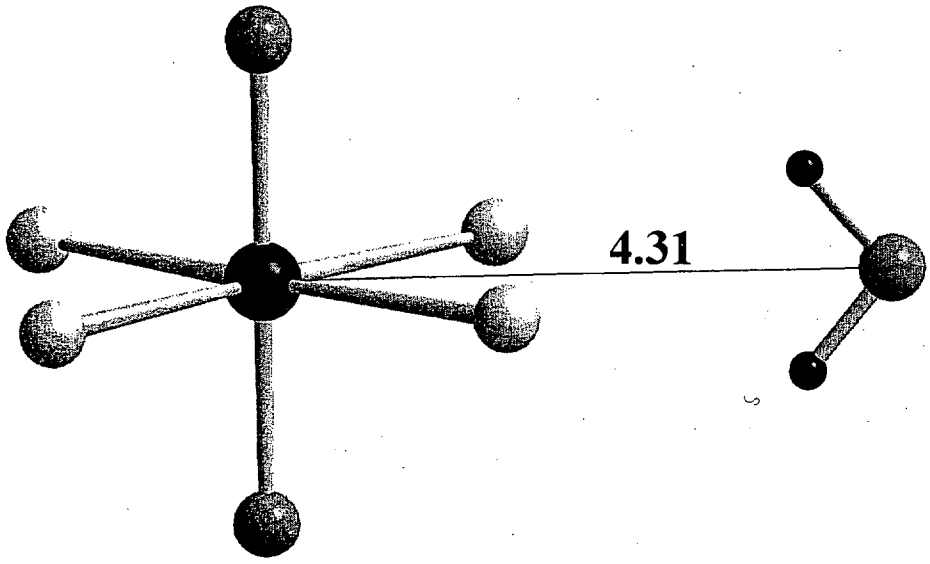
© 2001 American Chemical Society, Inorg. Chem., Vallet ic001405n Supporting Info Page 1

Supporting Information

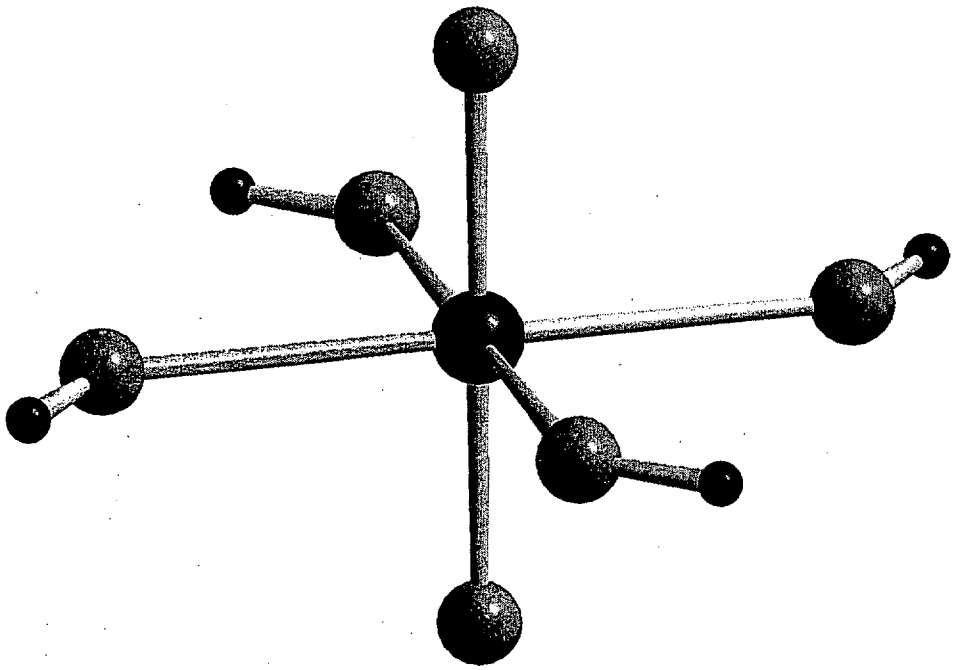
Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry

Valérie Vallet*[a], Ulf Wahlgren[a], Bernd Schimmelpfennig[b], Henry Moll[c], Zoltán Szabó[d] and Ingmar Grenthe*[d]

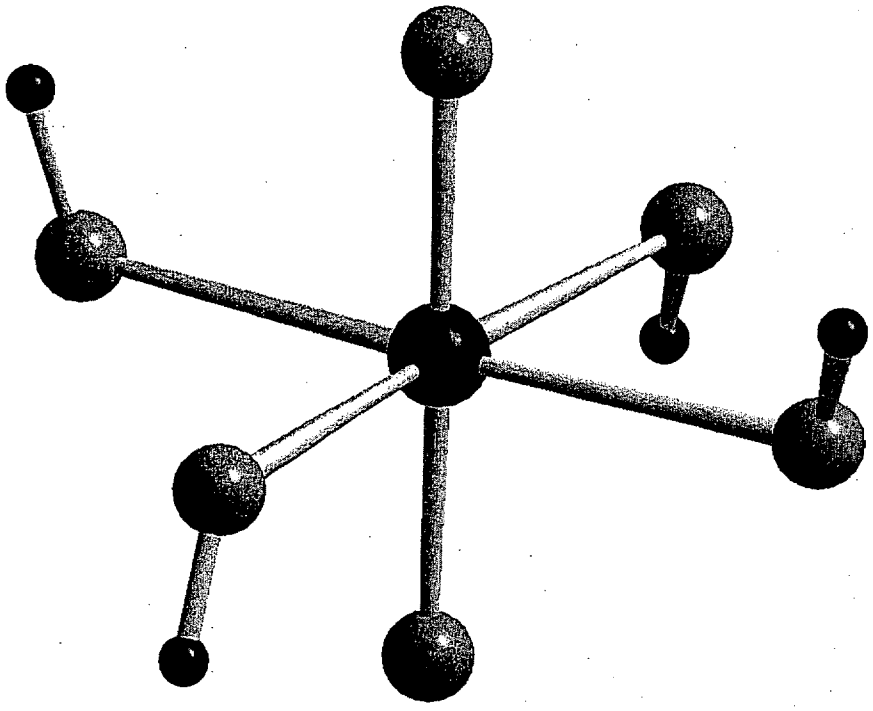


Structure 3.

S1. The uranium(VI) tetrafluoride structure 3.

