

Supporting Information

Promising Density Functional Theory Methods for Predicting the Structures of Uranyl Complexes

Hai-Zhu Yu, Can Li, Bai-Hua Chen, Chu-Ting Yang, Dong-Rui Wang, Yao Fu, Sheng Hu,* Zhi-Min Dang*

*Department of Polymer Science and Engineering, University of Science and Technology
Beijing, Beijing 100083, China*

Institute of Nuclear Physics and Chemistry, CAEP, Mianyang, 621900, China.

*Department of Chemistry, University of Science and Technology of China, Hefei 230026,
China.*

Emails: dangzm@ustb.edu.cn; husheng@126.com

Table of Contents

Full citation of reference 20	S3
Comparison between 6-311G(d,p) and 6-311++G(d,p)	S4
Calculated bond distances with BB1K, CAM-B3LYP and LC-BLYP methods.....	S5
NBO analysis on 8.....	S7
Cartesian coordinates of complexes calculated with M2-B1 method.....	S8

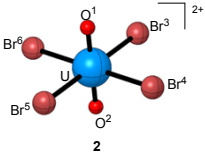
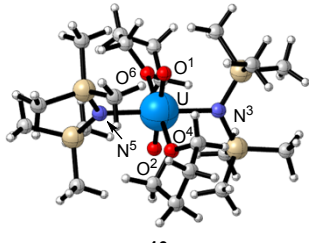
Full citation of reference 20

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

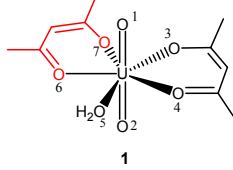
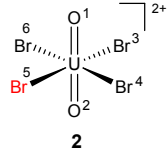
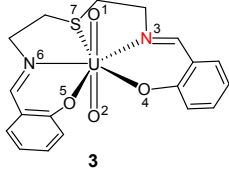
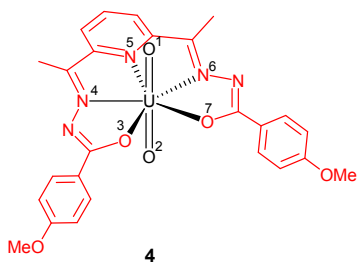
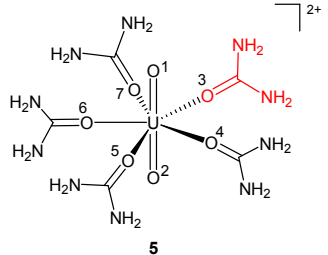
Comparison between 6-311G(d,p) and 6-311++G(d,p)

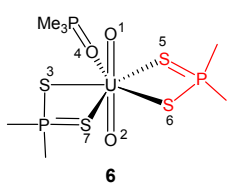
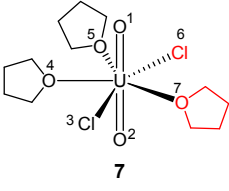
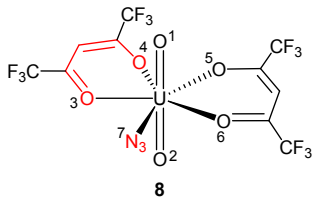
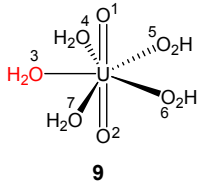
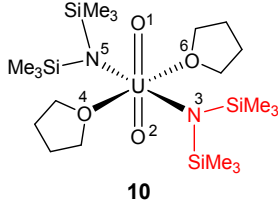
Considering that the two total electron basis set are mainly differentiated by the diffuse function, we chose complexes **2** and **10** as samples to evaluate the relative performance of them. The related calculation results in Table S1 indicate that the calculated bond distances of **2** are quite close with different basis sets, while the deviations of the bond distances calculated at 6-311++G(d,p) basis is relatively larger for bulky complex **10** (than the related ones calculated with 6-311G(d,p) method). The observation might be related to the inclusion of the diffuse functionals in 6-311++G(d,p) basis set, which slightly overestimates the steric hindrance between different ligand when the uranyl center is bulky. According to these additional calculation results, we suggest that 6-311G(d,p) is a better choice.

Table S1

Compound	U-X	BD ^{exp}	BD ^{6-311G(d,p)}	BD ^{6-311++G(d,p)}
	U-O ¹	1.766	1.730	1.730
	U-O ²	1.766	1.730	1.730
	U-Br ³	2.814	2.884	2.881
	U-Br ⁴	2.816	2.884	2.881
	U-Br ⁵	2.814	2.884	2.881
	U-Br ⁶	2.816	2.884	2.881
	U-O ¹	1.789	1.759	1.791
	U-O ²	1.789	1.759	1.791
	U-N ³	2.316	2.298	2.252
	U-O ⁴	2.432	2.447	2.398
	U-N ⁵	2.317	2.298	2.252
	U-O ⁶	2.445	2.439	2.402

