

***In situ* pre-concentration during the di-(2-ethylhexyl) phosphoric acid assisted dissolution of uranium trioxide in an ionic liquid: spectroscopic, electrochemical and theoretical studies<sup>†</sup>**

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**ELECTRONIC SUPPLEMENTARY INFORMATION**

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## S1. PURIFICATION OF THE IONIC LIQUID

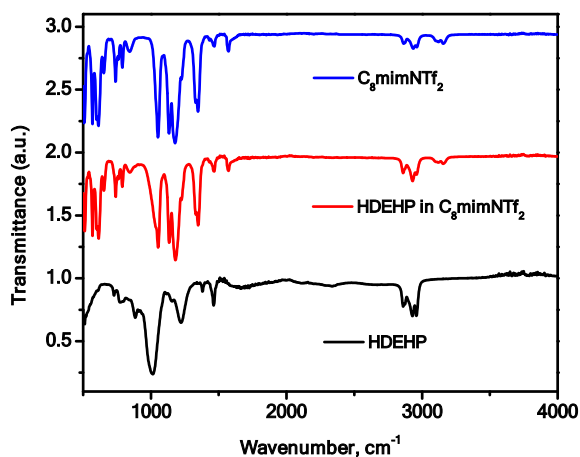
The ionic liquid,  $C_8\text{mim.NTf}_2$  was purified from colored impurities by contacting with activated carbon for 24 h.<sup>1,2</sup> Typically, 150 mg activated carbon was used for 10 mL of the ionic liquid. About 20 mL of dichloroethane (DCE) was used to make a slurry. Subsequently, the ionic liquid was filtered and the DCE was removed in a rotavap followed by drying at 50°C in vacuum before it was used for the dissolution studies.

## S2. SOLUBILITY OF HD2EHP

**Table S-1.** The resultant concentration of HD2EHP in different ionic liquids after its stepwise addition; T: 298 K.

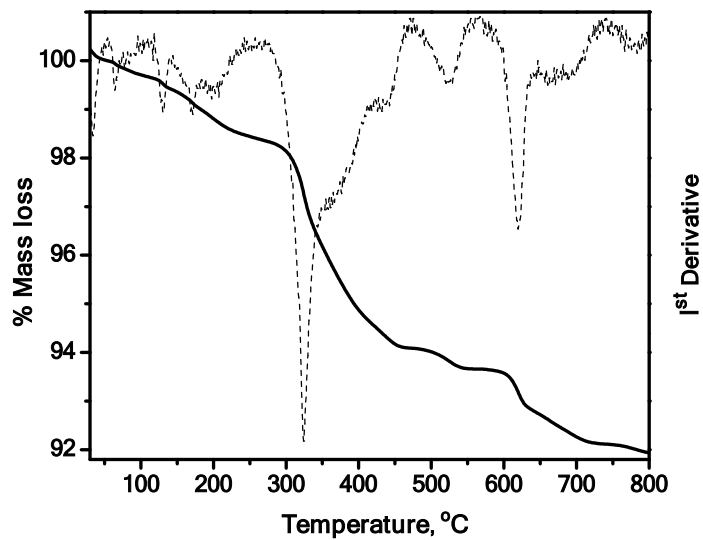
[HD2EHP], M	$C_4\text{mim.NTf}_2$	$C_6\text{mim.NTf}_2$	$C_8\text{mim.NTf}_2$
0.05	×	√	√
0.10	×	×	√
0.20	×	×	√
0.40	×	×	√
0.60	×	×	×

×Not soluble/hazy solution; √Soluble

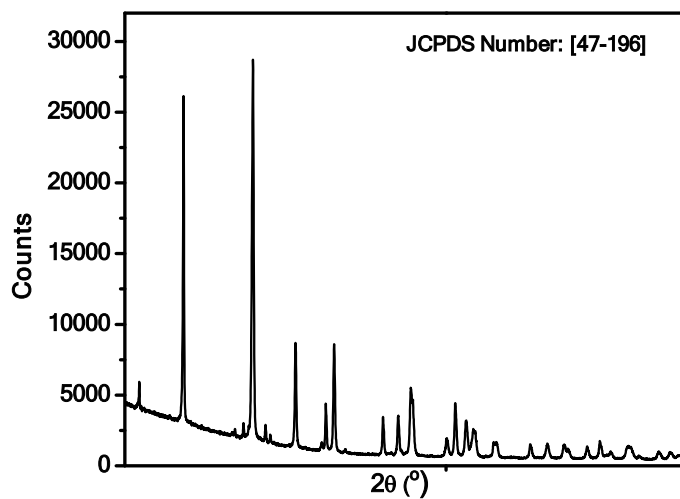


**Figure S1.** The FTIR spectra of  $C_8\text{mim.NTf}_2$ , neat HDEHP and 0.4 M HDEHP in  $C_8\text{mim.NTf}_2$

### S3. CHARACTERIZATION OF $\text{UO}_3$

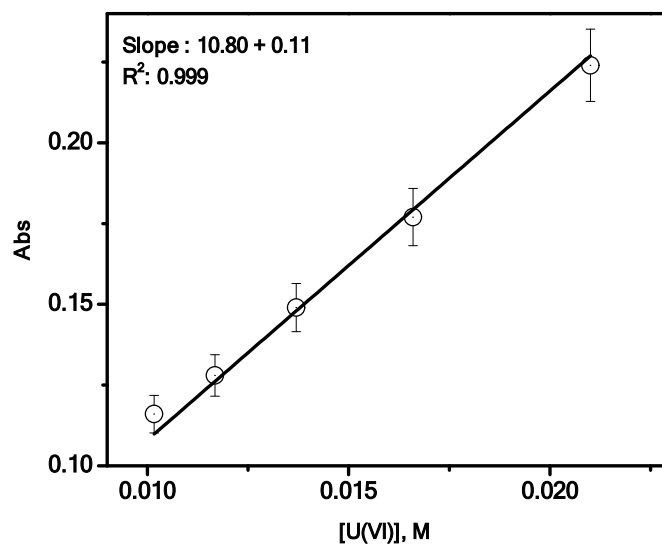


**Figure S2.** The TGA and its derivative plot for the thermal analysis of  $\text{UO}_3$ ; Heating rate:  $10\text{ }^\circ\text{C} / \text{minute}$ , inert atmosphere



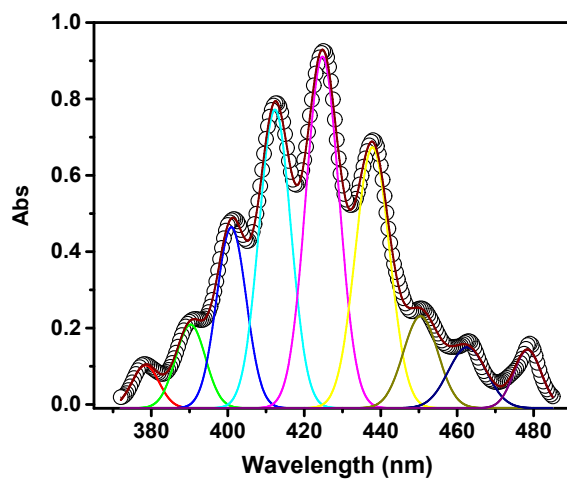
**Figure S3.** The XRD pattern for  $\text{UO}_3$ ; Instrument: Rigaku Ultima IV;  $2\theta$  range:  $10\text{-}80^\circ$