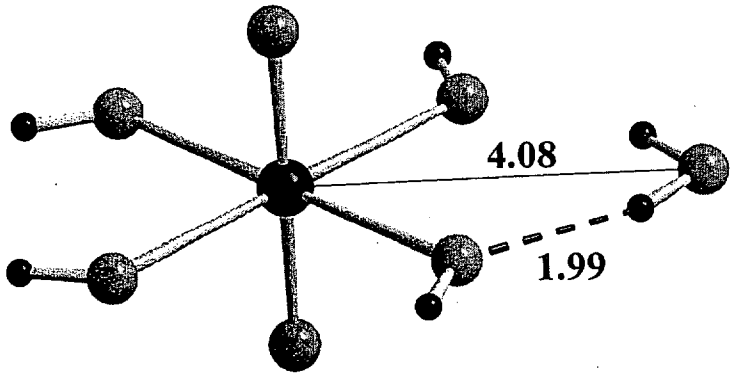


Structure 5 a.

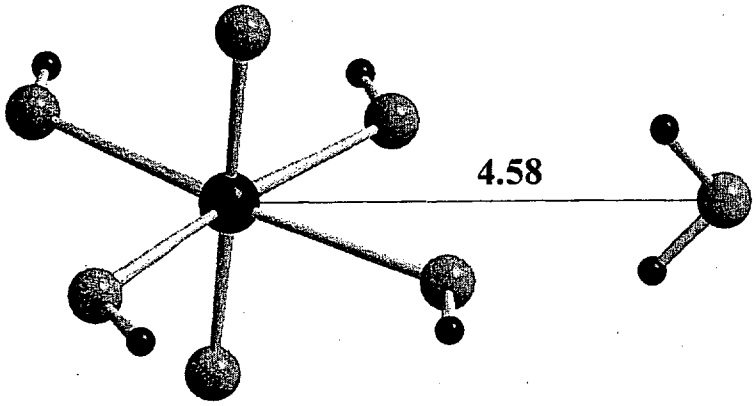


Structure 5 b.

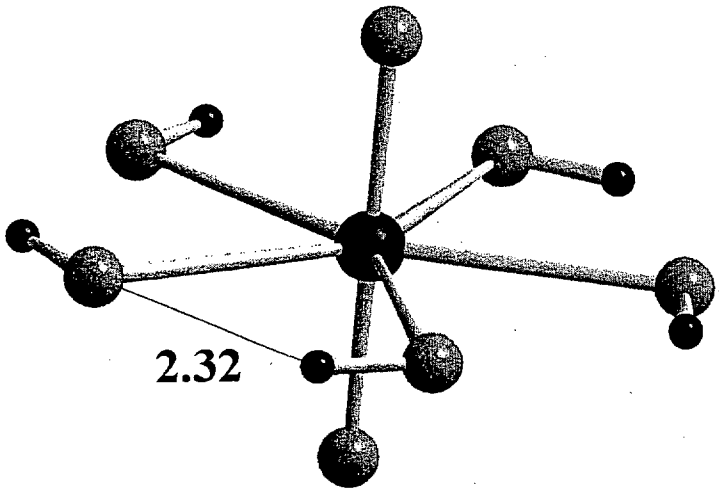
S2. The uranium(VI) tetrahydroxide structures 5a and 5b.



Structure 7 a.

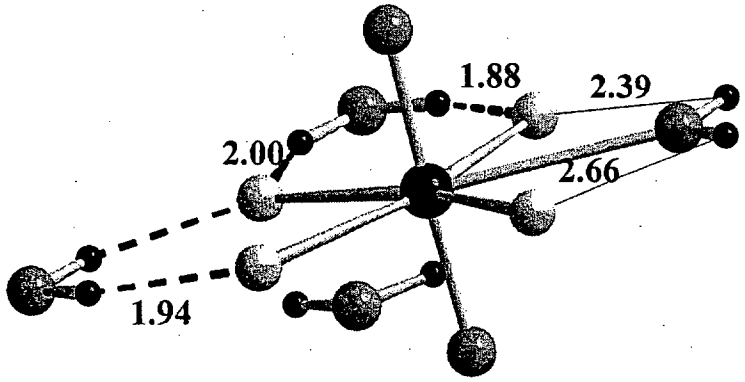


Structure 8.

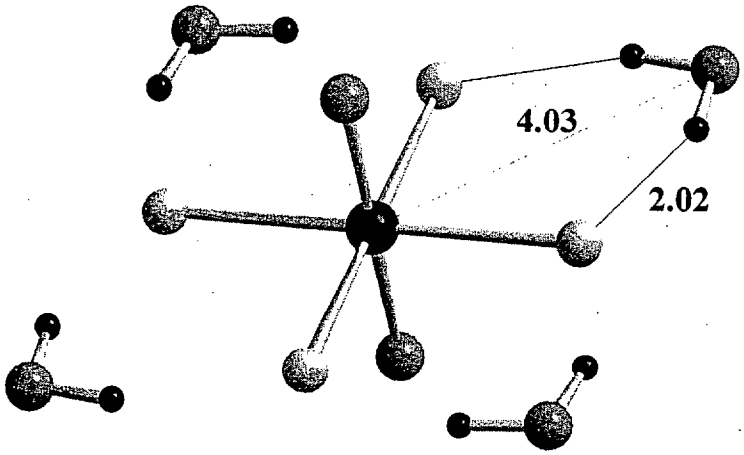


Structure 9.

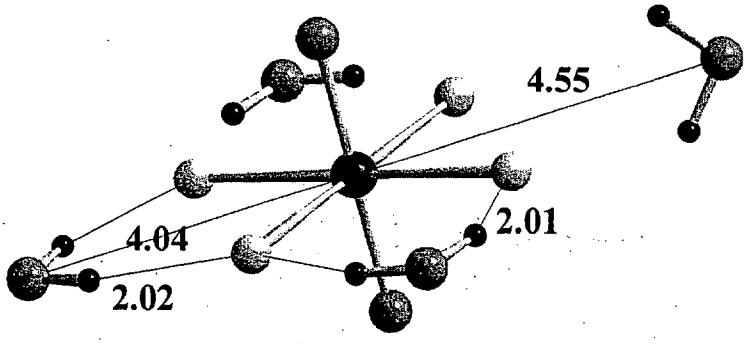
S3. The uranium(VI) tetrahydroxide structures 7a and 8 and the uranium(VI) pentahydroxide structure 9.



Structure 10.