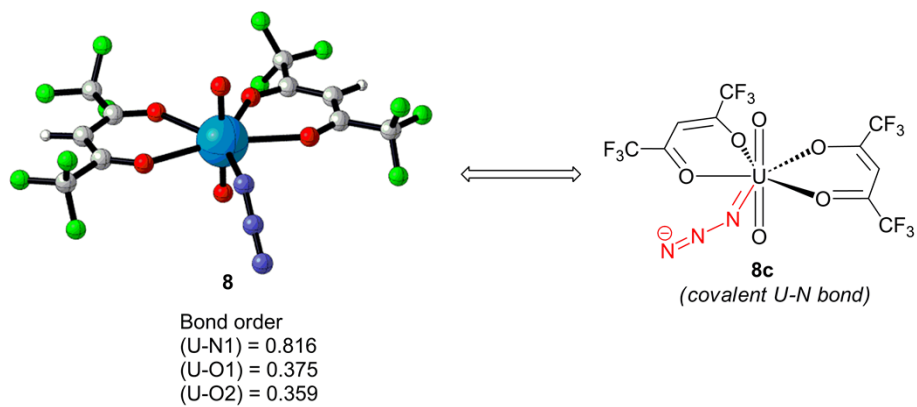
Calculated bond distances with BB1K, CAM-B3LYP and LC-BLYP methods

Compound	U-X	BD ^{exp}	BD ^{M2-B1}	BD ^{M6-B1}	BD ^{M7-B2}
 <p>1</p>	U-O ¹	1.733	1.735	1.757	1.738
	U-O ²	1.753	1.738	1.761	1.741
	U-O ³	2.338	2.319	2.329	2.318
	U-O ⁴	2.385	2.411	2.438	2.41
	U-O ⁵	2.488	2.531	2.537	2.496
	U-O ⁶	2.382	2.404	2.407	2.41
	U-O ⁷	2.349	2.319	2.327	2.318
 <p>2</p>	U-O ¹	1.766	1.73	1.751	1.729
	U-O ²	1.766	1.73	1.751	1.729
	U-Br ³	2.814	2.884	2.909	2.887
	U-Br ⁴	2.816	2.884	2.909	2.887
	U-Br ⁵	2.814	2.884	2.909	2.887
	U-Br ⁶	2.816	2.884	2.909	2.887
 <p>3</p>	U-O ¹	1.650	1.741	1.773	1.752
	U-O ²	1.662	1.751	1.764	1.744
	U-N ³	2.595	2.673	2.693	2.677
	U-O ⁴	2.299	2.209	2.217	2.207
	U-O ⁵	2.215	2.223	2.223	2.212
	U-N ⁶	2.601	2.625	2.674	2.656
	U-S ⁷	2.964	2.962	3.014	2.976
 <p>4</p>	U-O ¹	1.769	1.737	1.759	1.739
	U-O ²	1.768	1.737	1.759	1.739
	U-O ³	2.303	2.303	2.352	2.334
	U-N ⁴	2.493	2.582	2.619	2.604
	U-N ⁵	2.521	2.428	2.452	2.446
	U-N ⁶	2.470	2.6	2.603	2.59
	U-O ⁷	2.321	2.344	2.311	2.299
 <p>5</p>	U-O ¹	1.777	1.741	1.773	1.741
	U-O ²	1.778	1.748	1.761	1.753
	U-O ³	2.337	2.354	2.356	2.34
	U-O ⁴	2.337	2.354	2.356	2.341
	U-O ⁵	2.442	2.407	2.442	2.424
	U-O ⁶	2.366	2.369	2.388	2.375
	U-O ⁷	2.442	2.407	2.442	2.424

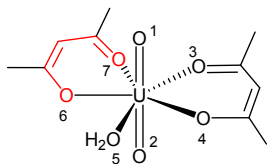
 <p style="text-align: center;">6</p>	U-O¹	1.741	1.739	1.758	1.738
	U-O²	1.743	1.729	1.747	1.727
	U-S³	2.867	2.874	2.924	2.896
	U-O⁴	2.317	2.345	2.36	2.336
	U-S⁵	2.867	2.902	2.929	2.901
	U-S⁶	2.881	2.869	2.917	2.889
	U-S⁷	2.881	2.862	2.914	2.886
 <p style="text-align: center;">7</p>	U-O¹	1.765	1.735	1.756	1.736
	U-O²	1.766	1.735	1.756	1.736
	U-Cl³	2.697	2.686	2.705	2.693
	U-O⁴	2.466	2.503	2.528	2.487
	U-O⁵	2.464	2.513	2.526	2.49
	U-Cl⁶	2.687	2.673	2.703	2.693
	U-O⁷	2.444	2.433	2.446	2.416
 <p style="text-align: center;">8</p>	U-O¹	1.688	1.736	1.759	1.739
	U-O²	1.725	1.737	1.758	1.739
	U-O³	2.417	2.454	2.465	2.444
	U-O⁴	2.424	2.474	2.489	2.467
	U-O⁵	2.412	2.474	2.489	2.467
	U-O⁶	2.401	2.454	2.465	2.444
	U-N⁷	2.382	2.279	2.293	2.287
 <p style="text-align: center;">9</p>	U-O¹	1.751	1.713	1.734	1.716
	U-O²	1.751	1.713	1.734	1.716
	U-O³	2.402	2.472	2.479	2.459
	U-O⁴	2.384	2.465	2.472	2.46
	U-O⁵	2.384	2.465	2.472	2.459
	U-O⁶	2.402	2.461	2.479	2.459
	U-N⁷	2.455	2.472	2.467	2.458
 <p style="text-align: center;">10</p>	U-O¹	1.789	1.759	1.779	1.759
	U-O²	1.789	1.759	1.779	1.759
	U-N³	2.316	2.298	2.327	2.311
	U-O⁴	2.432	2.447	2.485	2.448
	U-N⁵	2.317	2.298	2.327	2.311
	U-O⁶	2.445	2.439	2.481	2.444