#### S4. SOLUBILITY OF $\text{UO}_3$ USING HD2EHP



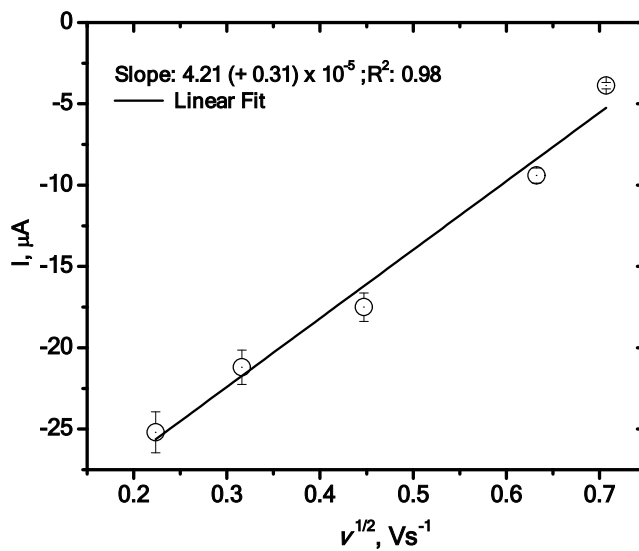
**Figure S4.** The calibration plot for the dissolved U(VI)-HD2EHP complex in  $\text{C}_8\text{mim.NTf}_2$

## S5. UV-VISIBLE SPECTROPHOTOMETRY



**Figure S5.** The peak deconvolution of the UV-Vis spectra U(VI)-H<sub>2</sub>DEHP complex in C<sub>8</sub>mim.NTf<sub>2</sub> using **multi-peak Gaussian functions**

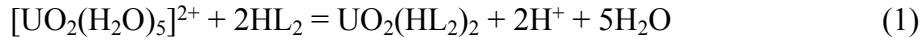
## S6. ELECTROCHEMICAL STUDIES



**Figure S6.** The linear relationship of I<sub>c</sub> variation with the square root of the scan rate at glassy carbon working electrode, Pt both as counter and reference electrode (all disk electrode with 2 mm dia), T: 298 K.

## S7. DFT STUDIES

The reaction free energy,  $\Delta G$  for the below mentioned complexation reaction can be evaluated as:



$$\Delta G = G_{\text{UO}_2(\text{HL}_2)_2} + 2G_{\text{H}^+} + 5G_{\text{H}_2\text{O}} - G_{[\text{UO}_2(\text{H}_2\text{O})_5]^{2+}} - 2G_{\text{HL}_2} \quad (2)$$

where  $G$  is the free energy of the respective chemical species. Next, we use the following standard thermodynamic relation for evaluating the free energy,  $G$ .

First, the value of enthalpy,  $H$  is obtained using  $U = E + \text{ZPE}$ , when zero point energy corrected total electronic energy ( $E$ ) of the chemical species are used.

$$H = U + RT \quad (3)$$

Here,  $T$  is the temperature and  $R$  is universal gas constant. Now, the free energy,  $G$  of the chemical species can be determined as:

$$G = H - TS \quad (4)$$

Here,  $E$  is the energy in COSMO phase and  $\text{ZPE}$  and  $S$  is evaluated at room temperature ( $T=298.15\text{K}$ ) in gas phase.

Only gas phase frequencies have been calculated to evaluate  $\text{ZPE}$  and entropy of the species as standard practice. Further it is approximated as  $S_{\text{sol}} \approx S_{\text{gas}}$ .

**Table S1:** Calculated values of energy, enthalpy, entropy and free energy of different chemical species in solution phase. The aqueous phase energy for hydrated  $[\text{UO}_2(\text{H}_2\text{O})_5]^{2+}$  and  $\text{H}_2\text{O}$  molecules is considered. All other species are in IL phase. (E is in COSMO phase and ZPE and S is evaluated in gas phase at 298.15K)

System	E(hartree)	H (kcal/mol)	S (kJ/mol)	G(kcal/mol)
solution phase				
$\text{H}_2\text{O}$	-76.42294987	-47950.98966	0.1949	-47964.89144
$[\text{UO}_2(\text{H}_2\text{O})_5]^{2+}$	-1009.458698	-633363.9233	0.559	-633403.7955
$(\text{HL})_2$	-2545.719951	-1596838.459	1.32253	-1596932.792
HL	-5717.859463	-798414.664	0.78964	-798470.9873
$\text{UO}_2(\text{HL}_2)_2$	-3172.491109	-3586772.98	2.60886	-3586959.064
$[\text{UO}_2\text{HL}_2]^+$	-3172.101661	-1990147.143	1.54592	-1990257.41
$\text{UO}_2\text{L}_2$	-1899.602279	-1989908.263	1.43289	-1990010.468
$[\text{UO}_2\text{L}]^+$	-4999.775117	-1191708.553	0.85471	-1191769.518
$\text{UO}_2\text{HL}_2\text{NTf}_2$	-3726.888205	-3136751.724	1.80533	-3136880.494
$\text{UO}_2\text{LNTf}_2$	-1827.209587	-2338313.381	1.22284	-2338400.604
$\text{NTf}_2^-$	-5717.859463	-1146557.337	0.50062	-1146593.045

## COORDINATES OF OPTIMIZED STRUCTURES

### HD2EHP (HL)

O 1.8404079 -2.0231635 1.3112930  
P 2.5003862 -2.1246523 2.8000791  
O 3.9276386 -2.8145403 2.5868383  
C 4.1011933 -4.0981300 1.9608272  
C 5.5752809 -4.3077739 1.6123905  
C 6.0522685 -3.2316526 0.6182948  
C 7.5413270 -3.2489838 0.2603771  
O 2.5366377 -0.8362966 3.5221219  
O 1.6633939 -3.3408160 3.4494614  
C 0.2805301 -3.1615051 3.8029366  
C -0.1544608 -4.2414527 4.7945049  
C 0.6963612 -4.1694129 6.0774555  
C 0.4559191 -5.2804422 7.1010020  
H 3.4781085 -4.1505560 1.0502607  
H 0.1463254 -2.1570844 4.2428356  
H -0.3228203 -3.2188469 2.8809815  
H 6.1381044 -4.1817042 2.5563822  
H 5.4574414 -3.3281338 -0.3106603  
H 8.1445339 -3.1802422 1.1847893  
H 0.0407749 -5.2145050 4.3046419

H	1.7571970	-4.1775140	5.7799756
H	1.1605755	-5.1917142	7.9437524
H	-0.5609621	-5.2479094	7.5244065
H	0.5992700	-6.2793716	6.6548209
H	1.7813182	-1.0932977	1.0457223
C	-1.6791435	-4.1126331	5.0383637
C	-2.4428737	-5.4400057	5.1354358
H	-2.1329581	-3.5250058	4.2186095
H	-1.8542825	-3.5165081	5.9524586
H	-2.2810086	-6.0170462	4.2057031
H	-2.0240974	-6.0601078	5.9470795
H	0.5247275	-3.1860575	6.5549053
H	5.7986632	-2.2442417	1.0390625
C	-3.9478263	-5.2618380	5.3613350
H	-4.3662985	-4.6474486	4.5425249
H	-4.1092755	-4.6762446	6.2850403
C	-4.7156199	-6.5820355	5.4533969
H	-4.3545692	-7.1992304	6.2938133
H	-5.7940185	-6.4131199	5.6051276
H	-4.5986542	-7.1795883	4.5334074
H	7.8101271	-4.2140999	-0.2053601
H	3.7529899	-4.8746808	2.6606711
C	7.9469651	-2.1190930	-0.6933244
C	9.4276567	-2.1455808	-1.0766080
H	7.7002743	-1.1456522	-0.2312570
H	7.3285160	-2.1804412	-1.6077515
H	10.0745233	-2.0401507	-0.1890561
H	9.6974143	-3.0963631	-1.5676576
H	9.6819128	-1.3292342	-1.7719192
C	5.7762309	-5.7618912	1.1127548
C	7.0618277	-6.4385002	1.5992249
H	5.7381630	-5.7768053	0.0084951
H	4.9223374	-6.3820221	1.4412077
H	7.1461747	-7.4636147	1.2026631
H	7.9631313	-5.8875719	1.2897389
H	7.0802985	-6.5060162	2.6998506