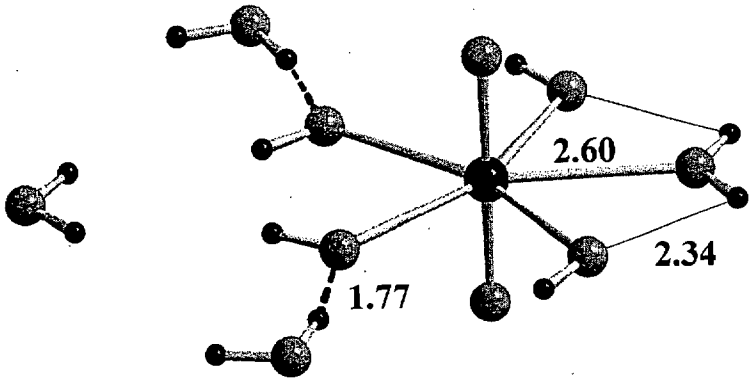


Structure 11.

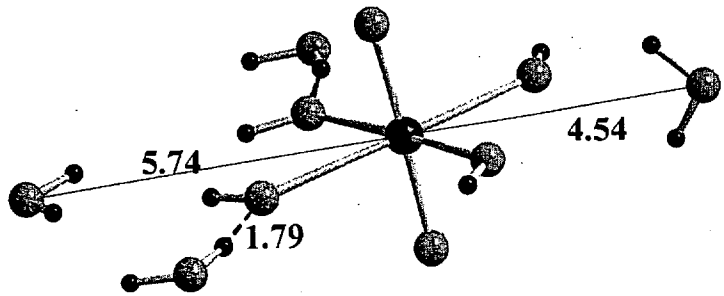


Structure 12.

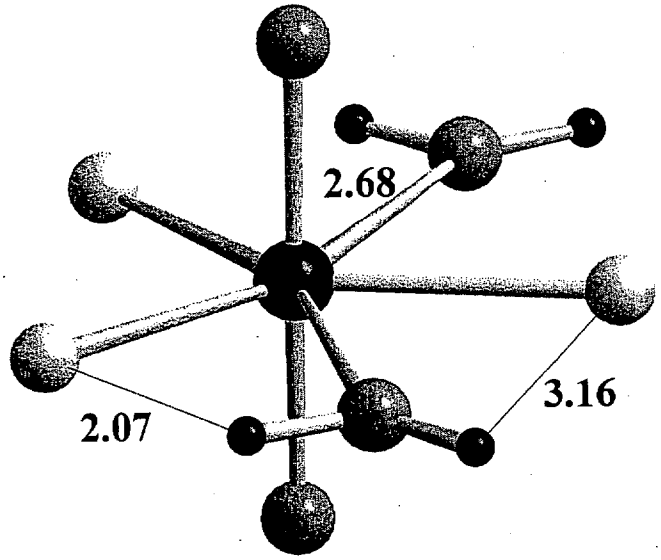
S4. The uranium(VI) tetrafluoride structure 10, 11 and 12, with a second coordination sphere.



Structure 13.

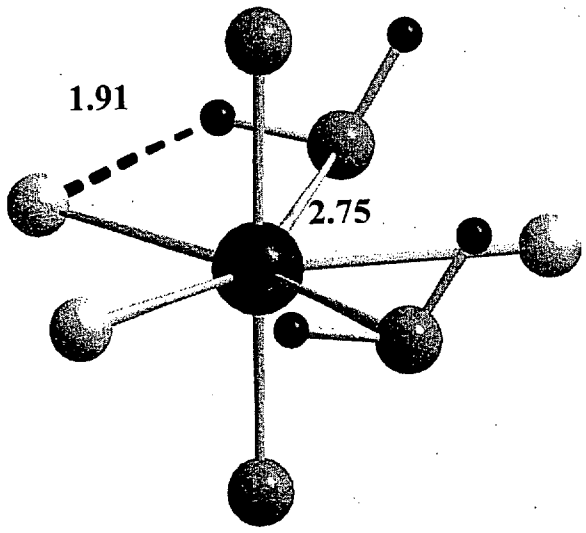


Structure 15.

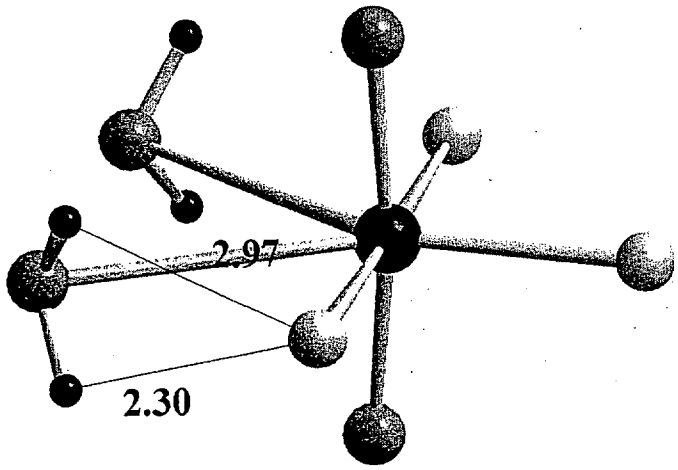


Structure 16.

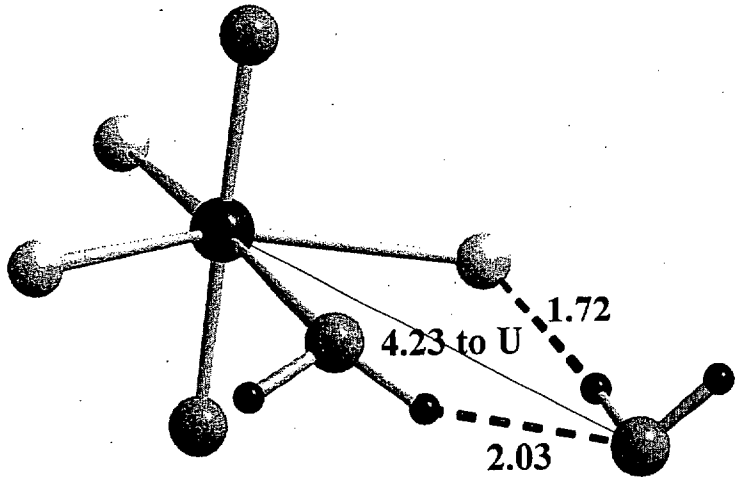
S5. The uranium(VI) tetrahydroxide structure 13 and 15, with a second coordination sphere. The following figure shows the uranium(VI) trifluoride structure 16.



