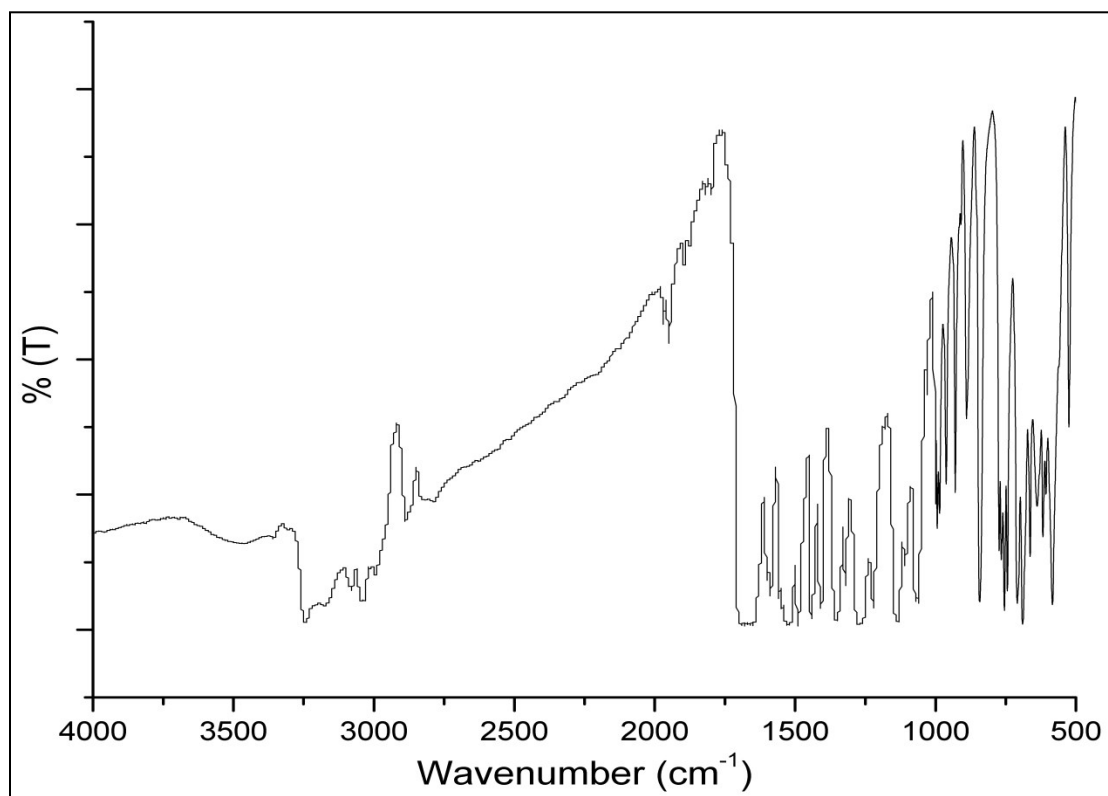


Fig. S4: FT-IR spectrum of H₂L

(a)



(b)