NBO analysis on 8

The Wiberg bond order of the equatorial U-X bonds are given in Figure S1. the Wiberg bond order of U-N bond is about double that of the dative/covalent U-O single bonds in the 1,3-diketone ligand. The observation provide extra evidence for the double bond character of the U-N(azide) bond, and thus supports our conclusion that **8c** represents the main resonance structure of **8**.

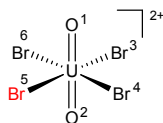


**Cartesian coordinates of all complexes
calculated at BB1K/(SDD-MWB60:6-
311G(d,p)) method.**



1

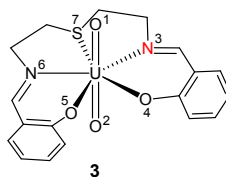
U	-0.00202800	-0.13795900	0.03127100
O	0.01788200	-2.66697500	0.11467100
O	-0.00268400	-0.08284700	1.76539800
O	-1.65065800	1.49143200	-0.03024900
O	-2.16329200	-1.18736400	-0.04243000
O	2.16826300	-1.18602500	-0.03842400
O	1.64642000	1.49240100	-0.02835600
O	0.00028600	-0.23973500	-1.70403100
C	-3.43801700	2.99399900	-0.04099300
C	-2.90257200	1.59963100	-0.02863600
C	-3.78092400	0.52019100	-0.01820100
C	-3.36179600	-0.80839600	-0.03140000
C	-4.38980400	-1.89567800	-0.03998000
C	4.39811200	-1.88483400	-0.03927000
C	3.36559700	-0.80181100	-0.03015200
C	3.77963400	0.52799000	-0.01938000
C	2.89762200	1.60480200	-0.02913000
C	3.42871000	3.00082300	-0.04333000
H	-3.05612500	3.50827200	-0.91895300
H	-3.05960000	3.52252200	0.83001400
H	-4.52099100	3.02506700	-0.04324700
H	-4.83684900	0.72140400	-0.01322300
H	-4.25768400	-2.49944000	-0.93453100
H	-5.40327000	-1.51366400	-0.01296500
H	-4.22371700	-2.54352200	0.81680500
H	5.40998600	-1.49850300	-0.01460700
H	4.26717600	-2.49019300	-0.93295300
H	4.23669500	-2.53232700	0.81871300
H	4.83487100	0.73280100	-0.01646400
H	3.05154400	3.52809600	0.82898400
H	3.04216300	3.51388600	-0.91994000
H	4.51156000	3.03537500	-0.04915700
H	-0.74301300	-2.98376800	-0.36731800
H	0.82472600	-2.94114300	-0.31794500



2

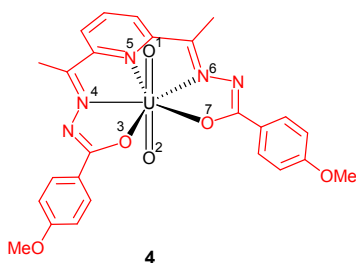
Br	0.00013700	-2.88389300	0.00000000
Br	-0.00041000	2.88391100	0.00000000
Br	0.00013700	-0.00001600	2.88390200
O	-1.72952800	-0.00013800	0.00000000
O	1.72952500	0.00015400	0.00000000