Structure 18 in gas-phase.

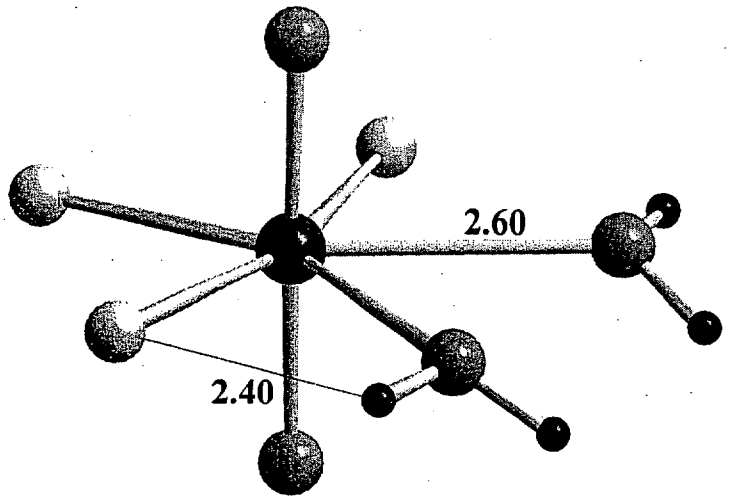


Structure 20.



Structure 21 in gas-phase.

S6. The uranium(VI) trifluoride structures 18, 20 and 21 in gas-phase.



Structure 21 in the solvent.

S7. The uranium(VI) trifluoride structure 21 in the solvent.

Table S1. Cartesians coordinates in Å of all the computed structures both in gas-phase and in the solvent

Chemical species	Complex	Method	Atoms	X (Å)	Y (Å)	Z (Å)
$UO_2F_4(H_2O)^{2-}$	Struct. 1	SCF Gas-phase	U	-0.089705	0.000000	0.000000
			F	1.117471	1.998458	0.000000
			F	1.117471	-1.998458	0.000000
			F	-1.798909	1.461563	0.000000
			F	-1.798909	-1.461563	0.000000
			O-yl	-0.050968	0.000000	1.738197
			O-yl	-0.050968	0.000000	-1.738197
			O-w	2.657954	0.000000	0.000000
			H-w	3.157012	0.794953	0.000000
			H-w	3.157012	-0.794953	0.000000
$UO_2F_4(H_2O)^{2-}$	Struct. 1	SCF + CPCM	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.750917
			O-yl	0.023591	0.000000	-1.750758
			Ow	2.619339	0.000000	0.017647
			F	0.958851	-2.050606	0.006460
			F	0.958851	2.050606	0.006460
			F	-1.770466	-1.396256	-0.011928
			F	-1.770466	1.396256	-0.011928
			H-w	3.170386	-0.776823	0.021359
			H-w	3.170386	0.776823	0.021359
$UO_2F_4(H_2O)^{2-}$ long distance water in the plane	Struct. 2	SCF Gas-phase	U	-0.214889	0.000000	0.000000
			F	1.485608	1.520565	0.000000
			F	1.485608	-1.520565	0.000000
			F	-1.757975	1.626659	0.000000
			F	-1.757975	-1.626659	0.000000
			O-yl	-0.215840	0.000000	1.735693
			O-yl	-0.215840	0.000000	-1.735693
			O-w	3.866588	0.000000	0.000000
			H-w	3.255755	0.730714	0.000000
			H-w	3.255755	-0.730714	0.000000
$UO_2F_4(H_2O)^{2-}$ long distance water in the plane	Struct. 2	SCF + CPCM	U	0.000000	0.000000	0.000000
			O	0.000000	0.000000	1.745498
			O	0.000000	0.000000	-1.745498
			O	4.070740	0.000000	0.000000
			F	1.683809	-1.491596	0.000000
			F	1.683809	1.491596	0.000000
			F	-1.518578	-1.627222	0.000000
			F	-1.518578	1.627222	0.000000
			H	3.478804	-0.741611	0.000000
			H	3.478804	0.741611	0.000000
$UO_2F_4(H_2O)^{2-}$ long distance water out of the plane	Struct. 3	SCF Gas-phase	U	-0.233156	0.000000	0.000000
			F	1.457106	1.494634	0.000000
			F	1.457106	-1.494634	0.000000
			F	-1.784406	1.628868	0.000000
			F	-1.784406	-1.628868	0.000000
			O-yl	-0.234763	0.000000	1.739637

			O-yl	-0.234763	0.000000	-1.739637
			Ow	4.257428	0.000000	0.000000
			Hw	3.647591	0.000000	0.722732
			Hw	3.647591	0.000000	-0.722732
$UO_2F_4(H_2O)^{2-}$ long distance water out of the plane	Struct. 3	SCF + CPCM	U	0.000000	0.000000	0.000000
			O	0.000000	0.000000	1.749008
			O	-0.015080	0.000000	-1.748943
			O	4.881838	0.000000	-0.021046
			F	1.551073	-1.598196	-0.006687
			F	1.551073	1.598196	-0.006687
			F	-1.591106	-1.568675	0.006859
			F	-1.591106	1.568675	0.006859
			H	4.308488	0.000000	0.736372
			H	4.301979	0.000000	-0.773491
$UO_2F_5^{3-}$	Struct. 4	SCF Gas-phase	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.764318
			O-yl	0.000000	0.000000	-1.764318
			F	2.344757	0.000000	0.000000
			F	0.724570	2.229996	0.000000
			F	0.724570	-2.229996	0.000000
			F	-1.896948	1.378213	0.000000
			F	-1.896948	-1.378214	0.000000
$UO_2F_5^{3-}$	Struct. 4	SCF + CPCM	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.759353
			O-yl	0.000000	0.000000	-1.759353
			F	2.292244	0.000000	0.000000
			F	0.708342	2.180054	0.000000
			F	0.708342	-2.180054	0.000000
			F	-1.854464	1.347347	0.000000
			F	-1.854464	-1.347347	0.000000
$UO_2(OH)_4^{2-}$ hydroxide in the plane	Struct. 5a	SCF Gas-phase	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.751060
			O-yl	0.000000	0.000000	-1.751060
			O-hyd	2.359157	-0.103701	0.000000
			O-hyd	-2.359157	0.103701	0.000000
			O-hyd	0.103701	2.359157	0.000000
			O-hyd	-0.103701	-2.359157	0.000000
			H-hyd	2.779736	0.738582	0.000000
			H-hyd	-2.779736	-0.738582	0.000000
			H-hyd	-0.738582	2.779736	0.000000
			H-hyd	0.738582	-2.779736	0.000000
$UO_2(OH)_4^{2-}$ hydroxide in the plane	Struct. 5a	SCF + CPCM	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.765821
			O-yl	0.000000	0.000000	-1.765821
			O-hyd	2.295698	0.000390	0.000000
			O-hyd	-2.295698	-0.000390	0.000000
			O-hyd	-0.000390	2.295698	0.000000
			O-hyd	0.000390	-2.295698	0.000000
			H-hyd	2.935574	0.700749	0.000000
			H-hyd	-2.935574	-0.700749	0.000000