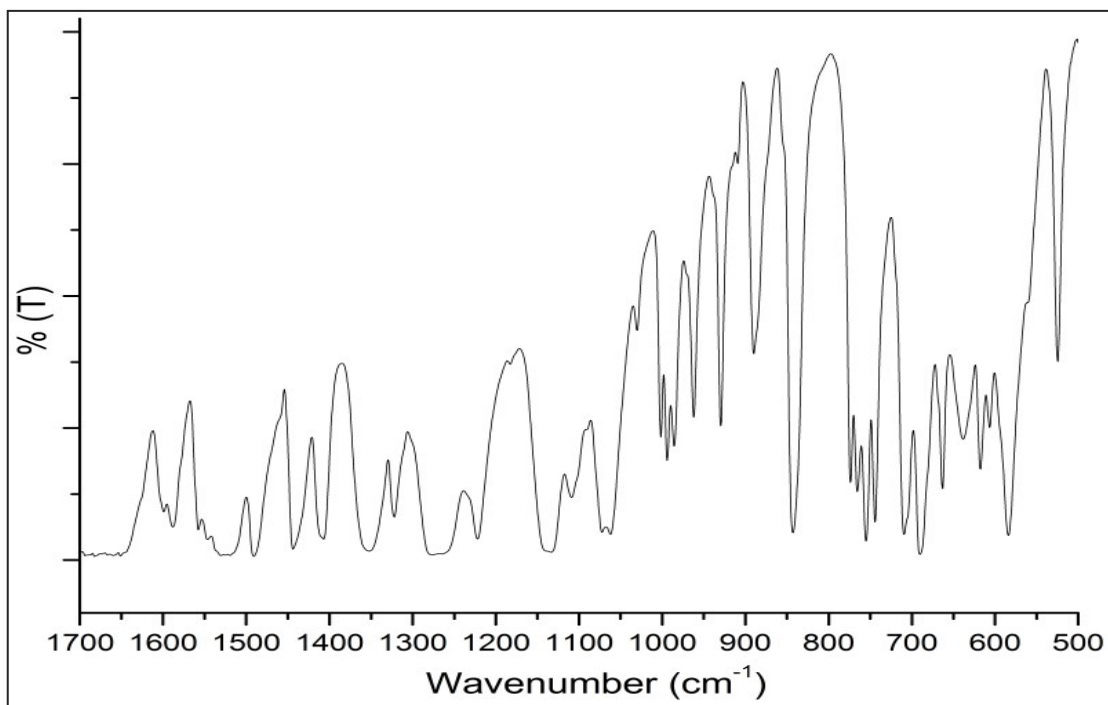
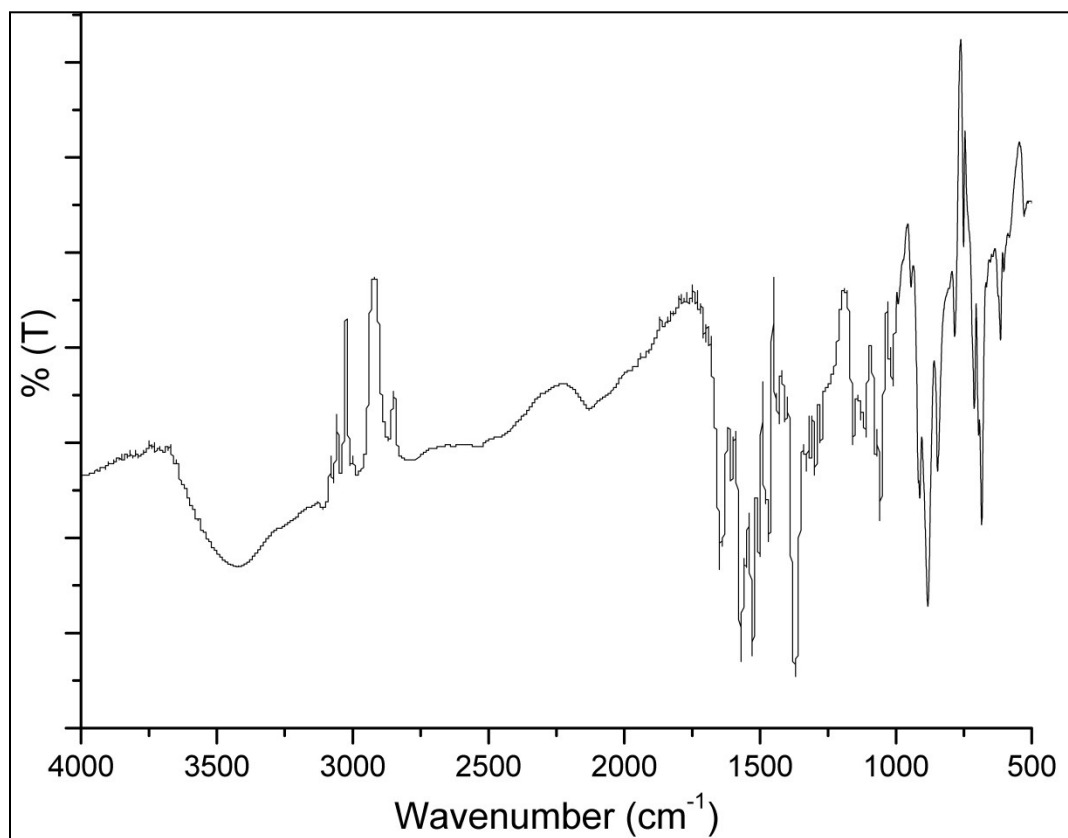


Fig. S5: FT-IR spectrum of uranyl complex **1**

(a)



(b)