#### **HD2EHP-dimer (HL)<sub>2</sub>**

C	-4.9245919	4.2752089	1.0050966
C	-3.6550747	3.7685412	0.3139016
C	-3.7227140	2.3483778	-0.2792258
C	-2.3528202	1.9250875	-0.8101602
O	-1.3777779	1.9792564	0.2444902
P	0.0946510	1.3784804	0.0151567
O	0.3533412	-2.1853640	0.9121482
P	1.1758613	-1.8466782	2.2225818
O	2.7142657	-2.1987642	1.9611123
C	3.1562197	-3.4385336	1.3823897
C	4.5919067	-3.2832993	0.8766293
C	4.6688983	-2.1813048	-0.1969732



C	6.0735760	-1.7957808	-0.6717109
O	1.0261656	-0.4466036	2.7384386
O	0.7190754	2.3812250	-1.0760819
O	0.7444044	-2.9850029	3.2701884
C	-0.5610281	-2.9677577	3.8769900
C	-0.6278149	-4.0077274	4.9952439
C	0.4461822	-3.7298766	6.0644431
C	0.5703115	-4.7856260	7.1644696
H	-2.0333226	2.5956193	-1.6291524
H	2.4780090	-3.7211423	0.5579442
H	-0.7592442	-1.9555145	4.2718435
H	-1.3122937	-3.1895683	3.0999943
H	-3.9728494	1.6443702	0.5369217
H	-3.3766396	4.4721396	-0.4945287
H	-5.7552589	4.3425897	0.2792946
H	-5.2465876	3.5415585	1.7679161
H	5.1928259	-2.9581361	1.7469242
H	4.0638960	-2.4988542	-1.0687119
H	6.6987673	-1.5347158	0.2031102
H	-0.4016829	-4.9849493	4.5277759
H	1.4165457	-3.6254289	5.5530637
H	1.4015281	-4.5427497	7.8459446
H	-0.3417414	-4.8601473	7.7787403
H	0.7703021	-5.7858177	6.7436692
H	0.2190158	-1.3671138	0.3135448
O	0.8429896	1.6812241	1.3583114
O	0.1052722	-0.0518711	-0.4627570
H	0.9331613	0.8619343	1.9674114
C	-2.0720835	-4.0531182	5.5559223
C	-2.6237497	-5.4610454	5.8150286
H	-2.7585707	-3.5461105	4.8525770
H	-2.1215039	-3.4593318	6.4864830
H	-2.6229781	-6.0273310	4.8649155
H	-1.9465775	-6.0128734	6.4905846
H	0.2368829	-2.7443414	6.5218515
H	-2.8223066	3.7949407	1.0364232
H	4.1741753	-1.2817917	0.2059479
C	-4.0379129	-5.4652771	6.4043938
H	-4.7125724	-4.9014753	5.7336495
H	-4.0335474	-4.9080631	7.3591634
C	-4.6020698	-6.8685836	6.6343120
H	-3.9678754	-7.4477041	7.3270538
H	-5.6160538	-6.8321374	7.0644867
H	-4.6610533	-7.4368767	5.6905030
H	-2.3953144	0.8959007	-1.2046609
H	6.5675248	-2.6605051	-1.1500925
H	3.1020831	-4.2212384	2.1574941
C	1.5257857	1.9284890	-2.1782109
C	2.3373849	3.0961767	-2.7449251
H	0.8593547	1.5065451	-2.9514375
H	2.1934702	1.1186388	-1.8437739

C	3.2501620	2.5196032	-3.8507083
H	2.9813920	3.4553958	-1.9203456
C	4.2802726	3.4541063	-4.5166567
H	3.8002419	1.6732906	-3.4030199
H	2.6149839	2.0700625	-4.6381352
H	5.1575405	2.8477696	-4.8060036
H	4.6624800	4.1803546	-3.7760522
C	3.7976133	4.1926858	-5.7727791
C	4.8781205	5.0691356	-6.4084576
H	2.9165446	4.8127271	-5.5389221
H	3.4490746	3.4458287	-6.5095359
H	5.2283216	5.8469336	-5.7083126
H	5.7586847	4.4723312	-6.7019990
C	-4.7422573	5.6439216	1.6708691
C	-6.0072422	6.1650167	2.3549286
H	-4.4055663	6.3740311	0.9118431
H	-3.9212286	5.5805384	2.4083959
H	-6.8357744	6.2786013	1.6349288
H	-6.3504536	5.4740737	3.1439202
C	6.0753290	-0.6214127	-1.6574005
C	7.4730361	-0.2234788	-2.1353336
H	5.5854988	0.2488505	-1.1830042
H	5.4467316	-0.8805600	-2.5298951
H	8.1151193	0.0781534	-1.2902856
H	7.9765918	-1.0612268	-2.6472946
H	7.4347828	0.6223860	-2.8408898
H	4.5061491	5.5794397	-7.3117030
H	-5.8392260	7.1478358	2.8246088
C	-4.7697143	2.1812768	-1.4103941
C	-6.1327168	1.6464022	-0.9594025
H	-4.3713466	1.4884802	-2.1740131
H	-4.8982979	3.1470661	-1.9317103
H	-6.8238444	1.5530454	-1.8131323
H	-6.0333678	0.6471921	-0.5028511
H	-6.6111464	2.3011187	-0.2149025
C	1.4121430	4.2625965	-3.1668989
C	2.0070110	5.6622213	-2.9820657
H	0.4977766	4.2101258	-2.5555403
H	1.0889920	4.1164571	-4.2139327
H	1.2845371	6.4398528	-3.2796359
H	2.2642562	5.8391836	-1.9242994
H	2.9219443	5.8204283	-3.5730428
C	5.1177907	-4.6633018	0.4045903
C	6.5764567	-4.9571443	0.7704288
H	4.9792476	-4.7511412	-0.6882044
H	4.4907962	-5.4615137	0.8418691
H	6.8866023	-5.9483453	0.4011501
H	7.2679152	-4.2130560	0.3464429
H	6.7183264	-4.9516636	1.8643279

**NTf<sub>2</sub>**

N	-0.0422321	-0.6540294	0.1100049
S	-1.6319565	-0.4915656	0.0057535
S	1.0461132	0.2758391	-0.6351407
O	0.8634749	0.4836164	-2.0760928
C	2.4769175	-0.9354038	-0.5169410
O	1.4776121	1.4176604	0.1839474
O	-2.1659494	-0.1315432	-1.3119960
O	-2.2541284	-1.5817991	0.7607508
F	2.2448793	-2.0373009	-1.2346516
F	3.5752883	-0.3437134	-1.0109263
F	2.7368381	-1.2967849	0.7406518
C	-2.0009963	1.0358239	1.0485953
F	-3.3120282	1.0816190	1.3316270
F	-1.3308558	1.0278043	2.2018622
F	-1.6829766	2.1497773	0.3825555