			H-hyd	-0.700749	2.935574	0.000000
			H-hyd	0.700749	-2.935574	0.000000
$UO_2(OH)_4^{2-}$ trans "2 up, 2 down"	Struct. 5b	SCF Gas-phase	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.762796
			O-yl	0.000000	0.000000	-1.762796
			O-hyd	0.000000	2.335674	0.007767
			O-hyd	0.000000	-2.335674	0.007767
			O-hyd	-2.335674	0.000000	-0.007767
			O-hyd	2.335674	0.000000	-0.007767
			H-hyd	0.000000	2.690959	-0.863182
			H-hyd	0.000000	-2.690959	-0.863182
			H-hyd	-2.690959	0.000000	0.863182
			H-hyd	2.690959	0.000000	0.863182
$UO_2(OH)_4^{2-}$ trans "2 up, 2 down"	Struct. 5b	SCF + CPCM	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.767643
			O-yl	0.000000	0.000000	-1.767643
			O-hyd	0.000000	2.298455	0.038069
			O-hyd	0.000000	-2.298455	0.038069
			O-hyd	-2.298455	0.000000	-0.038069
			O-hyd	2.298455	0.000000	-0.038069
			H-hyd	0.000000	2.756587	-0.794296
			H-hyd	0.000000	-2.756587	-0.794296
			H-hyd	-2.756587	0.000000	0.794296
			H-hyd	2.756587	0.000000	0.794296
$UO_2(OH)_4(H_2O)^{2-}$	Struct. 6a	SCF Gas-phase	U	-0.067401	0.000000	0.000000
			O-yl	-0.044284	0.000000	1.737139
			O-yl	-0.044284	0.000000	-1.737139
			O-w	2.543892	0.000000	0.000000
			O-hyd	1.103195	2.115442	0.000000
			O-hyd	1.103195	-2.115442	0.000000
			O-hyd	-1.874678	1.560099	0.000000
			O-hyd	-1.874678	-1.560099	0.000000
			H-w	3.027143	0.805440	0.000000
			H-w	3.027143	-0.805440	0.000000
			H-hyd	0.434240	2.778581	0.000000
			H-hyd	0.434240	-2.778581	0.000000
			H-hyd	-2.741136	1.196245	0.000000
			H-hyd	-2.741136	-1.196245	0.000000
$UO_2(OH)_4(H_2O)^{2-}$	Struct. 6a	SCF + CPCM	U	-0.065803	0.000000	0.000000
			O-yl	-0.044048	0.000000	1.764302
			O-yl	-0.044048	0.000000	-1.764302
			O-w	2.527089	0.000000	0.000000
			O-hyd	0.955757	2.127911	0.000000
			O-hyd	0.955757	-2.127911	0.000000
			O-hyd	-1.875468	1.482039	0.000000
			O-hyd	-1.875468	-1.482039	0.000000
			H-w	3.067584	0.782301	0.000000
			H-w	3.067584	-0.782301	0.000000
			H-hyd	0.325041	2.837661	0.000000
			H-hyd	0.325041	-2.837661	0.000000
			H-hyd	-2.763967	1.148608	0.000000

			H-hyd	-2.763967	-1.148608	0.000000
$UO_2(OH)_4(H_2O)^{2-}$ Trans "1 up 1 down"	Struct. 6b	SCF Gas-phase	U	-0.077564	0.000000	0.000000
			O-yl	-0.089137	0.235034	1.728356
			O-yl	-0.089137	-0.235034	-1.728356
			O-hyd	1.152084	2.083662	-0.300865
			O-hyd	1.152084	-2.083662	0.300865
			O-hyd	-1.828108	1.554030	-0.235197
			O-hyd	-1.828108	-1.554030	0.235197
			O-w	2.535176	0.000000	0.000000
			H-hyd	0.483421	2.729316	-0.449999
			H-hyd	0.483421	-2.729316	0.449999
			H-hyd	-2.310760	1.624535	0.569573
			H-hyd	-2.310760	-1.624535	-0.569573
			H-w	3.013813	0.798573	-0.125245
			H-w	3.013813	-0.798573	0.125245
$UO_2(OH)_4(H_2O)^{2-}$ water in the plane at long distance	Struct. 7a	SCF Gas-phase	U	-0.198636	0.000000	0.000000
			O-yl	-0.209751	0.000000	1.736570
			O-yl	-0.209751	0.000000	-1.736570
			O-w	3.882782	0.000000	0.000000
			O-hyd	1.496662	1.637006	0.000000
			O-hyd	1.496662	-1.637006	0.000000
			O-hyd	-1.859497	1.667449	0.000000
			O-hyd	-1.859497	-1.667449	0.000000
			H-w	3.274229	0.735878	0.000000
			H-w	3.274229	-0.735878	0.000000
			H-hyd	1.239593	2.541260	0.000000
			H-hyd	1.239593	-2.541260	0.000000
			H-hyd	-2.778549	1.473368	0.000000
			H-hyd	-2.778549	-1.473368	0.000000
$UO_2(OH)_4(H_2O)^{2-}$ water in the plane at long distance	Struct. 7a	SCF + CPCM	U	-0.243669	0.000000	0.000000
			O-yl	-0.251286	0.000000	1.763482
			O-yl	-0.251286	0.000000	-1.763482
			O-w	3.733740	0.000000	0.000000
			O-hyd	1.431037	1.606860	0.000000
			O-hyd	1.431037	-1.606860	0.000000
			O-hyd	-1.856480	1.620875	0.000000
			O-hyd	-1.856480	-1.620875	0.000000
			H-w	3.130028	0.739748	0.000000
			H-w	3.130028	-0.739748	0.000000
			H-hyd	1.323511	2.551020	0.000000
			H-hyd	1.323511	-2.551020	0.000000
			H-hyd	-2.799479	1.520229	0.000000
			H-hyd	-2.799479	-1.520229	0.000000
$UO_2(OH)_4(H_2O)^{2-}$ Trans "2 up, 2 down" water in the plane at long distance	Struct. 7b	SCF Gas-phase	U	-0.216204	0.000000	0.000000
			O-yl	-0.223891	0.012429	1.750023
			O-yl	-0.223891	-0.012429	-1.750023
			O-hyd	1.509422	1.604966	-0.056941
			O-hyd	1.509422	-1.604966	0.056941
			O-hyd	-1.798681	1.686769	-0.032581
			O-hyd	-1.798681	-1.686769	0.032581
			O-w	3.896731	0.000000	0.000000