U	-0.00000100	0.00000400	0.00000000
Br	0.00013700	-0.00001600	-2.88390200



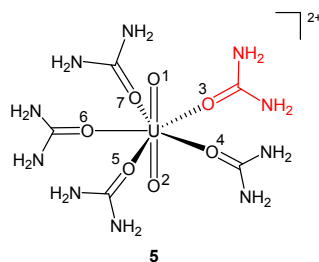
3

U	-0.03920900	0.12288000	0.02283300
S	-0.26485600	3.02569300	-0.52254300
O	0.43153900	0.60448300	1.63939400
O	-0.53284800	-0.13633800	-1.62688600
O	1.55290200	-1.40216500	-0.11266200
O	-1.53277600	-1.38318000	0.68724800
N	2.30310700	1.24114100	-0.61569300
N	-2.36624100	1.24939100	0.47616700
C	1.43036000	3.44874900	-0.07642200
C	2.34026600	2.64247100	-0.97657000
C	3.44974400	0.68780500	-0.49323100
C	3.78161300	-0.66579500	-0.16294200
C	5.13701900	-0.98839100	-0.04048700
C	5.54536100	-2.26012100	0.26039500
C	4.57674900	-3.24690600	0.43750400
C	3.24104000	-2.96487300	0.31608900
C	2.80542000	-1.66678800	0.01524600
C	-3.46372600	0.65067400	0.20553200
C	-3.67620000	-0.74114300	-0.05257900
C	-2.69993600	-1.71649300	0.24897500
C	-3.05482500	-3.06433700	0.09489600
C	-4.29620700	-3.41791300	-0.36506600
C	-5.25895600	-2.45612200	-0.67044300
C	-4.94395700	-1.13665200	-0.49390000
C	-1.16790900	3.30544800	1.01596200
C	-2.51422600	2.64315800	0.86717000
H	1.58987500	4.51373600	-0.20980300
H	1.59443700	3.17443400	0.96224100
H	2.01633800	2.75438400	-2.01242200
H	3.35474000	3.03963700	-0.91134600
H	4.32908900	1.31387000	-0.65977000
H	5.86802500	-0.20595400	-0.18756600
H	6.59210100	-2.49509300	0.35554200
H	4.88217000	-4.25506500	0.67315700
H	2.48991700	-3.72580800	0.44866000
H	-4.38081500	1.24458400	0.19802700
H	-2.31223200	-3.80600500	0.33838900
H	-4.53269300	-4.46389700	-0.48839500
H	-6.23318100	-2.74843200	-1.02455700
H	-5.67927400	-0.37197500	-0.70004800
H	-0.60691600	2.84419400	1.82267800
H	-1.27888200	4.36955300	1.19686800
H	-3.02939400	2.70866000	1.82471300
H	-3.11678000	3.18034400	0.13283000

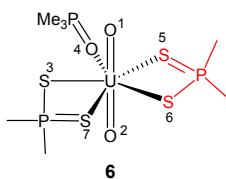


U	0.01246700	0.40008700	0.00020700
O	0.00654000	0.42944200	-1.73621900
O	0.00639700	0.43024200	1.73661700
O	-1.97379900	-0.84527600	0.00039100
O	1.96198600	-0.82646300	0.00056100
O	-7.37007100	-4.00565100	-0.00008200
O	7.33033500	-4.03751200	-0.00022600
N	-2.27922500	1.62707700	-0.00013800
N	-0.00795400	2.82809000	-0.00015700
N	2.26695100	1.65708000	0.00004900
N	-3.40690900	0.93410400	-0.00013200
N	3.40752300	0.94040200	0.00006900
C	-3.14207200	-0.36948100	0.00008600
C	-4.28109100	-1.28692400	0.00007200
C	-5.58715300	-0.82464200	-0.00059900
C	-6.65024300	-1.70351400	-0.00068300
C	-6.40863800	-3.07100700	-0.00006100
C	-5.10026000	-3.54327500	0.00064300
C	-4.05237800	-2.66011600	0.00069000
C	-2.36011900	2.91960800	-0.00020800
C	-1.07105300	3.55622600	-0.00018500
C	-0.71301600	5.00297400	-0.00025500
C	0.77511700	4.94037200	-0.00023000
C	1.12465200	3.64596300	-0.00017700
C	2.38499500	2.93850900	-0.00011200
C	3.14129500	-0.34376600	0.00031700
C	4.27154200	-1.27827500	0.00028000
C	5.58293800	-0.83370100	-0.00016100
C	6.63540700	-1.72610100	-0.00031800
C	6.37768400	-3.09029500	-0.00048000
C	5.06461300	-3.54488500	0.00045700
C	4.02711900	-2.64735700	0.00060500
C	-8.70567000	-3.58268800	-0.00085800
C	-3.64772100	3.65467600	-0.00023700
C	3.69317300	3.63503800	-0.00027500
C	8.66855800	-3.62641900	-0.00130100
H	-5.76084700	0.23798700	-0.00106400
H	-7.65563400	-1.31955300	-0.00122000
H	-4.94181000	-4.60888200	0.00113000
H	-3.03507500	-3.01402500	0.00119900
H	-1.12421000	5.51078800	-0.87450400
H	-1.12424700	5.51095300	0.87387600
H	1.42521800	5.79423600	-0.00020800
H	5.76916400	0.22701300	-0.00038600
H	7.64538600	-1.35394200	-0.00062900
H	4.89177300	-4.60836600	0.00068000
H	3.00575500	-2.98901700	0.00095600
H	-9.30714800	-4.48239000	-0.00085500
H	-8.93598900	-2.99574200	0.88743300
H	-8.93513200	-2.99631600	-0.88974800
H	-4.23523900	3.37529800	0.87097600
H	-3.49741700	4.72908800	-0.00044700

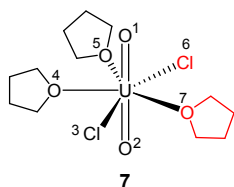
H	-4.23540200	3.37498400	-0.87123500
H	3.57247500	4.71231700	0.00009200
H	4.26997300	3.33467500	0.87040000
H	4.26942000	3.33525500	-0.87153100
H	8.90528400	-3.04143500	0.88690400
H	9.26311700	-4.53092100	-0.00200800
H	8.90370800	-3.04104200	-0.88966200