### **UO<sub>2</sub>(HL<sub>2</sub>)<sub>2</sub>**

C	-5.4023621	3.1765064	0.7217212
C	-4.0125512	2.9738923	0.1099258
C	-3.8712976	1.8102234	-0.8893697
C	-2.4062879	1.6255802	-1.2917523
O	-1.6145068	1.3756041	-0.1254658
P	-0.0318935	1.0959554	-0.1978923
O	1.7103163	-2.3611651	0.5033391
P	2.3869267	-1.8169330	1.7669924
O	3.8991708	-2.2846982	1.9263982
C	4.2908107	-3.6658160	2.0252740
C	5.8159430	-3.7669159	1.9791519
C	6.3554853	-3.1972409	0.6531514
C	7.8791389	-3.0920977	0.5330535
O	2.4436786	-0.2787502	1.8797189
O	0.6069286	2.4587150	-0.7814665
O	1.6788188	-2.4729895	3.0522642
C	0.2572817	-2.3205398	3.2661285
C	-0.0939214	-2.7235317	4.6972379
C	0.6541669	-1.8471287	5.7194280
C	0.4940341	-2.2721154	7.1798713
H	-2.0356227	2.5342227	-1.8030374
H	3.8373813	-4.2352078	1.1941450
H	-0.0305205	-1.2721868	3.0701254
H	-0.2728144	-2.9610895	2.5424141
H	-4.1702654	0.8768945	-0.3759117
H	-3.6979761	3.9087607	-0.3937057
H	-6.1348959	3.4316089	-0.0649332
H	-5.7519434	2.2245158	1.1641791
H	6.1915972	-3.1351326	2.8060982
H	5.9660746	-3.8172546	-0.1773993
H	8.2752395	-2.5129630	1.3883878
H	0.2555716	-3.7663357	4.8215237

H	1.7244411	-1.8500939	5.4573583
H	1.0960118	-1.6301074	7.8430357
H	-0.5512989	-2.2039933	7.5224891
H	0.8267527	-3.3126193	7.3359824
O	0.4148729	0.8824905	1.2343239
O	0.2530790	-0.0365576	-1.2075791
H	1.5489154	0.2821765	1.5787479
C	-1.6356992	-2.6973726	4.8664237
C	-2.2266944	-3.9273724	5.5666499
H	-2.1187073	-2.6044205	3.8762613
H	-1.9283282	-1.7843047	5.4155564
H	-1.9760906	-4.8304713	4.9784272
H	-1.7421786	-4.0676064	6.5497080
H	0.3148930	-0.8012716	5.5983066
H	-3.2872591	2.8097179	0.9238580
H	5.9201945	-2.1942917	0.5108318
C	-3.7450232	-3.8550484	5.7576036
H	-4.2278042	-3.7015541	4.7746098
H	-3.9923115	-2.9580384	6.3548804
C	-4.3378864	-5.0948118	6.4298078
H	-3.9011487	-5.2569103	7.4301715
H	-5.4291327	-5.0052487	6.5546082
H	-4.1450044	-6.0044153	5.8358915
H	-2.3063663	0.7736880	-1.9856518
H	8.3413159	-4.0932744	0.6047229
H	3.9035762	-4.0686070	2.9750761
C	1.2168876	2.6007326	-2.0734298
C	1.7951179	4.0128273	-2.2086015
H	0.4628832	2.4195812	-2.8610360
H	2.0085592	1.8438019	-2.1902593
C	2.5867550	4.0598419	-3.5347274
H	2.5141012	4.1323792	-1.3763800
C	3.3719212	5.3430585	-3.8746038
H	3.3013478	3.2187038	-3.5094617
H	1.8968198	3.8331946	-4.3702946
H	4.2762681	5.0564729	-4.4409672
H	3.7486086	5.8094400	-2.9462016
C	2.6137352	6.3823756	-4.7125814
C	3.4431011	7.6300225	-5.0202722
H	1.6815355	6.6801605	-4.2039111
H	2.2967588	5.9080793	-5.6596440
H	3.7394495	8.1532266	-4.0950611
H	4.3695150	7.3732347	-5.5620003
C	-5.4340591	4.2701137	1.7956737
C	-6.8180765	4.4842636	2.4108421
H	-5.0741828	5.2191725	1.3571761
H	-4.7098337	4.0165250	2.5911550
H	-7.5573951	4.7768723	1.6458401
H	-7.1907411	3.5635518	2.8914196
C	8.3358745	-2.4341300	-0.7741086
C	9.8556194	-2.3131604	-0.8999759

H	7.8756569	-1.4326751	-0.8561634
H	7.9403918	-3.0145179	-1.6283713
H	10.2781589	-1.6975922	-0.0875782
H	10.3437676	-3.3016161	-0.8502395
H	10.1475999	-1.8468542	-1.8550791
H	2.8822229	8.3469986	-5.6415984
H	-6.8029983	5.2757732	3.1777554
C	-4.7312149	1.9643806	-2.1695800
C	-6.0963540	1.2703387	-2.1219010
H	-4.1743326	1.5543945	-3.0321971
H	-4.8634019	3.0386620	-2.3923682
H	-6.6520202	1.4229949	-3.0617691
H	-5.9803732	0.1831903	-1.9777361
H	-6.7249668	1.6456262	-1.3001704
C	0.6874664	5.0783753	-2.0346266
C	1.1392009	6.3987183	-1.4020545
H	-0.0897529	4.6514581	-1.3809117
H	0.2004337	5.2650183	-3.0097700
H	0.2863545	7.0858073	-1.2758842
H	1.5707255	6.2230598	-0.4024438
H	1.8988398	6.9250706	-1.9994859
C	6.2317883	-5.2347425	2.2560870
C	7.4727159	-5.3996465	3.1396389
H	6.3836867	-5.7569899	1.2941444
H	5.3947172	-5.7646208	2.7463161
H	7.7100874	-6.4648538	3.2945630
H	8.3608864	-4.9216638	2.6995018
H	7.3139278	-4.9474189	4.1331204
U	1.1490542	-2.0926197	-1.7485551
O	2.7361741	-1.3440093	-2.0145643
O	-0.4331797	-2.8499641	-1.4752292
C	2.2397354	0.2998248	-10.2479356
C	1.4088407	-0.1509888	-9.0423271
C	1.6506703	0.6090677	-7.7245287
C	0.8771287	-0.0481829	-6.5784873
O	1.2786984	-1.4156819	-6.4474794
P	0.5702643	-2.4291106	-5.4186834
O	2.0435648	-4.1970246	-2.2379239
P	2.0789876	-5.5562890	-2.9399596
O	1.6847232	-6.7696933	-1.9921456
C	2.4268517	-7.1235915	-0.8103428
C	1.6066110	-8.1035283	0.0292169
C	0.2844769	-7.4525283	0.4777842
C	-0.7111703	-8.3657889	1.1996524
O	1.1248474	-5.7003201	-4.1508177
O	-0.9808303	-2.4349618	-5.8697139
O	3.5936402	-5.8998977	-3.3477173
C	4.3495402	-5.0105983	-4.2046054
C	5.5610123	-5.7488594	-4.7714256
C	5.1261602	-6.9776466	-5.5921005
C	6.2665471	-7.8718529	-6.0813169