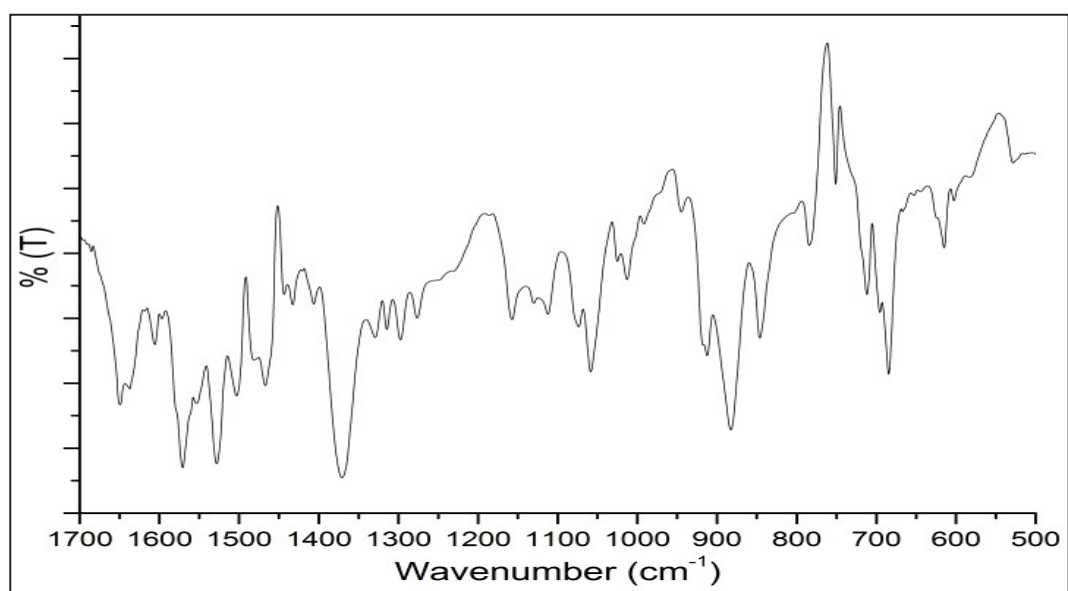
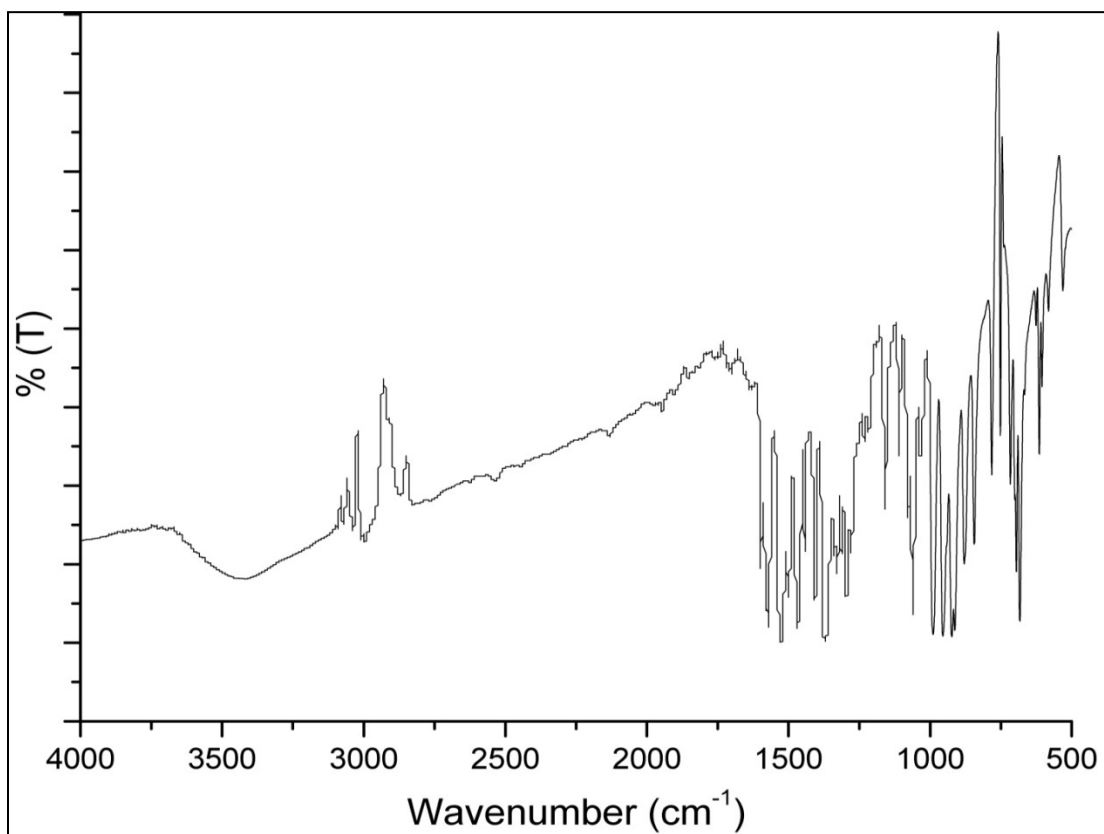


Fig. S6: FT-IR spectrum of uranyl complex **2**

(a)



(b)

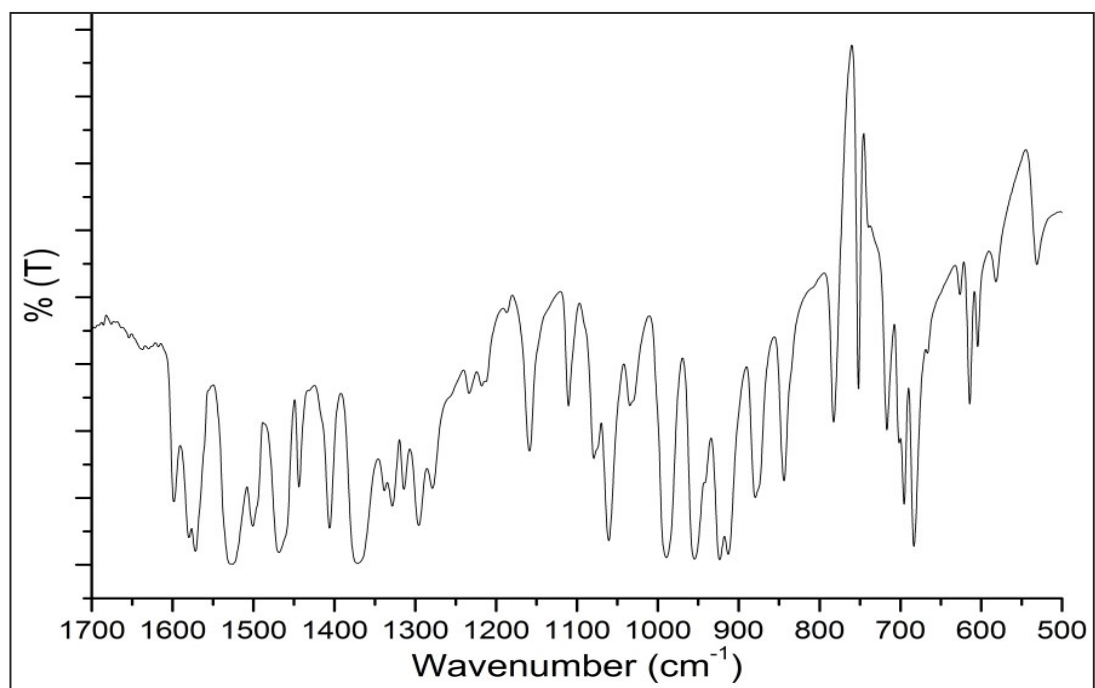
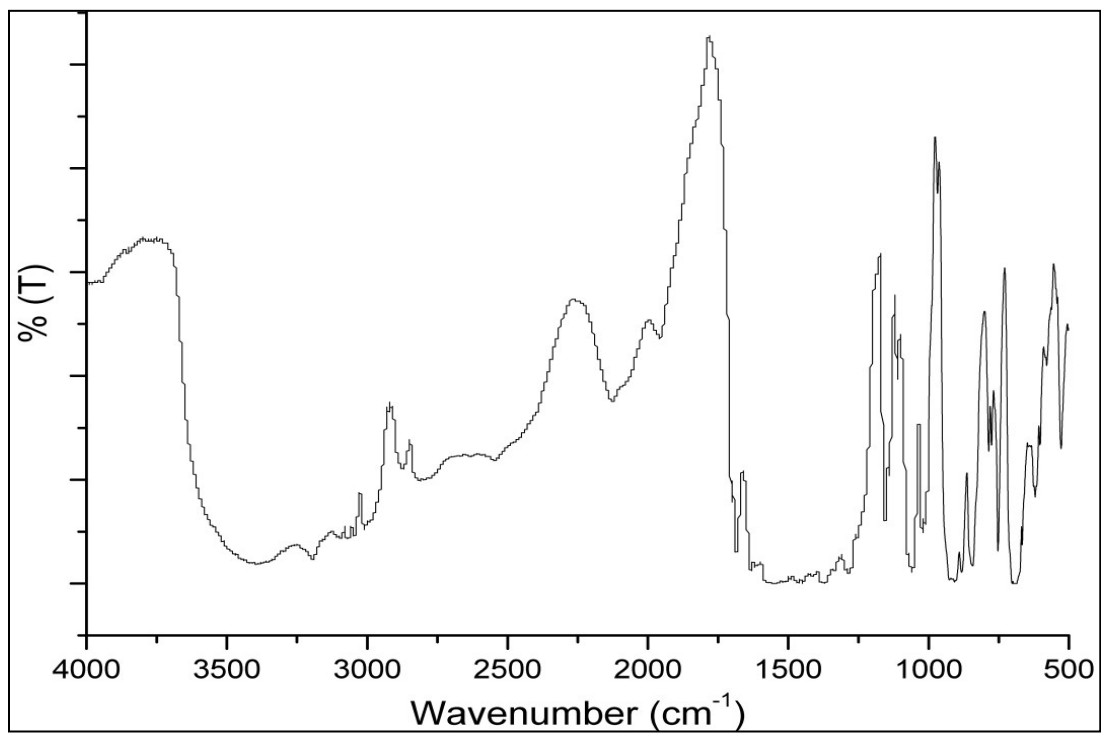