U	0.00003700	0.07851200	0.07568700
O	1.42335700	1.94544100	0.25143900
O	2.28136500	-0.68693500	0.02759600
O	-0.00057400	-2.26439700	-0.27262000
O	0.00002500	0.24909500	-1.65722800
O	0.00004500	-0.13832900	1.80979500
C	2.31910900	2.55494700	-0.36937000
C	3.12137000	-1.10775300	0.85585600
C	-0.00097000	-3.10749300	-1.19336900
N	3.02907700	1.95273700	-1.32111900
N	2.57088600	3.82849300	-0.08033400
N	2.90105900	-1.05429000	2.16516400
N	4.27314800	-1.61632900	0.42051500
N	-0.00084700	-2.74473300	-2.47443200
N	-0.00153800	-4.40459500	-0.89317000
O	-1.42237000	1.94615400	0.25142200
O	-2.28169500	-0.68583600	0.02779000
C	-2.31775300	2.55597200	-0.36962200
C	-3.12186400	-1.10612100	0.85615700
N	-3.02806200	1.95383100	-1.32115900
N	-2.56878600	3.82976700	-0.08104100
N	-2.90149600	-1.05248600	2.16544800
N	-4.27387700	-1.61427500	0.42094900
H	3.73160600	2.42223300	-1.85496400
H	3.32079300	4.34485400	-0.49286200
H	2.03268000	-0.67499400	2.49176900
H	4.98035300	-1.96825900	1.03320800
H	-0.00046000	-1.76723900	-2.69210900
H	-0.00152800	-4.66299000	0.07233300
H	-3.73032300	2.42353700	-1.85517100
H	-3.31840800	4.34640900	-0.49373600
H	-2.03291800	-0.67355600	2.49194600
H	-4.98124000	-1.96573100	1.03373200
H	-2.04627500	4.25298600	0.65846800
H	-2.86931100	0.97671500	-1.47068000
H	2.04863800	4.25174700	0.65934200
H	2.86970900	0.97579200	-1.47107900
H	3.55921000	-1.39268500	2.83725000
H	4.41448000	-1.69798500	-0.56502300
H	-0.00175000	-5.12754900	-1.58332600
H	-0.00117500	-3.40528600	-3.22453800
H	-4.41528200	-1.69605200	-0.56457000
H	-3.55975200	-1.39050900	2.83761900

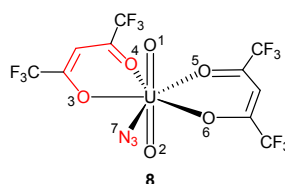


U	-0.12458400	-0.18583100	-0.17725300
P	2.81694500	-1.86472700	0.14022800
P	1.03268200	3.25465000	0.07874100
S	2.72750200	-0.03600800	-0.69428500
S	1.04708600	-2.79431000	0.05681500
C	3.36762300	-1.72670500	1.85375100
C	4.07827000	-2.84795300	-0.69070100
C	2.36460600	3.88622800	-0.93755300
C	-0.16501100	4.56626400	0.31012000
O	0.28945500	0.11408200	1.48510800
O	-0.52542200	-0.45759900	-1.83725800
O	0.38011600	2.06700400	-0.59005600
S	-2.59509900	1.25418900	0.10651900
S	-2.19540700	-2.00158500	0.60185900
C	1.72860900	2.85701800	1.67761600
P	-3.48223900	-0.54920100	0.10307200
C	-4.88858100	-0.55264000	1.23181400
C	-4.17781700	-0.87002700	-1.52974900
H	3.43189300	-2.71607700	2.29665100
H	2.62513900	-1.14357400	2.38881100
H	4.33119600	-1.22783800	1.89759300
H	4.13420800	-3.83064800	-0.23176700
H	3.79503400	-2.95152700	-1.73199700
H	5.03801000	-2.34395100	-0.62416000
H	3.09662900	3.09404400	-1.06525300
H	1.97073000	4.15698800	-1.91190000
H	2.83673600	4.75057800	-0.48032800
H	-0.98874900	4.17661000	0.90125000
H	-0.55077000	4.86746500	-0.65854400
H	0.27459100	5.42284300	0.81196300
H	0.94408800	2.47449800	2.32206400
H	2.46215300	2.06764500	1.53606200
H	2.19472700	3.73014000	2.12450400
H	-5.37197000	-1.52478900	1.20484500
H	-4.52269100	-0.35964400	2.23378700
H	-5.58953000	0.22552400	0.94434200
H	-4.66587200	-1.83998000	-1.53639000
H	-3.35786200	-0.87417900	-2.24072500
H	-4.88151300	-0.08608400	-1.79287500



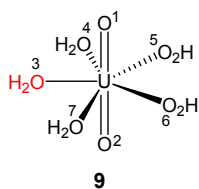
U	0.15089600	-0.04847400	-0.05764800
Cl	0.57854400	-2.67270600	-0.33123700
Cl	1.17141700	2.41306400	0.27957800
O	0.06467900	-0.21789900	1.66726700
O	0.14784500	0.14310900	-1.78223100
O	-2.07972400	-1.19774900	0.07049300