H	-0.2099422	0.0008918	-6.7767931
H	2.6556132	-6.2113310	-0.2305396
H	3.6971315	-4.6435563	-5.0167137
H	4.6695734	-4.1436880	-3.6035187
H	2.7229888	0.5189838	-7.4675091
H	0.3330258	-0.0803539	-9.2953485
H	1.9937604	1.3434127	-10.5150586
H	3.3123646	0.3004439	-9.9762827
H	1.3667210	-8.9526416	-0.6377167
H	0.5241729	-6.5890487	1.1279068
H	-0.9119083	-9.2567125	0.5751530
H	6.1438202	-6.1079577	-3.9018074
H	4.4369649	-7.5767930	-4.9753340
H	5.8719209	-8.7544964	-6.6100779
H	6.9382795	-7.3476238	-6.7805336
H	6.8812482	-8.2375498	-5.2410950
O	1.2062011	-3.7811467	-5.6574382
O	0.6449769	-1.8599534	-3.9838561
H	1.1092892	-4.8666630	-4.8338653
C	6.4340149	-4.7452490	-5.5692737
C	7.9389036	-4.8323793	-5.2851961
H	6.1068782	-3.7118661	-5.3520609
H	6.2529558	-4.8831071	-6.6506159
H	8.1134547	-4.6363659	-4.2101109
H	8.2954667	-5.8627613	-5.4626497
H	4.5325219	-6.6275584	-6.4571533
H	1.6063047	-1.2194407	-8.8561781
H	-0.2079910	-7.0313303	-0.4143452
C	8.7774970	-3.8575100	-6.1176989
H	8.4096816	-2.8282945	-5.9502514
H	8.6111950	-4.0626097	-7.1913720
C	10.2750421	-3.9205559	-5.8115329
H	10.6820373	-4.9284071	-6.0019327
H	10.8453895	-3.2099951	-6.4313648
H	10.4796355	-3.6778487	-4.7547468
H	1.0787376	0.4797656	-5.6305205
H	-0.2724130	-8.7466629	2.1394480
H	3.3779552	-7.5813800	-1.1268461
C	-2.0856899	-2.0317700	-5.0452409
C	-3.3979727	-2.4844738	-5.6923947
H	-2.0730812	-0.9317801	-4.9339844
H	-1.9776550	-2.4682915	-4.0400328
C	-4.5342955	-2.1625207	-4.6956840
H	-3.3298263	-3.5841631	-5.7900662
C	-5.9667810	-2.6161622	-5.0433511
H	-4.2541701	-2.6243812	-3.7330825
H	-4.5433201	-1.0719348	-4.5044606
H	-6.4920945	-2.8551939	-4.1011387
H	-5.9332116	-3.5674816	-5.6045462
C	-6.8229061	-1.5917141	-5.8011410
C	-8.2355395	-2.0934441	-6.1059841

H	-6.3287835	-1.2993219	-6.7427114
H	-6.8824181	-0.6675240	-5.1975302
H	-8.2128803	-2.9944571	-6.7424929
H	-8.7758635	-2.3595261	-5.1813654
C	2.0364679	-0.5853191	-11.4833256
C	2.8585755	-0.1442829	-12.6954060
H	0.9632823	-0.5954261	-11.7491563
H	2.2891182	-1.6298724	-11.2247750
H	2.6007325	0.8834494	-13.0034951
H	3.9397186	-0.1590571	-12.4748219
C	-2.0381351	-7.6699829	1.5235162
C	-3.0441963	-8.5718674	2.2405099
H	-2.4843590	-7.2874743	0.5876913
H	-1.8360521	-6.7770431	2.1438280
H	-3.3005489	-9.4538142	1.6289391
H	-2.6411163	-8.9428681	3.1983379
H	-3.9828318	-8.0374923	2.4598580
H	-8.8319237	-1.3303591	-6.6320695
H	2.6883308	-0.8031620	-13.5623171
C	1.2847286	2.1135948	-7.7825003
C	2.4516222	3.0533231	-8.1013847
H	0.8601180	2.4218323	-6.8093700
H	0.4717508	2.2618826	-8.5160382
H	2.1186661	4.1039267	-8.1280596
H	3.2420195	2.9747617	-7.3360213
H	2.9141073	2.8271463	-9.0742935
C	-3.5451165	-1.8906468	-7.1131025
C	-4.2981938	-2.7702129	-8.1164381
H	-2.5330691	-1.7270937	-7.5161807
H	-4.0148166	-0.8919064	-7.0475040
H	-4.3237061	-2.2974751	-9.1120710
H	-3.7985982	-3.7469783	-8.2279545
H	-5.3397634	-2.9667766	-7.8202367
C	2.4832284	-8.6295624	1.1951264
C	2.3072149	-10.1180254	1.5124963
H	2.2853721	-8.0270408	2.0999384
H	3.5492314	-8.4578612	0.9579605
H	2.9558577	-10.4251536	2.3491492
H	1.2702597	-10.3627510	1.7887949
H	2.5712758	-10.7416731	0.6418782

**[UO<sub>2</sub>-HL<sub>2</sub>]<sup>+</sup>**

C	-5.1471617	3.1697008	0.6066596
C	-3.8026301	2.9265325	-0.0863318
C	-3.7484923	1.7213163	-1.0446864
C	-2.3231505	1.4917947	-1.5414846
O	-1.4547036	1.2170497	-0.4064988
P	0.1022082	0.9785877	-0.4505072
O	1.7494378	-2.7104877	0.4205249
P	2.3648831	-2.0874256	1.7731175

O	3.8238221	-2.6517035	1.9501757
C	4.1661533	-4.0427095	2.2082754
C	5.6345912	-4.2799652	1.8624248
C	5.9074010	-3.9533001	0.3811571
C	7.3693535	-4.0277598	-0.0710688
O	2.3664626	-0.5826650	1.6996764
O	0.8301541	2.2154586	-1.1094026
O	1.5301392	-2.7337446	2.9595779
C	0.1431281	-2.3838053	3.2340350
C	-0.2607692	-2.8819234	4.6183248
C	0.6246992	-2.2626545	5.7163466
C	0.3734634	-2.7982566	7.1266235
H	-1.9457011	2.3842067	-2.0694276
H	3.5089886	-4.6942097	1.6059408
H	0.0352535	-1.2880726	3.1594871
H	-0.4805561	-2.8561307	2.4574136
H	-4.0303116	0.8122822	-0.4813765
H	-3.5146141	3.8348237	-0.6504924
H	-5.9329478	3.3673847	-0.1432452
H	-5.4574161	2.2501743	1.1379485
H	6.2193221	-3.5777105	2.4848390
H	5.3012361	-4.6394871	-0.2447914
H	7.9897558	-3.3969961	0.5919286
H	-0.0970895	-3.9757434	4.6183163
H	1.6811600	-2.4335060	5.4507247
H	1.0770284	-2.3485729	7.8447533
H	-0.6438421	-2.5708524	7.4826095
H	0.5070911	-3.8921296	7.1727721
O	0.5158449	0.8633165	1.0240799
O	0.4236773	-0.3138254	-1.2884473
H	1.3602134	0.2725318	1.3238200
C	-1.7770380	-2.6101467	4.8106229
C	-2.5752890	-3.7869094	5.3865705
H	-2.2343896	-2.3325136	3.8421428
H	-1.9082650	-1.7217721	5.4535939
H	-2.4747347	-4.6562245	4.7095223
H	-2.1331548	-4.1046775	6.3472084
H	0.4809018	-1.1657475	5.7054879
H	-3.0293081	2.7906051	0.6885334
H	5.5333001	-2.9351563	0.1778384
C	-4.0607582	-3.4730481	5.5904891
H	-4.4945355	-3.1340941	4.6312884
H	-4.1577640	-2.6153834	6.2811874
C	-4.8681475	-4.6562469	6.1268703
H	-4.4853874	-4.9937271	7.1045880
H	-5.9292673	-4.3922313	6.2593591
H	-4.8235253	-5.5185173	5.4399953
H	-2.2795548	0.6244943	-2.2200321
H	7.7522524	-5.0573693	0.0420165
H	3.9694374	-4.2380305	3.2729214
C	1.2069972	2.4261612	-2.4999023