			H-hyd	1.514110	2.054691	-0.884011
			H-hyd	1.514110	-2.054691	0.884011
			H-hyd	-2.034719	1.991520	0.825255
			H-hyd	-2.034719	-1.991520	-0.825255
			H-w	3.276682	0.726362	0.043227
			H-w	3.276682	-0.726362	-0.043227
$UO_2(OH)_4(H_2O)^{2-}$ long water out of the plane	Struct. 8	SCF Gas-phase	U	-0.248638	0.000000	0.000000
			O-yl	-0.260050	0.000000	1.739631
			O-yl	-0.260050	0.000000	-1.739631
			O-w	4.331538	0.000000	0.000000
			O-hyd	1.507107	1.558457	0.000000
			O-hyd	1.507107	-1.558457	0.000000
			O-hyd	-1.787777	1.772317	0.000000
			O-hyd	-1.787777	-1.772317	0.000000
			H-w	3.714137	0.000000	0.717466
			H-w	3.714137	0.000000	-0.717466
			H-hyd	1.370969	2.487593	0.000000
			H-hyd	1.370969	-2.487593	0.000000
			H-hyd	-1.511341	2.670105	0.000000
			H-hyd	-1.511341	-2.670105	0.000000
$UO_2(OH)_4(H_2O)^{2-}$ long water out of the plane	Struct. 8	SCF + CPCM	U	-0.242072	0.000000	0.000000
			O-yl	-0.248406	0.000000	1.762374
			O-yl	-0.248406	0.000000	-1.762374
			O-w	3.729168	0.000000	0.000000
			O-hyd	1.429237	1.610826	0.000000
			O-hyd	1.429237	-1.610826	0.000000
			O-hyd	-1.858978	1.616734	0.000000
			O-hyd	-1.858978	-1.616734	0.000000
			H-w	3.125606	0.739915	0.000000
			H-w	3.125606	-0.739915	0.000000
			H-hyd	1.318938	2.554525	0.000000
			H-hyd	1.318938	-2.554525	0.000000
			H-hyd	-2.800725	1.504417	0.000000
			H-hyd	-2.800725	-1.504417	0.000000
$UO_2(OH)_5^{3-}$	Struct. 9	SCF Gas-phase	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.755757
			O-yl	0.000000	0.000000	-1.755757
			O-hyd	2.471243	-0.094024	0.000000
			O-hyd	0.853078	2.321237	0.000000
			O-hyd	-1.944012	1.528628	0.000000
			O-hyd	0.674234	-2.379347	0.000000
			O-hyd	-2.054544	-1.376493	0.000000
			H-hyd	2.625466	0.837128	0.000000
			H-hyd	0.015158	2.755653	0.000000
			H-hyd	-2.616098	0.865959	0.000000
			H-hyd	-1.631995	-2.220461	0.000000
			H-hyd	1.607470	-2.238280	0.000000
$UO_2F_4.(H_2O)(H_2O)_3^{2-}$	Struct. 10	SCF Gas-phase	U	0.175775	0.000000	0.000000
			F	1.301914	2.035728	0.000000
			F	1.301914	-2.035728	0.000000
			F	-1.584804	1.466198	0.000000

			F	-1.584804	-1.466198	0.000000
			O-yl	0.206449	0.000000	1.725969
			O-yl	0.206449	0.000000	-1.725969
			O-w	2.836696	0.000000	0.000000
			O-ws	-0.535213	4.123515	0.000000
			O-ws	-0.535213	-4.123515	0.000000
			O-ws	-4.001351	0.000000	0.000000
			H-w	3.339979	0.793188	0.000000
			H-w	3.339979	-0.793188	0.000000
			H-ws	-1.181074	3.426509	0.000000
			H-ws	-1.181074	-3.426509	0.000000
			H-ws	0.264040	3.604374	0.000000
			H-ws	0.264040	-3.604374	0.000000
			H-ws	-3.389764	0.728353	0.000000
			H-ws	-3.389764	-0.728353	0.000000
$UO_2F_4.(H_2O)_4^{2-}$	Struct. 11	SCF Gas-phase	U	0.000492	0.000000	0.000000
			F	1.607645	1.606475	0.000000
			F	1.607645	-1.606475	0.000000
			F	-1.607054	1.607225	0.000000
			F	-1.607054	-1.607225	0.000000
			O-yl	0.000904	0.000000	1.724197
			O-yl	0.000904	0.000000	-1.724197
			O-ws	4.031386	0.000000	0.000000
			O-ws	0.000343	4.035838	0.000000
			O-ws	0.000343	-4.035838	0.000000
			O-ws	-4.041367	0.000000	0.000000
			H-ws	3.435262	0.739029	0.000000
			H-ws	3.435262	-0.739029	0.000000
			H-ws	-0.738986	3.440042	0.000000
			H-ws	-0.738986	-3.440042	0.000000
			H-ws	0.739006	3.439281	0.000000
			H-ws	0.739006	-3.439281	0.000000
			H-ws	-3.445138	0.738936	0.000000
			H-ws	-3.445138	-0.738936	0.000000
$UO_2F_4.(H_2O)(H_2O)_3^{2-}$ Long water out of the equatorial plane	Struct. 12	SCF Gas-phase	U	-0.020089	0.000000	0.000000
			F	1.566550	1.598250	0.000000
			F	1.566550	-1.598250	0.000000
			F	-1.636576	1.607514	0.000000
			F	-1.636576	-1.607514	0.000000
			O-yl	-0.018788	0.000000	1.727500
			O-yl	-0.018788	0.000000	-1.727500
			O-w	4.530416	0.000000	0.000000
			O-ws	-0.010876	4.027364	0.000000
			O-ws	-0.010876	-4.027364	0.000000
			O-ws	-4.061044	0.000000	0.000000
			H-w	3.933046	0.000000	0.731577
			H-w	3.933046	0.000000	-0.731577
			H-ws	-0.753798	3.435924	0.000000
			H-ws	-0.753798	-3.435924	0.000000
			H-ws	0.723402	3.424565	0.000000
			H-ws	0.723402	-3.424565	0.000000
			H-ws	-3.463874	0.738527	0.000000