O	2.57000700	-0.30692000	-0.03374000
O	-1.74450600	1.58320900	-0.14708500
C	-2.39790700	-1.98569500	1.22853900
H	-1.49962500	-2.51680800	1.53160400
H	-2.69998600	-1.30703300	2.01857300
C	-3.47998700	-2.92991700	0.76725100
H	-4.45562800	-2.44984900	0.81023700
H	-3.51450300	-3.83269000	1.36758600
C	-3.06933900	-3.18014200	-0.67238000
H	-3.87025100	-3.57043200	-1.29154500
H	-2.22621400	-3.86445100	-0.70854700
C	-2.62272300	-1.80713400	-1.11041000
H	-1.84648300	-1.82933000	-1.86810900
H	-3.45231100	-1.19109800	-1.45144900
C	3.27894900	-0.79245600	1.11445100
H	2.89524000	-1.78083500	1.34285200
H	3.07168700	-0.11585800	1.94008400
C	4.73326200	-0.76459500	0.70743000
H	5.39195800	-0.63564200	1.55961700
H	5.00242300	-1.68830100	0.20077300
C	4.76641100	0.40171700	-0.26429800
H	5.63049200	0.39441500	-0.92030800
H	4.74208500	1.34634900	0.27344400
C	3.47361800	0.21056600	-1.01628900
H	3.04701900	1.12830100	-1.40408400
H	3.56407200	-0.52556700	-1.81206000
C	-2.24793500	2.09935000	1.09257200
H	-1.40007800	2.27971000	1.74996500
H	-2.89517900	1.34508700	1.52736100
C	-2.95082200	3.38357700	0.72601300
H	-3.96861400	3.18423100	0.39698000
H	-2.98838100	4.07837200	1.55815900
C	-2.09925100	3.87255900	-0.43095500
H	-2.59660600	4.60699900	-1.05579500
H	-1.16738300	4.29137700	-0.06105400
C	-1.81339600	2.58987600	-1.17029900
H	-0.86872300	2.59338300	-1.70007000
H	-2.61844400	2.31700600	-1.84978000

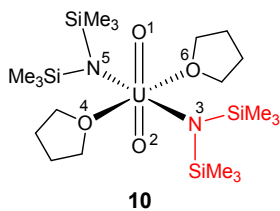


U	0.00000300	-0.68295000	0.08771200
N	0.00004200	-2.96042200	0.16619300
N	0.00094300	-3.91282700	-0.54521800
N	0.00176400	-4.84671800	-1.18688000
O	-0.00043400	-0.56134000	1.82035500
O	0.00035500	-0.72313100	-1.64778200
O	2.40976300	-1.14791000	0.10393600
O	1.38177900	1.36652700	-0.00779800
O	-1.38202800	1.36658700	-0.00808500
O	-2.40950400	-1.14823900	0.10353100
C	3.48003800	-0.53542800	0.06272400
C	3.67862800	0.83659900	-0.01334400
C	2.57381800	1.67833800	-0.03998000
C	4.71076300	-1.43791800	0.11784300

C	2.81362100	3.18513800	-0.11648500
C	-2.57415900	1.67804700	-0.03977600
C	-3.67878000	0.83603200	-0.01320600
C	-3.47991100	-0.53595400	0.06246600
C	-2.81439800	3.18481000	-0.11583200
C	-4.71043700	-1.43872500	0.11738700
F	4.67287600	-2.34419400	-0.84476000
F	4.76471800	-2.07678600	1.27803100
F	5.85195400	-0.76185900	-0.01504600
F	2.25349500	3.69055100	-1.20478200
F	2.28509100	3.79444500	0.93394800
F	4.10737600	3.50368500	-0.15094200
F	-2.25591600	3.69035700	-1.20495700
F	-2.28448100	3.79418100	0.93382200
F	-4.10826800	3.50309300	-0.14845300
F	-4.76423900	-2.07788800	1.27742000
F	-5.85178600	-0.76290300	-0.01534200
F	-4.67235700	-2.34477100	-0.84542900
H	4.67121600	1.23757400	-0.04714900
H	-4.67145900	1.23680700	-0.04667700



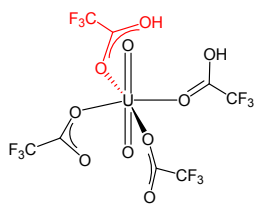
U	0.00598600	-0.00042700	0.00000600
O	0.02759200	0.00022700	-1.71238800
O	0.02760700	-0.00338800	1.71238500
O	0.58908500	-2.38470900	0.22257300
O	-2.06449100	-1.29873900	-0.37306600
O	-1.91868600	1.50563000	0.37338300
O	0.83284900	2.31106400	-0.22323100
O	2.46382100	-0.12677200	0.00027100
H	0.70691800	-3.03654800	-0.47004700
H	-2.39021600	-1.54674200	-1.23969100
H	-2.49483200	1.92019600	-0.27039400
H	1.03403800	2.73816800	-1.05741700
H	3.03468300	-0.13040000	-0.76967300
H	1.01852300	2.94677300	0.46948700
H	3.03148300	-0.18332900	0.77051100
H	0.74421400	-2.83058500	1.05678900
H	-2.68082500	-1.65106000	0.27057000
H	-2.21691300	1.78631800	1.23993400