C	1.6101297	3.8870997	-2.6994833
H	0.3566230	2.1606013	-3.1510832
H	2.0478990	1.7511461	-2.7228907
C	2.2072882	4.0004562	-4.1222707
H	2.4195865	4.0831835	-1.9721983
C	2.8180415	5.3511551	-4.5498242
H	2.9977595	3.2330575	-4.2022370
H	1.4351155	3.7095845	-4.8601317
H	3.6364147	5.1399939	-5.2599720
H	3.3046994	5.8330022	-3.6826080
C	1.8607593	6.3383985	-5.2317501
C	2.5577777	7.6166546	-5.7022227
H	1.0317901	6.6049607	-4.5550992
H	1.3909682	5.8353373	-6.0968405
H	3.0164092	8.1591559	-4.8582391
H	3.3602641	7.3936704	-6.4251230
C	-5.1078817	4.3379830	1.5987812
C	-6.4404420	4.5804167	2.3089299
H	-4.8019220	5.2558270	1.0636819
H	-4.3169370	4.1509036	2.3480010
H	-7.2465715	4.7975624	1.5882145
H	-6.7503083	3.6985129	2.8947647
C	7.5710862	-3.5798573	-1.5236778
C	9.0252750	-3.6521979	-1.9916932
H	7.1971216	-2.5451811	-1.6374274
H	6.9401113	-4.2028409	-2.1855858
H	9.6792592	-3.0199782	-1.3679973
H	9.4146250	-4.6827583	-1.9383319
H	9.1310276	-3.3115785	-3.0340337
H	1.8502783	8.3038136	-6.1926144
H	-6.3771224	5.4337144	3.0026302
C	-4.6861438	1.8482673	-2.2758343
C	-6.0329673	1.1327476	-2.1316284
H	-4.1796991	1.4427566	-3.1713771
H	-4.8496858	2.9179925	-2.4952463
H	-6.6503056	1.2719540	-3.0330387
H	-5.8934791	0.0482053	-1.9884065
H	-6.6095389	1.5078300	-1.2726686
C	0.4318230	4.8381331	-2.3779219
C	0.8344906	6.1733971	-1.7441786
H	-0.2440360	4.3311486	-1.6690350
H	-0.1606740	5.0095851	-3.2944159
H	-0.0541572	6.7874092	-1.5280091
H	1.3639694	6.0099455	-0.7910255
H	1.4953499	6.7686006	-2.3912618
C	6.0087318	-5.7298772	2.2701221
C	7.3890224	-5.8789299	2.9167229
H	5.9352140	-6.3840609	1.3832966
H	5.2563888	-6.1181463	2.9806641
H	7.5922828	-6.9312556	3.1713344
H	8.1971198	-5.5358836	2.2530350

H	7.4549225	-5.2932003	3.8483994
U	1.3866420	-2.2579367	-1.6287676
O	2.9664087	-1.5243362	-1.8598324
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### UO<sub>2</sub>-L<sub>2</sub>

C	-3.8180250	4.3597061	-1.5685769
C	-2.5836377	3.8460640	-2.3159996
C	-2.7109426	2.4527406	-2.9605963
C	-1.3692023	2.0074553	-3.5418211
O	-0.3745005	1.9812438	-2.4976920
P	1.0735348	1.3524134	-2.7197792
O	2.5662229	-3.3752763	-1.2817041
P	3.3279366	-3.4140865	0.0673003
O	4.8202845	-3.9516312	-0.0735697
C	5.1407657	-5.1945021	-0.7326441
C	6.6238266	-5.2095746	-1.1042094
C	6.9562742	-4.0391137	-2.0492364
C	8.4381785	-3.8397074	-2.3824067
O	3.3253626	-1.9649499	0.5892311
O	1.7053665	2.3185499	-3.8313219
O	2.6947321	-4.4662679	1.0952049
C	1.3486076	-4.3289907	1.6030955
C	1.1470438	-5.2825943	2.7800849
C	2.1560985	-4.9840035	3.9054207
C	2.1448918	-5.9665308	5.0779474
H	-1.0363407	2.7012832	-4.3342087
H	4.5109638	-5.3005777	-1.6331345
H	1.1852149	-3.2825425	1.9132641
H	0.6436959	-4.5614616	0.7883536
H	-2.9623993	1.7253902	-2.1662386
H	-2.3077932	4.5726120	-3.1047082
H	-4.6685697	4.4712056	-2.2649929
H	-4.1337342	3.6085134	-0.8205253
H	7.1816334	-5.0611703	-0.1602061
H	6.3863272	-4.1735899	-2.9887691
H	9.0202130	-3.7734829	-1.4440390
H	1.3520971	-6.3004034	2.3970552
H	3.1651591	-4.9636311	3.4632177
H	2.9358984	-5.7162437	5.8031478
H	1.1879948	-5.9557430	5.6244353
H	2.3233011	-7.0014192	4.7393637
O	1.8300576	1.3456191	-1.3795684
O	1.0532311	-0.1197963	-3.2026410
C	-0.3338026	-5.2169378	3.2347579
C	-0.9764420	-6.5756347	3.5417686
H	-0.9413538	-4.7235518	2.4537400
H	-0.4147957	-4.5610666	4.1203954
H	-0.9471336	-7.2008188	2.6296519
H	-0.3732871	-7.1160516	4.2923418

H	1.9683132	-3.9600854	4.2805570
H	-1.7314369	3.8207693	-1.6165252
H	6.5700297	-3.1124959	-1.5939649
C	-2.4226034	-6.4720242	4.0372949
H	-3.0238577	-5.9194385	3.2917787
H	-2.4473404	-5.8564777	4.9553345
C	-3.0731582	-7.8284333	4.3145269
H	-2.5133168	-8.3930390	5.0794666
H	-4.1079534	-7.7153192	4.6764400
H	-3.1054293	-8.4515065	3.4045928
H	-1.4538331	0.9969369	-3.9745540
H	8.8327186	-4.7195667	-2.9222083
H	4.9049563	-6.0200564	-0.0411754
C	2.7559778	1.8808878	-4.7239060
C	3.4104643	3.0907322	-5.3951318
H	2.3088834	1.2071938	-5.4747871
H	3.5050743	1.3069123	-4.1555871
C	4.5566944	2.5440394	-6.2766155
H	3.8585320	3.6924391	-4.5822909
C	5.5297369	3.5448874	-6.9302834
H	5.1522834	1.8655972	-5.6413694
H	4.1226869	1.8995295	-7.0649355
H	6.5123404	3.0484227	-7.0239010
H	5.7008356	4.3992606	-6.2498895
C	5.1428819	4.0565979	-8.3251647
C	6.2191545	4.9445948	-8.9529655
H	4.1915466	4.6120886	-8.2829959
H	4.9522260	3.1889093	-8.9830641
H	6.4259487	5.8291509	-8.3265071
H	7.1701908	4.3978307	-9.0714019
C	-3.5816016	5.7009300	-0.8649330
C	-4.8108860	6.2276483	-0.1226273
H	-3.2526444	6.4478961	-1.6108372
H	-2.7390464	5.5944987	-0.1574461
H	-5.6610175	6.3792144	-0.8096039
H	-5.1414508	5.5213420	0.6580299
C	8.7010658	-2.5860246	-3.2251964
C	10.1779570	-2.3728428	-3.5613343
H	8.3113497	-1.7018577	-2.6886472
H	8.1143299	-2.6487975	-4.1599386
H	10.7866036	-2.2689842	-2.6468476
H	10.5878091	-3.2232842	-4.1327855
H	10.3290347	-1.4636308	-4.1656285
H	5.9170829	5.3070769	-9.9488171
H	-4.6053486	7.1926211	0.3686326
C	-3.7911205	2.3619859	-4.0692993
C	-5.1548375	1.8436242	-3.6014488
H	-3.4333295	1.6932090	-4.8733370
H	-3.9076430	3.3525592	-4.5447694
H	-5.8721939	1.8064377	-4.4375824
H	-5.0701755	0.8231883	-3.1915431