Fig. S7: FT-IR spectrum of uranyl complex **3**

(a)



(b)

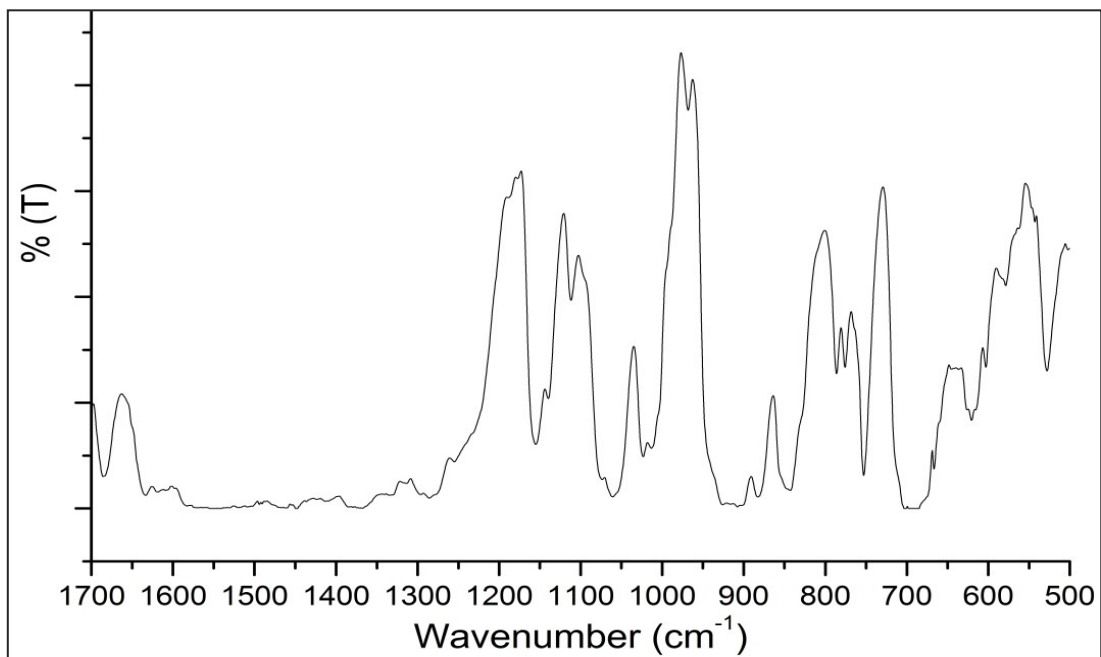


Fig. S8: Thermal decomposition diagram of 1.