U	0.00000000	0.02003200	0.00000100
O	-0.00724000	0.01825200	1.75934000
N	2.29778400	-0.00722200	-0.00041300

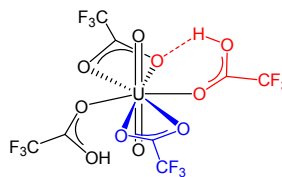
Si	3.10972000	0.46785400	1.46172600
C	4.91058500	0.96196100	1.23187400
H	5.58402100	0.11698300	1.13319000
H	5.21580300	1.52454000	2.11339000
H	5.05382600	1.60930800	0.36824300
C	2.34762200	2.00612700	2.22791700
H	1.32434000	1.85046300	2.55084700
H	2.37561200	2.84678800	1.53653300
H	2.93508500	2.28664800	3.10147000
C	3.06198000	-0.89991300	2.74093800
H	2.03340900	-1.13759700	3.00168000
H	3.58095500	-0.60732200	3.65216800
H	3.53994800	-1.80199500	-2.36207900
Si	3.10333600	-0.51079900	-1.45743400
C	4.89034200	-1.04831500	-1.21626100
H	5.58282200	-0.21957500	-1.11172400
H	5.18819000	-1.61673400	-2.09654900
H	5.01272800	-1.69985100	-0.35260000
C	3.09622100	0.85427600	-2.74075100
H	3.62845400	1.73294500	-2.37920900
H	2.07484800	1.14206500	-2.97923100
H	3.57890800	0.53212800	-3.66189500
C	2.31370000	-2.02878500	-2.23825700
H	1.30003600	-1.84579900	-2.57646000
H	2.31256600	-2.87783600	-1.55697400
H	2.90727800	-2.31334500	-3.10649000
O	-0.00001100	-2.41878400	-0.00002100
C	0.73560800	-3.22947100	0.92484200
H	0.58916000	-2.81948300	1.91757400
H	1.78974500	-3.15990800	0.66623200
C	0.18201300	-4.62091800	0.73739700
H	-0.70658400	-4.75588800	1.34939300
H	0.90223700	-5.38702400	1.00348100
O	0.00002000	2.46747300	0.00001700
C	0.80046300	3.27879600	-0.86940800
H	0.37663900	3.21976100	-1.86911300
H	1.80217100	2.86236200	-0.87657500
C	0.70136400	4.67001300	-0.29100500
H	0.85633000	5.43655400	-1.04257500
H	1.43706100	4.80729100	0.49772400
O	0.00725400	0.01829100	-1.75933900
N	-2.29778900	-0.00720300	0.00041600
Si	-3.10972500	0.46792700	-1.46170900
C	-4.91057900	0.96206100	-1.23182300
H	-5.58402700	0.11709300	-1.13313700
H	-5.21580100	1.52465600	-2.11332700
H	-5.05379500	1.60939900	-0.36818300
C	-2.34760600	2.00620200	-2.22787800
H	-1.32432700	1.85052800	-2.55081600
H	-2.37557700	2.84685200	-1.53648100
H	-2.93506800	2.28675000	-3.10142300
C	-3.06203600	-0.89981200	-2.74095400
H	-2.03347700	-1.13752100	-3.00171300
H	-3.58101200	-0.60718500	-3.65217200
H	-3.54002900	-1.80188600	-2.36211000
Si	-3.10335000	-0.51082400	1.45742300
C	-4.89035300	-1.04833200	1.21621500
H	-5.58283200	-0.21959000	1.11168500
H	-5.18821300	-1.61677100	2.09648700
H	-5.01272700	-1.69985000	0.35253800
C	-3.09625200	0.85420900	2.74078700
H	-3.62848100	1.73289000	2.37926700

H	-2.07488200	1.14198600	2.97928900
H	-3.57895100	0.53203300	3.66191500
C	-2.31372300	-2.02883300	2.23821500
H	-1.30005800	-1.84585800	2.57642300
H	-2.31259200	-2.87787000	1.55691500
H	-2.90730400	-2.31341000	3.10643900
C	-0.73562700	-3.22946000	-0.92489500
H	-0.58918000	-2.81945400	-1.91761900
H	-1.78976300	-3.15990800	-0.66628200
C	-0.18202400	-4.62090600	-0.73747300
H	0.70657300	-4.75586200	-1.34947100
H	-0.90224400	-5.38701200	-1.00357000
C	-0.80040400	3.27881100	0.86944400
H	-0.37658800	3.21975800	1.86915200
H	-1.80212300	2.86240500	0.87660100
C	-0.70126700	4.67002900	0.29105200
H	-0.85621300	5.43656900	1.04262700
H	-1.43696000	4.80733200	-0.49767700