H	-5.5928271	2.4778075	-2.8155842
C	2.3604105	3.9692643	-6.1166573
C	2.6447324	5.4742325	-6.0907024
H	1.3864859	3.8105687	-5.6272212
H	2.2387777	3.6181778	-7.1574234
H	1.8261168	6.0368104	-6.5690574
H	2.7325613	5.8380159	-5.0532776
H	3.5755242	5.7429301	-6.6131561
C	6.9852295	-6.6063204	-1.6726087
C	8.3497519	-7.1473636	-1.2342139
H	6.9299279	-6.5743721	-2.7755919
H	6.2158989	-7.3375516	-1.3638796
H	8.5456627	-8.1372317	-1.6781324
H	9.1739108	-6.4809080	-1.5305425
H	8.3963689	-7.2603105	-0.1380808
U	2.1994667	-1.0156011	-1.3002309
O	3.7562817	-0.7699819	-2.1078028
O	0.6438348	-1.2590402	-0.4924078

**[UO<sub>2</sub>-L]<sup>+</sup>**

C	-3.8331150	5.0092835	-1.5089286
C	-2.6594073	4.4253042	-2.3019140
C	-2.9038241	3.0437289	-2.9387254
C	-1.6459727	2.5268404	-3.6255325
O	-0.5535981	2.4244363	-2.6389786
P	0.9461829	2.1072109	-2.9277144
O	1.3477771	2.8602569	-4.2379912
H	-1.3099078	3.2050652	-4.4253005
H	-3.1456245	2.3238896	-2.1350572
H	-2.3716613	5.1352451	-3.1012185
H	-4.6954380	5.1763635	-2.1777206
H	-4.1699988	4.2738509	-0.7547611
O	1.7805299	2.4851484	-1.6472731
O	1.2970250	0.5652644	-2.9811695
H	-1.7857554	4.3515450	-1.6315835
H	-1.8017064	1.5185839	-4.0378775
C	2.2655987	2.4029825	-5.3003830
C	2.8948871	3.5942337	-6.0157472
H	1.6560373	1.7959162	-5.9871240
H	3.0321617	1.7611179	-4.8425813
C	3.8979093	2.9887024	-7.0290556
H	3.4696119	4.1561459	-5.2560557
C	4.7881879	3.9505878	-7.8435706
H	4.5612673	2.3119400	-6.4616257
H	3.3427305	2.3385721	-7.7315159
H	5.7558017	3.4482480	-8.0164173
H	5.0306703	4.8437521	-7.2399336
C	4.2342342	4.3693295	-9.2129014
C	5.1978340	5.2578332	-10.0013814
H	3.2679255	4.8891426	-9.0975158

H	4.0126807	3.4576045	-9.7974786
H	5.4218683	6.1917838	-9.4586898
H	6.1570285	4.7449763	-10.1840478
C	-3.4900698	6.3289447	-0.8075422
C	-4.6659966	6.9300694	-0.0363064
H	-3.1300546	7.0559950	-1.5586340
H	-2.6408088	6.1632615	-0.1193096
H	-5.5148356	7.1488246	-0.7055957
H	-5.0300612	6.2401894	0.7437741
H	4.7779863	5.5361290	-10.9807202
H	-4.3833307	7.8721998	0.4593559
C	-4.0551942	3.0169872	-3.9815425
C	-5.4027541	2.5389433	-3.4327340
H	-3.7776707	2.3566892	-4.8239074
H	-4.1611606	4.0226584	-4.4245210
H	-6.1723420	2.5515733	-4.2204462
H	-5.3335771	1.5058263	-3.0533081
H	-5.7609753	3.1719097	-2.6072266
C	1.8148124	4.5354343	-6.5996719
C	2.2165495	6.0116680	-6.6787902
H	0.9160361	4.4716799	-5.9643853
H	1.5084539	4.1648968	-7.5939665
H	1.3774961	6.6229742	-7.0469148
H	2.4968115	6.3983442	-5.6848193
H	3.0679167	6.1848478	-7.3524309
U	2.4933595	0.4491909	-1.0978447
O	4.0577158	0.6371442	-1.8621073
O	1.1139968	0.0384795	-0.1046578

**[UO<sub>2</sub>-HL<sub>2</sub>-NTf<sub>2</sub>]**

C	-10.6391444	2.7281211	4.7435638
C	-9.3067999	2.9007091	4.0073706
C	-8.9690696	1.8190838	2.9636644
C	-7.5614836	2.0263717	2.4062175
O	-6.5978332	1.9784463	3.4797891
P	-5.0295784	1.9332021	3.1973834
O	-2.9950280	-1.5544004	3.7749867
P	-2.5689378	-1.1004068	5.1905253
O	-1.0508580	-1.5411794	5.3728102
C	-0.2753552	-1.2403227	6.5530694
C	0.8598379	-2.2558114	6.6917862
C	0.2930015	-3.6835864	6.8097186
C	1.3141762	-4.8250302	6.7872477
O	-2.7714769	0.3841089	5.4849173
O	-4.7652529	3.3006893	2.4072812
O	-3.3309752	-2.0027615	6.2819167
C	-4.7473695	-1.8509514	6.5034018
C	-5.1683459	-2.6256862	7.7514808
C	-4.4234645	-2.1149008	8.9992818
C	-4.6688294	-2.9162890	10.2790427

H	-7.4803319	3.0048418	1.9013944
H	-0.9280067	-1.2663292	7.4429588
H	-4.9851233	-0.7768482	6.6079281
H	-5.2805626	-2.2398183	5.6192678
H	-8.9617902	0.8372210	3.4729807
H	-9.2941001	3.8871778	3.5050781
H	-11.4792553	2.7627792	4.0264928
H	-10.6760772	1.7237004	5.2059027
H	1.4489218	-2.1929699	5.7576087
H	-0.3051622	-3.7478381	7.7390442
H	1.9627177	-4.7200904	5.8972773
H	-4.8670716	-3.6759720	7.5798440
H	-3.3437115	-2.1144517	8.7778530
H	-4.0615530	-2.5222460	11.1099955
H	-5.7222961	-2.8778496	10.6007019
H	-4.3998686	-3.9779189	10.1469663
O	-4.3423170	1.9385910	4.5622345
O	-4.6841672	0.7347580	2.2818466
H	-3.5855978	1.1734773	4.9769880
C	-6.7128872	-2.5712942	7.8829661
C	-7.3783894	-3.9147041	8.2075818
H	-7.1534043	-2.1937415	6.9417105
H	-6.9901939	-1.8255869	8.6499395
H	-7.1359899	-4.6380800	7.4066658
H	-6.9417953	-4.3352892	9.1306638
H	-4.7019398	-1.0572474	9.1657366
H	-8.4912997	2.9287243	4.7497297
H	-0.4199903	-3.8353258	5.9826538
C	-8.8998463	-3.8249993	8.3634533
H	-9.3340554	-3.3905710	7.4439031
H	-9.1400182	-3.1110336	9.1728758
C	-9.5649080	-5.1713186	8.6550622
H	-9.1768114	-5.6168569	9.5867824
H	-10.6565252	-5.0686187	8.7656929
H	-9.3794098	-5.8945413	7.8428761
H	-7.3196307	1.2359087	1.6771028
H	1.9854224	-4.7577938	7.6622885
H	0.1218967	-0.2183347	6.4461915
C	-3.6715745	3.4832066	1.4783485
C	-3.4425637	4.9742485	1.2220966
H	-3.9256555	2.9604438	0.5397131
H	-2.7589923	3.0220611	1.8873927
C	-2.2043814	5.0819201	0.3014269
H	-3.1843792	5.4215972	2.2004241
C	-1.6544389	6.4833445	-0.0330044
H	-1.3952870	4.5068692	0.7841331
H	-2.4164948	4.5477678	-0.6443902
H	-0.5624180	6.3954851	-0.1735325
H	-1.7813320	7.1552697	0.8353652
C	-2.2275758	7.1430457	-1.2949882
C	-1.5933234	8.5003683	-1.6049956