			H-ws	-3.463874	-0.738527	0.000000
$UO_2(OH)_4.(H2O)(H_2O)_4^{2-}$	Struct. 13	SCF Gas-phase	U	0.442004	0.000000	0.000000
			O-yl	0.440426	0.000000	1.730935
			O-yl	0.440426	0.000000	-1.730935
			O-w	3.037564	0.000000	0.000000
			O-hyd	1.569928	2.086763	0.000000
			O-hyd	1.569928	-2.086763	0.000000
			O-hyd	-1.468118	1.545179	0.000000
			O-hyd	-1.468118	-1.545179	0.000000
			O-ws	-2.231232	4.162592	0.000000
			O-ws	-2.231232	-4.162592	0.000000
			O-ws	-5.295604	0.000000	0.000000
			H-w	3.523379	0.804361	0.000000
			H-w	3.523379	-0.804361	0.000000
			H-hyd	0.980810	2.820488	0.000000
			H-hyd	0.980810	-2.820488	0.000000
			H-hyd	-2.271099	1.057107	0.000000
			H-hyd	-2.271099	-1.057107	0.000000
			H-ws	-3.155747	3.991616	0.000000
			H-ws	-3.155747	-3.991616	0.000000
			H-ws	-1.834764	3.273229	0.000000
			H-ws	-1.834764	-3.273229	0.000000
			H-ws	-4.719875	0.747424	0.000000
			H-ws	-4.719875	-0.747424	0.000000
$UO_2(OH)_4.(H_2O)_4^{2-}$	Struct. 14	SCF Gas-phase	U	0.000000	0.000000	0.000000
			O-yl	0.000000	0.000000	1.728567
			O-yl	0.000000	0.000000	-1.728567
			O-hyd	2.288054	-0.612997	0.000000
			O-hyd	-2.288054	0.612997	0.000000
			O-hyd	0.622237	2.284519	0.000000
			O-hyd	-0.622237	-2.284519	0.000000
			O-ws	3.020119	3.617104	0.000000
			O-ws	-3.020119	-3.617104	0.000000
			O-ws	-3.731992	2.940345	0.000000
			O-ws	3.731992	-2.940345	0.000000
			H-hyd	2.897392	0.104398	0.000000
			H-hyd	-2.897392	-0.104398	0.000000
			H-hyd	-0.082721	2.907987	0.000000
			H-hyd	0.082721	-2.907987	0.000000
			H-ws	2.142663	3.205423	0.000000
			H-ws	-2.142663	-3.205423	0.000000
			H-ws	3.272376	-2.086496	0.000000
			H-ws	-3.272376	2.086496	0.000000
			H-ws	-3.032921	3.569930	0.000000
			H-ws	3.032921	-3.569930	0.000000
			H-ws	-3.611100	-2.885078	0.000000
			H-ws	3.611100	2.885078	0.000000
$UO_2(OH)_4.(H2O)(H_2O)_4^{2-}$ long water out of the plane	Struct. 15	SCF Gas-phase	U	0.281252	0.000000	0.000000
			O-yl	0.248097	0.000000	1.733639
			O-yl	0.248097	0.000000	-1.733639
			O-w	4.821617	0.000000	0.000000
			O-hyd	1.893307	1.620222	0.000000

			O-hyd	1.893307	-1.620222	0.000000
			O-hyd	-1.519599	1.631529	0.000000
			O-hyd	-1.519599	-1.631529	0.000000
			O-ws	-2.020594	4.332578	0.000000
			O-ws	-2.020594	-4.332578	0.000000
			O-ws	-5.464650	0.000000	0.000000
			H-w	4.213546	0.000000	0.724171
			H-w	4.213546	0.000000	-0.724171
			H-hyd	1.795075	2.553557	0.000000
			H- hyd	1.795075	-2.553557	0.000000
			H- hyd	-2.370184	1.230618	0.000000
			H- hyd	-2.370184	-1.230618	0.000000
			H-ws	-2.956650	4.244299	0.000000
			H-ws	-2.956650	-4.244299	0.000000
			H-ws	-1.705347	3.414807	0.000000
			H-ws	-1.705347	-3.414807	0.000000
			H-ws	-4.890143	0.747944	0.000000
			H-ws	-4.890143	-0.747944	0.000000
$UO_2F_3(H_2O)_2^-$ non neighbourging water in the plane	Struct. 16	SCF Gas-phase	U	-0.042509	0.000000	0.000000
			F	2.174518	0.000000	0.000000
			F	-1.557892	1.654125	0.000000
			F	-1.557892	-1.654125	0.000000
			O-yl	-0.033720	0.000000	1.722109
			O-yl	-0.033720	0.000000	-1.722109
			O-w	0.810468	2.542416	0.000000
			O-w	0.810468	-2.542416	0.000000
			H-w	-0.001195	3.026222	0.000000
			H-w	-0.001195	-3.026222	0.000000
			H-w	1.565862	3.098850	0.000000
			H-w	1.565862	-3.098850	0.000000
$UO_2F_3(H_2O)_2^-$ non neighbourging water out of the plane	Struct. 17	SCF Gas-phase	U	0.236338	0.000000	0.000000
			F	2.396463	0.000000	0.000000
			F	-0.850603	1.899933	0.000000
			F	-0.850603	-1.899933	0.000000
			O-yl	0.227327	0.000000	1.717668
			O-yl	0.227327	0.000000	-1.717668
			O-w	-2.161719	4.420931	0.000000
			O-w	-2.161719	-4.420931	0.000000
			H-w	-1.882347	3.889519	0.728354
			H-w	-1.882347	-3.889519	0.728354
			H-w	-1.882347	3.889519	-0.728354
			H-w	-1.882347	-3.889519	-0.728354
$UO_2F_3(H_2O)_2^-$ non neighbourging water molecules (C_1)	Struct. 18	SCF Gas-phase	U	-0.044575	-0.000729	-0.032699
			O	0.019817	-0.001384	1.702939
			O	-0.081423	0.001222	-1.759973
			O	0.812099	2.611226	0.111597
			O	0.866938	-2.594129	0.113023
			F	2.153688	0.022675	0.005426
			F	-1.563153	1.640221	0.069476
			F	-1.530749	-1.669675	0.065057
			H	-0.090480	2.833072	0.308603
			H	1.322295	2.669873	0.901309