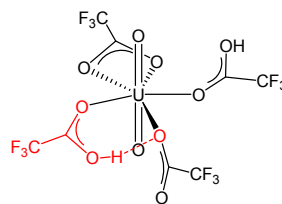
11-a

U	-0.10854000	-0.50425100	-0.04649300
O	-0.04496100	-0.30324100	-1.76025100
O	-0.17816500	-0.57102400	1.67755900
O	2.68149600	-3.22276100	-1.29968400
O	1.84268200	-1.55470400	-0.06739000
C	2.76370900	-2.21507600	-0.67455300
C	4.13169900	-1.54068700	-0.48803500
F	4.51478600	-1.56998300	0.79037100
F	5.07207600	-2.09050900	-1.21073300
F	4.06223100	-0.23864800	-0.82514300
O	1.54646700	1.43917400	0.18301700
O	2.81538000	0.61123400	1.77117900
C	2.58361300	1.41205500	0.78442900
C	3.68424300	2.42408400	0.44308300
F	3.76045300	2.62433600	-0.84269000
F	4.85372600	1.98563000	0.89497100
F	3.41074900	3.56572800	1.04827000
O	-1.87615000	-1.78195400	-0.19399500
O	-2.73711900	-3.62809800	0.72384400
C	-2.79730600	-2.49910700	0.35972200
C	-4.09754100	-1.69635500	0.50150800
F	-4.59758500	-1.38644700	-0.68936800
F	-3.85885900	-0.54335800	1.13788700
F	-5.01282400	-2.35056600	1.17832900
O	-1.52604200	1.55634700	-0.03866600
O	-1.65891700	3.73492700	-0.22082200
C	-2.16461000	2.54094800	-0.25499900
C	-3.66899400	2.44454900	-0.56004200
F	-3.91458800	1.43923800	-1.34895500
F	-4.06266900	3.57485600	-1.15244300
F	-4.33635900	2.31773700	0.56222700
H	3.74747300	0.58206900	2.00297800
H	-2.30830000	4.39524500	-0.47514400



11-b

U	0.02066700	0.01007200	-0.10688200
O	0.11040400	-0.02630300	-1.82528600
O	-0.05232700	0.08035900	1.61234500
O	-0.22122300	2.53417400	-0.13491100
O	1.81736100	1.79023400	-0.06246900
C	0.98769600	2.72862800	-0.08384600
C	1.52319800	4.15820200	-0.00161200
F	2.72221800	4.23702400	-0.55120700
F	0.72007400	5.00291700	-0.60928700
F	1.62666600	4.51339700	1.27089500
O	-2.36077800	0.94876500	-0.29399100
O	-3.20688100	0.40424100	1.66195000
C	-3.29547600	0.82108900	0.43654600
C	-4.69563100	1.19584300	-0.06920600
F	-4.77684300	2.49610100	-0.23485300
F	-5.61149400	0.83013400	0.83014000
F	-4.95195900	0.59277500	-1.20014800
O	2.37967200	-0.85773200	0.01946100
O	4.07896300	0.59014100	0.00911400
C	3.55168800	-0.57836900	0.04597800
C	4.60888100	-1.68237300	0.14312900
F	5.46905000	-1.56969300	-0.85226800
F	4.04926500	-2.86432700	0.09594000
F	5.26693300	-1.56066400	1.28320500
O	0.18233300	-2.43826000	-0.01438900
O	-1.83385800	-1.62000700	-0.09635700
C	-1.04586200	-2.58047400	-0.04400000
C	-1.63100900	-3.99300000	-0.05108000
F	-1.84877300	-4.37499600	-1.30141600
F	-2.78377900	-4.02283600	0.59538100
F	-0.81036200	-4.85449000	0.51160700
H	-4.07269900	0.31682700	2.06593400
H	3.36215000	1.26626300	-0.03391400



11-c

U	0.02318800	0.00085000	-0.08431400
O	0.15049800	-0.02566400	-1.80054300
O	-0.09076600	0.06146700	1.63317200
O	-0.24478500	2.52434800	-0.10646100
O	1.80065400	1.80233100	-0.00712400
C	0.96115800	2.73192400	-0.04301200
C	1.48388000	4.16614000	0.03614900
F	1.66359500	4.49579600	1.30707400
F	2.64597000	4.26983300	-0.58512700
F	0.63608100	5.01361800	-0.50190100
O	-2.35475000	0.92247500	-0.32688600

O	-3.24388500	0.37043600	1.60787100
C	-3.30445700	0.79936300	0.38490200
C	-4.69024000	1.19709700	-0.14173100
F	-4.92287800	0.63292800	-1.29721200
F	-4.76179300	2.50276000	-0.26611800
F	-5.62805400	0.80733900	0.72426900
O	2.38820100	-0.83968500	0.05835700
O	4.07119400	0.62602500	-0.00057000
C	3.55772700	-0.54811300	0.04472400
C	4.62736400	-1.64418200	0.07069000
F	5.28986100	-1.63685600	-1.07309900
F	4.07916200	-2.82045200	0.24023700
F	5.48118000	-1.41844400	1.05222000
O	0.20399100	-2.44620900	0.00809800
O	-1.81659800	-1.64591300	-0.12455300
C	-1.02188600	-2.59897300	-0.04141700
C	-1.60936700	-4.01014800	-0.00630000
F	-2.20095700	-4.27799000	-1.16059700
F	-2.52046900	-4.09728400	0.95189200
F	-0.68348000	-4.91708300	0.21163500
H	3.34616600	1.29542700	-0.02026400
H	-4.11852800	0.28338500	1.99275000