H	-3.3199127	7.2636841	-1.2050648
H	-2.0730854	6.4609522	-2.1507812
H	-1.7557704	9.2182261	-0.7827043
H	-0.5033212	8.4102733	-1.7509933
C	-10.8734957	3.7883961	5.8256893
C	-12.2038995	3.6252547	6.5628552
H	-10.8277943	4.7921511	5.3644372
H	-10.0406171	3.7558086	6.5520020
H	-13.0587834	3.6886900	5.8678971
H	-12.2646228	2.6471231	7.0697513
C	0.6616527	-6.2123988	6.7716812
C	1.6684059	-7.3633222	6.7404237
H	-0.0101125	-6.2853415	5.8969363
H	0.0095112	-6.3163645	7.6585073
H	2.3121726	-7.3082807	5.8460710
H	2.3301106	-7.3441964	7.6233800
H	1.1635758	-8.3428158	6.7255366
H	-2.0158625	8.9442282	-2.5208022
H	-12.3415214	4.4053596	7.3289879
C	-9.9690061	1.7495381	1.7793142
C	-11.0514149	0.6741826	1.9129955
H	-9.4142314	1.5579424	0.8428791
H	-10.4381404	2.7400062	1.6409598
H	-11.7279339	0.6826723	1.0428753
H	-10.6037026	-0.3318515	1.9747178
H	-11.6670490	0.8165298	2.8144150
C	-4.7310192	5.6602887	0.7094010
C	-4.9089584	7.1144983	1.1572593
H	-5.5970219	5.0909023	1.0829628
H	-4.7727978	5.5881190	-0.3924849
H	-5.8560446	7.5313423	0.7773140
H	-4.9359584	7.1831221	2.2578770
H	-4.0976763	7.7709517	0.8076644
C	1.7694136	-1.8350945	7.8745988
C	3.2687912	-2.0507056	7.6451081
H	1.4475762	-2.3704049	8.7861381
H	1.6114814	-0.7634280	8.0950191
H	3.8526201	-1.7416655	8.5274974
H	3.5095803	-3.1047496	7.4396959
H	3.6268795	-1.4581630	6.7864675
U	-3.1530208	-0.8290066	1.6384870
O	-1.8711624	0.3543114	1.9328277
O	-4.4116626	-2.0208251	1.2997047
N	-2.3004089	-2.1750366	-1.9954328
S	-1.3551630	-2.8176768	-0.8858526
S	-2.8531191	-0.6731668	-2.0379643
O	-3.2281333	-0.1456061	-0.6705898
C	-4.5221014	-0.9700463	-2.8474110
O	-2.1211412	0.2483313	-2.8892451
O	-1.5677214	-2.2072308	0.4807193
O	-1.3345361	-4.2621266	-0.9727908

F	-5.2646335	-1.7526408	-2.0817249
F	-5.1129463	0.2108032	-2.9864760
F	-4.3495921	-1.5253707	-4.0338366
C	0.3739371	-2.2054026	-1.2957972
F	1.2286387	-2.6935931	-0.4101892
F	0.7072209	-2.6058189	-2.5113316
F	0.3817425	-0.8770779	-1.2432870

### [UO<sub>2</sub>-L-NTf<sub>2</sub>]

C	-2.2555508	4.7240750	-3.6383748
C	-1.0225293	4.1086838	-4.3079589
C	-1.1760325	2.6587792	-4.8066669
C	0.1613260	2.1212319	-5.3154137
O	1.1319417	2.1615892	-4.2455344
P	2.6566472	1.7520268	-4.4132115
O	3.1809529	2.7418100	-5.5523578
H	0.5330251	2.7272569	-6.1597368
H	-1.4588439	2.0242527	-3.9458091
H	-0.7178029	4.7431920	-5.1629792
H	-3.0918388	4.7829720	-4.3580189
H	-2.6015409	4.0598070	-2.8243356
O	3.3588659	1.9111305	-3.0470272
O	2.8983127	0.2687796	-4.8050543
H	-0.1822533	4.1385829	-3.5942209
H	0.0585460	1.0761304	-5.6501202
C	4.3172067	2.4170669	-6.3944092
C	4.7971517	3.6667229	-7.1333033
H	4.0011564	1.6342506	-7.1037584
H	5.1260574	2.0062826	-5.7700279
C	6.0618337	3.2543032	-7.9226815
H	5.0998165	4.3922785	-6.3553825
C	6.8524281	4.3449580	-8.6728197
H	6.7473907	2.7753595	-7.2019038
H	5.7881860	2.4572609	-8.6395260
H	7.9142222	4.0408970	-8.6915263
H	6.8315093	5.2882139	-8.0972550
C	6.4247417	4.6060984	-10.1238376
C	7.3036368	5.6386091	-10.8324531
H	5.3733897	4.9354787	-10.1629257
H	6.4586548	3.6513154	-10.6797626
H	7.2738542	6.6139812	-10.3173664
H	8.3581492	5.3154743	-10.8621791
C	-1.9977407	6.1239704	-3.0689450
C	-3.2264332	6.7481031	-2.4048497
H	-1.6398564	6.7852703	-3.8797309
H	-1.1690673	6.0710701	-2.3392380
H	-4.0608127	6.8505984	-3.1196130
H	-3.5869316	6.1291653	-1.5655571
H	6.9765375	5.8025567	-11.8719982
H	-3.0059430	7.7515569	-2.0064020



C	-2.2419079	2.4813677	-5.9192635
C	-3.6226655	2.0395011	-5.4239601
H	-1.8881813	1.7307558	-6.6494994
H	-2.3305947	3.4234866	-6.4894529
H	-4.3300888	1.9383405	-6.2630448
H	-3.5669021	1.0615791	-4.9171194
H	-4.0554173	2.7556958	-4.7088605
C	3.6577907	4.3041288	-7.9635566
C	3.7039217	5.8330282	-8.0499534
H	2.6961600	4.0279287	-7.5021420
H	3.6466853	3.8602397	-8.9751083
H	2.8578666	6.2211747	-8.6402919
H	3.6399480	6.2819703	-7.0447383
H	4.6285385	6.2058417	-8.5162923
U	4.1140993	-0.3104712	-2.8533774
O	5.6386040	0.1575902	-3.6135598
O	2.6179757	-0.8449979	-2.0883882
N	6.0632406	-2.9159380	-0.4647907
S	5.4873491	-3.5823158	-1.7901406
S	5.5987033	-1.5590320	0.2420936
O	5.2246036	-0.4867767	-0.7653882
C	7.2566539	-0.9404009	0.8769134
O	4.7119370	-1.7038512	1.3813826
O	4.8802356	-2.5667585	-2.7354465
O	6.4182638	-4.5285102	-2.3651135
F	8.1024764	-0.8021457	-0.1299253
F	7.0515970	0.2324258	1.4580976
F	7.7331925	-1.8027006	1.7571789
C	3.9782904	-4.5580211	-1.2348588
F	3.3928898	-5.0854083	-2.2995750
F	4.3592761	-5.5162292	-0.4079639
F	3.1372299	-3.7362403	-0.6181174

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