			H	1.380324	-2.635630	0.901829
			H	-0.029439	-2.836035	0.313814
$UO_2F_3(H_2O)_2^-$ non neighbourging water molecules (C_1)	Struct. 18	SCF + CPCM	U	-0.000016	-0.110310	-0.000711
			O	0.002801	-0.112208	-1.740195
			O	-0.001224	-0.094415	1.738807
			O	-2.382473	0.843781	-0.007750
			O	2.381732	0.848985	0.007151
			F	-1.494567	-1.759554	0.004472
			F	1.499821	-1.755692	0.003491
			F	-0.006939	2.127083	-0.009398
			H	-2.548254	1.779615	-0.057928
			H	-3.214090	0.388729	0.076290
			H	2.561627	1.779570	0.092265
			H	3.208013	0.382295	-0.065924
$UO_2F_3(H_2O)_2^-$ neighbourging water molecules in the plane	Struct. 19	SCF Gas-phase	U	0.147801	0.000000	0.000000
			F	2.299875	0.000000	0.000000
			F	0.078219	2.259158	0.000000
			F	0.078219	-2.259158	0.000000
			O-yl	0.080838	0.000000	1.717048
			O-yl	0.080838	0.000000	-1.717048
			O-w	-2.32944	1.545844	0.000000
			O-w	-2.32944	-1.545844	0.000000
			H-w	-1.70910	2.268976	0.000000
			H-w	-3.21124	1.865618	0.000000
			H-w	-1.70910	-2.268976	0.000000
			H-w	-3.21124	-1.865618	0.000000
$UO_2F_3(H_2O)_2^-$ neighbourging water out of the plane	Struct. 20	SCF Gas-phase	U	0.147801	0.000000	0.000000
			F	2.299875	0.000000	0.000000
			F	0.078219	2.259158	0.000000
			F	0.078219	-2.259158	0.000000
			O	0.080838	0.000000	1.717048
			O	0.080838	0.000000	-1.717048
			O	-2.32944	1.545844	0.000000
			O	-2.32944	-1.545844	0.000000
			H	-1.70910	2.268976	0.000000
			H	-3.21124	1.865618	0.000000
			H	-1.70910	-2.268976	0.000000
			H	-3.21124	-1.865618	0.000000
$UO_2F_3(H_2O)_2^-$ neighbourging water molecules (C_1)	Struct. 21	SCF Gas-phase	U	0.282356	0.072163	0.010594
			F	2.383851	-0.374889	-0.315857
			F	-0.016081	2.251951	0.087382
			F	-0.876007	-1.853167	0.059260
			O	0.516618	0.002126	1.723008
			O	0.009092	0.132672	-1.697652
			O	-2.265753	0.708746	0.344827
			O	-3.499449	-1.791030	-0.332488
			H	-2.338541	1.573276	-0.026595
			H	-2.913194	0.125176	-0.032262
			H	-3.853148	-2.197696	0.439451

			H	-2.554911	-1.959062	-0.291366
$UO_2F_3(H_2O)_2^-$ neighbourging water molecules (C_1)	Struct. 21	SCF + CPCM	U	0.125891	-0.000301	0.000359
			O	0.045146	0.000805	-1.737146
			O	0.149462	-0.003720	1.738448
			O	-2.069919	1.394331	0.074174
			O	-2.076494	-1.382059	0.079965
			F	2.341097	-0.005303	-0.071406
			F	0.471217	-2.208156	-0.002037
			F	0.485516	2.202174	0.004766
			H	-2.911836	-1.198140	-0.341260
			H	-1.926928	-2.321328	0.008808
			H	-2.895024	1.238764	-0.377829
			H	-1.914195	2.335094	0.051850

Table S2. Mulliken atomic charges for the different compounds and population of the *7s*, *6p*, *6d* and *5f* orbitals on the uranium atom.

Complex	Method	U	O_{uranyl}	(OH)/F	*7s*	*6p*	*6d*	*5f*
$UO_2F_4^{2-}$	Gas Phase	2.44	-0.70	-0.76	0.092	5.934	1.447	2.087
	SCF + CPCM	2.36	-0.68	-0.75	0.091	5.940	1.497	2.110
$UO_2(OH)_4^{2-}$	Gas Phase	2.48	-0.70	-0.77	0.006	5.906	1.484	2.129
	SCF + CPCM	2.49	-0.74	-0.75	-0.032	5.915	1.513	2.093
$UO_2F_5^{3-}$	SCF	2.64	-0.78	-0.81	0.087	5.936	1.360	1.975
	SCF + CPCM	2.43	-0-72	-0.80	0.092	5.954	1.499	2.026
$UO_2F_4(H2O)^{2-}$	SCF + CPCM	2.43	-0.68	-0.77	0.083	5.931	1.493	2.061
$UO_2(OH)_4(H2O)^{2-}$	SCF + CPCM	2.47	-0.73	-0.77	0.021	5.909	1.557	2.041
$UO_2F_3(H_2O)_2^-$ non-neighbouring water molecules in the plane	SCF Gas-phase	2.47	-0.64	-0.73	0.047	5.885	1.474	2.115
$UO_2F_3(H_2O)_2^-$ non-neighbouring water molecules out of the plane	SCF Gas-phase	2.29	-0.58	-0.72	0.080	5.884	1.573	2.169
$UO_2F_3(H_2O)_2^-$ Neighbouring water molecules in the plane	SCF Gas-phase	2.41	-0.61	-0.72	0.073	5.883	1.482	2.150
$UO_2F_3(H_2O)_2^-$ Neighbouring water molecules out of the plane	SCF Gas-phase	2.30	-0.62	-0.72	0.098	5.906	1.531	2.163
$UO_2F_3(H_2O)_2^-$	SCF Gas Phase	2.34	-0.62	-0.72	0.076	5.903	1.537	2.143
Non-neighbouring water molecules	SCF + CPCM	2.45	-0.66	-0.74	0.059	5.906	1.488	2.093

$UO_2F_3(H_2O)_2^-$	SCF Gas Phase	2.35	-0.62	-0.72	0.071	5.879	1.539	2.150
Neighbouring water	SCF + CPCM	2.41	-0.64	-0.75	0.080	5.909	1.488	2.107
molecules								