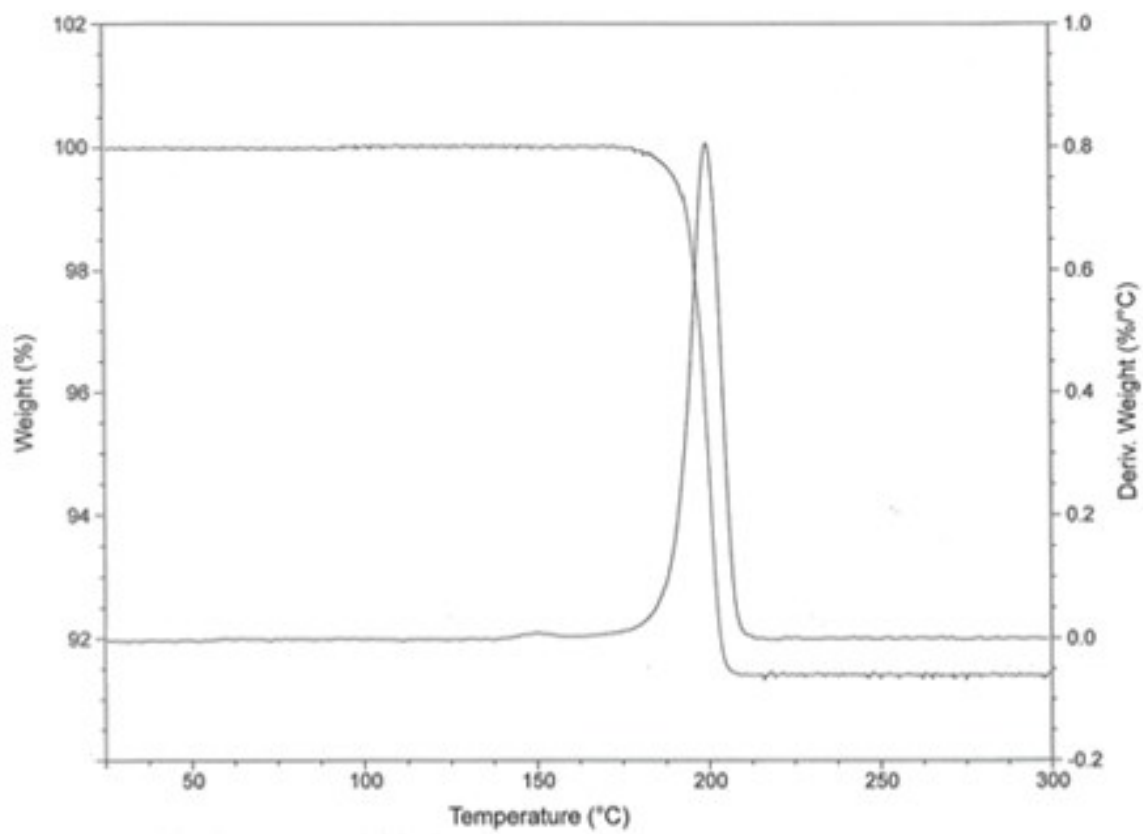


Fig. S9: Thermal decomposition diagram of **3**.

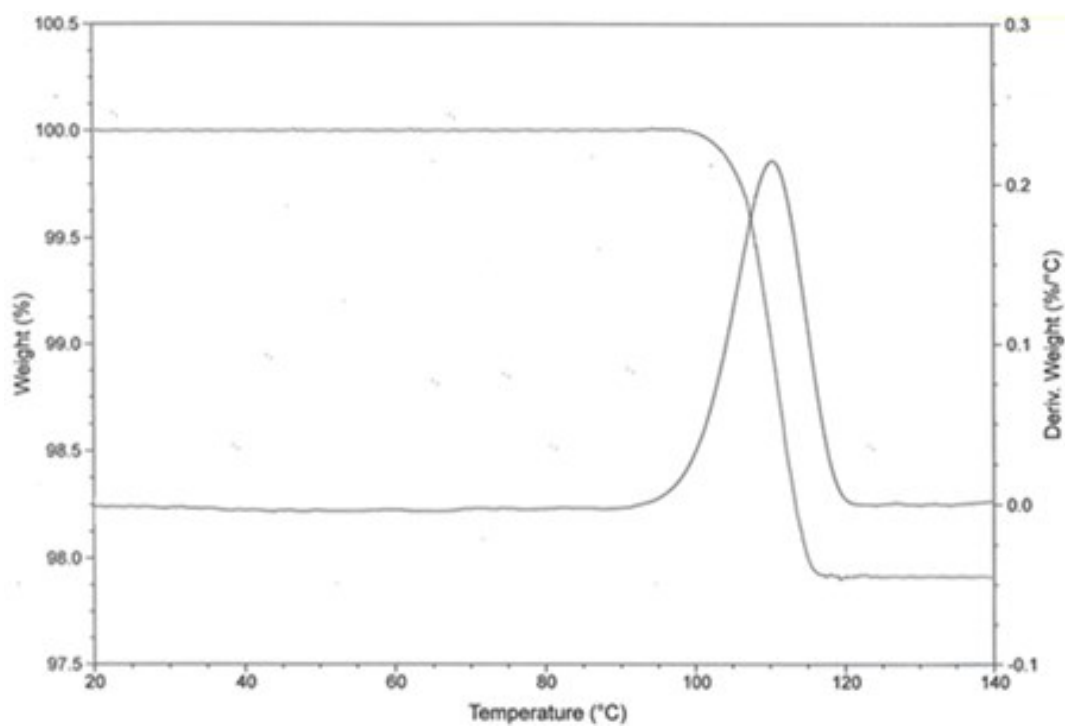


Fig. S10: Cyclic voltammogram of H_2L at its 1×10^{-3} M $CHCl_3$ solution with added ferrocene (Fc) using $[Bu_4N][ClO_4]$ (0.1M) as supporting electrolyte, scan rate: 100mV/sec, initial scan direction: cathodic.

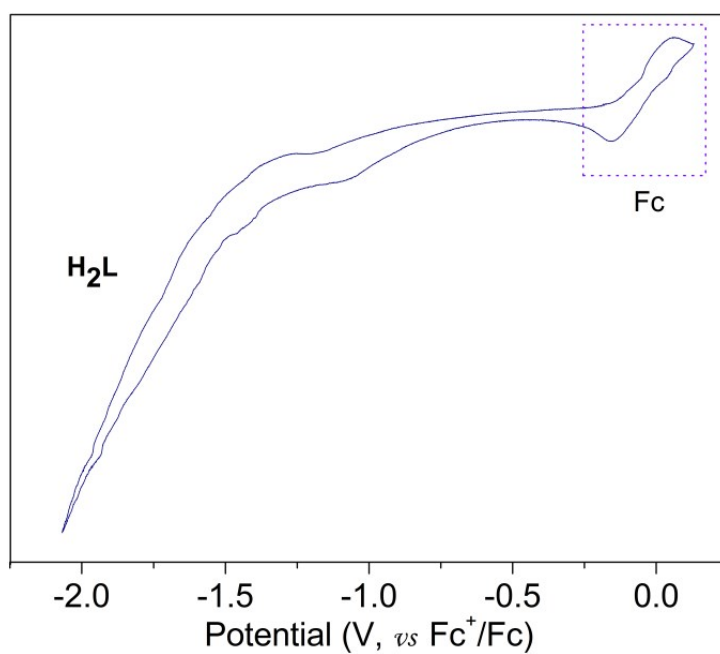


Fig. S11: Powder XRD pattern of complex 1

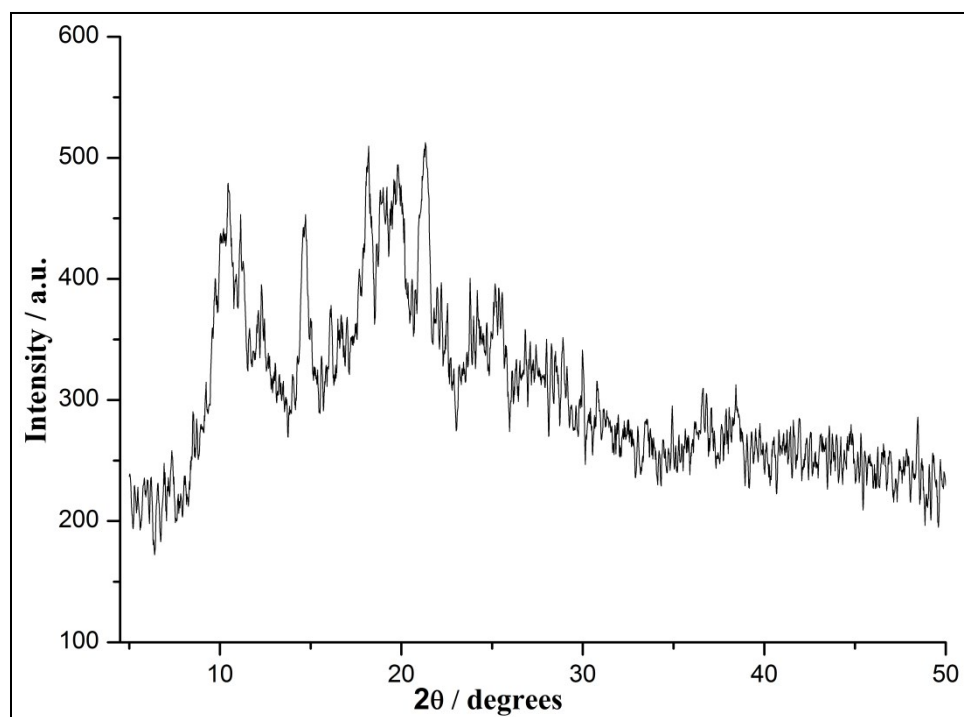


Fig. S12: Powder XRD pattern of complex 2

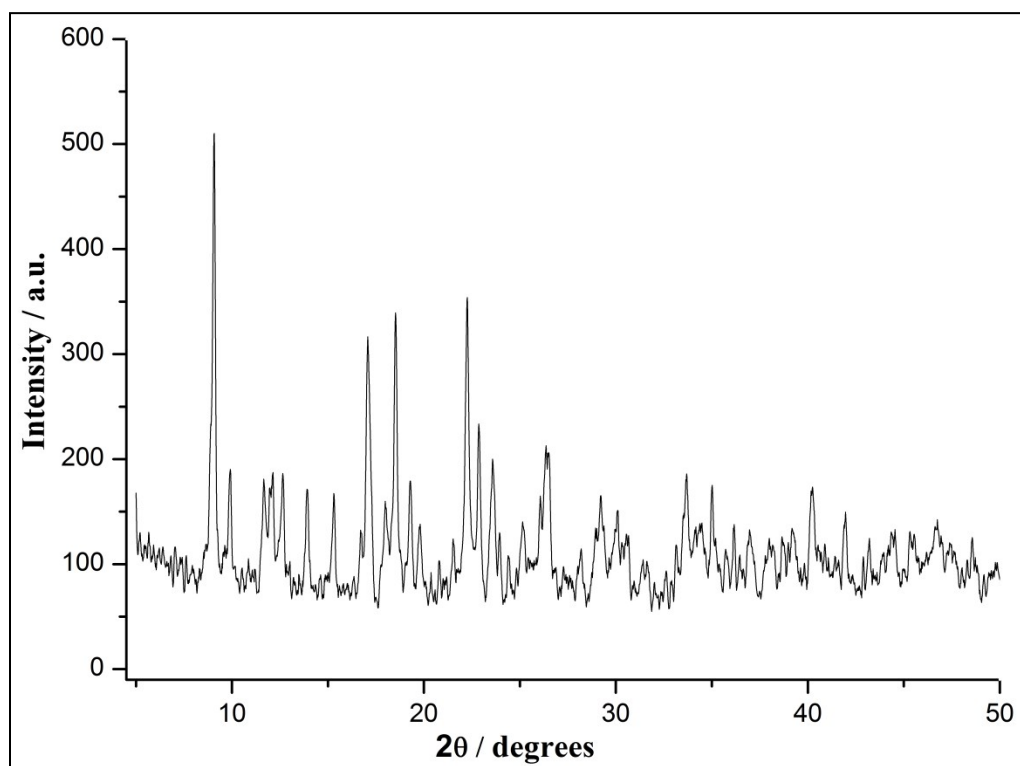


Fig. S13: Powder XRD pattern of complex **3**

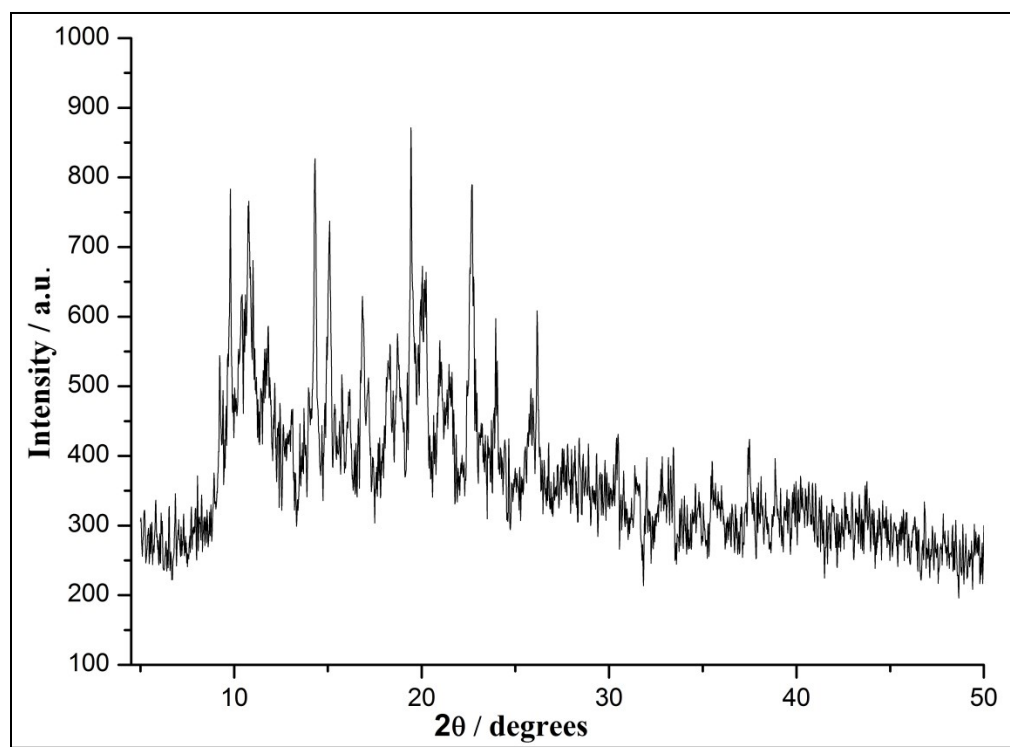
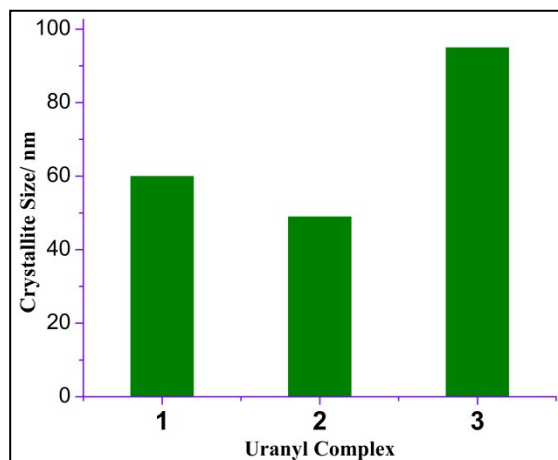
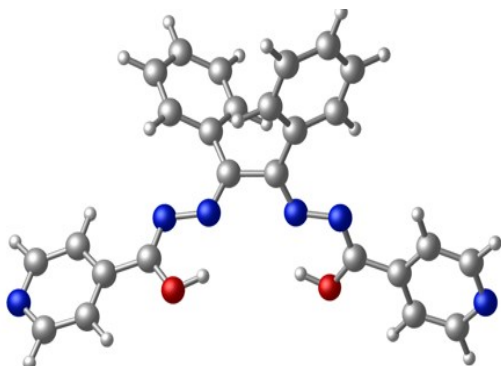


Fig. S14: Diagram showing the crystallite size of complexes **1-3**.



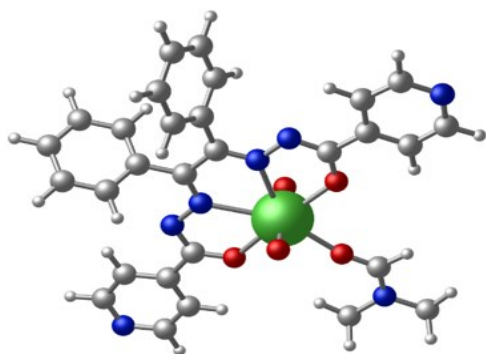
Geometry of the ligand in XYZ format



Atoms	X	Y	Z
C	-0.74092	0.7856	-0.13664
C	0.74093	0.78559	0.13664
C	-1.31048	1.93065	-0.88485
C	-0.52002	2.5611	-1.86577
C	-2.60612	2.42667	-0.64295
C	-1.01303	3.64228	-2.59428
H	0.47673	2.19363	-2.06688
C	-3.0886	3.51948	-1.3621
H	-3.22519	1.95082	0.09879
C	-2.29849	4.12799	-2.3417
H	-0.39529	4.106	-3.35129
H	-4.0823	3.89534	-1.15852
H	-2.67977	4.97225	-2.90031
C	1.3105	1.93066	0.88483
C	0.52002	2.56113	1.86572
C	2.60616	2.42665	0.64297
C	1.01302	3.64231	2.59424
H	-0.47674	2.19368	2.06679
C	3.08862	3.51946	1.36214
H	3.22528	1.95077	-0.09871
C	2.29849	4.12801	2.34169
H	0.39525	4.10605	3.35121
H	4.08235	3.8953	1.15859
H	2.67976	4.97227	2.9003
N	1.36186	-0.26506	-0.31687
N	-1.36187	-0.26505	0.31687
N	-2.74536	-0.41241	0.0437
N	2.74538	-0.41238	-0.04375
C	-3.19169	-1.51109	0.60336
C	3.19167	-1.51112	-0.60331
O	-2.40082	-2.33273	1.35273
O	2.40075	-2.33287	-1.35251
C	-4.58658	-1.93615	0.45443
C	-5.47598	-1.21437	-0.35747
C	-5.06078	-3.07634	1.11918
C	-6.79095	-1.65647	-0.46677
H	-5.13239	-0.33917	-0.88737
C	-6.3952	-3.44321	0.95067
H	-4.39958	-3.65305	1.74694
N	-7.25888	-2.75343	0.17366

H	-7.50646	-1.13064	-1.08304
H	-6.79949	-4.31442	1.44651
C	4.58657	-1.93617	-0.45442
C	5.06075	-3.07638	-1.11914
C	5.476	-1.21435	0.35741
C	6.39519	-3.44323	-0.95069
H	4.39953	-3.65313	-1.74685
C	6.79099	-1.65643	0.46667
H	5.13243	-0.33915	0.88731
N	7.2589	-2.75342	-0.17374
H	6.79945	-4.31446	-1.44651
H	7.50652	-1.13058	1.08289
H	-1.49304	-1.93905	1.34251
H	1.49297	-1.93919	-1.34231

Geometry of the uranyl complex **1** in XYZ format



Atoms	X	Y	Z
U	12.73056	9.28959	8.69726
O	14.72899	8.10764	8.40243
O	13.86953	11.13398	7.81599
O	11.86482	7.26760	9.47738
O	12.17564	8.86885	7.07651
O	13.21641	9.73580	10.33440
N	16.63024	6.99447	8.71586
N	12.06169	12.55802	8.00453
N	11.43522	11.44852	8.53588
N	10.36650	9.32509	9.53615
N	9.79752	8.15132	9.99159
N	15.53176	15.52180	5.99544
N	9.28816	3.35780	11.25018
C	10.24934	11.61282	9.02561
C	10.65925	7.16023	9.91201
C	8.24611	10.40493	10.10545
C	10.18337	5.84677	10.37847
C	13.29958	12.27344	7.66418
C	9.61984	10.39536	9.57410
C	7.18879	10.81189	9.31455
H	7.33944	11.06674	8.43304
C	9.54599	12.90902	9.09539

C	7.99335	10.03131	11.41913
H	8.68941	9.72700	11.95538
C	5.91232	10.84154	9.83120
H	5.20220	11.09515	9.28639
C	10.78190	4.68178	9.96098
H	11.50585	4.70470	9.37821
C	15.72653	7.50586	7.96291
H	15.82157	7.42287	7.04223
C	5.67572	10.50123	11.13999
H	4.81282	10.53805	11.48647
C	14.06450	13.38512	7.05937
C	6.71614	10.10800	11.92967
H	6.56227	9.89120	12.82097
C	9.04409	13.35578	10.30624
H	9.16625	12.84867	11.07633
C	15.44369	13.34186	6.96387
H	15.91275	12.59013	7.24669
C	9.36207	13.68399	7.95434
H	9.70849	13.39988	7.14017
C	9.12960	5.73541	11.27711
H	8.70243	6.49468	11.60400
C	8.72750	4.47050	11.67869
H	8.02449	4.40421	12.28227
C	13.43374	14.50396	6.55250
H	12.50549	14.56594	6.55006
C	8.17359	15.32570	9.22272
H	7.71991	16.13635	9.26680
C	10.29065	3.47902	10.42132
H	10.70082	2.70026	10.12014
C	16.11369	14.42713	6.44354
H	17.04230	14.38421	6.40559
C	16.60045	7.11837	10.15075
H	17.36539	6.67583	10.52661
H	15.79795	6.71630	10.48988
H	16.61922	8.04727	10.39194
C	14.21127	15.52708	6.04686
H	13.77156	16.27830	5.71875
C	8.66220	14.87705	8.03024
H	8.52339	15.37846	7.25893
C	8.35711	14.56382	10.36868
H	8.01760	14.86165	11.18162
C	17.75229	6.27691	8.14533
H	18.32763	5.96944	8.85053
H	18.24429	6.86129	7.56378
H	17.43002	5.52497	7.64459