Supplementary Tables
for

Reduction of uranyl(VI) by iron (II) in solutions: ab initio study.

by

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Table S1. Calculated structure of four-ligand complexes of Fe(II) systems. The structures are obtained on the SCF level, bond distances are in Å. Ground state configurations are marked as (*), bond angles are given by numbers in square brackets [...].Label (b) marks the OH group of the bridge.

Complex	U-Oyl [OUOangle]	U-O (bridge) [angle]	U-Fe	Fe-O (bridge) [angle]	U-O(lig) [angle]	O-H bonds	Fe-O (lig) [angle]
Fig. S1a	1.82641 1.74032 [170.142]	2.34317 [73.216]	3.3091	2.03505 2.11684 [74.957]	2.10554 [122.978]	0.93944 0.9439 (b) 0.93486	1.81491 [----]
Fig. S1b	1.7525 [172.2]	2.66828 [66.524]	3.3604	1.84850 [104.690]	2.15 [116.925]	0.93894 0.94084	-----
Fig. 1a (*)	1.73584 [179.117]	2.35 [71.391]	3.42176	2.04143 [84.528]	2.12013	0.93983 0.94430(b) 0.93495	1.82658
Fig. S1c	1.7340 [163.080]	2.12541 [90.507]	3.39951	2.42923 [76.837]	-----	0.94230(b) 0.93522	1.85448 [149.665]

Table S2. Calculated structure of four-ligand complexes of Fe(III) systems. The structures are obtained on the SCF level, bond distances are in Å. Ground state configurations are marked as (*), bond angles are given by numbers in square brackets [...].Label (b) marks the OH group of the bridge.

Complex	U-Oyl [OUOangle]	U-O (bridge) [angle]	U-Fe	Fe-O (bridge) [angle]	U-O(lig) [angle]	O-H bonds	Fe-O (lig) [angle]
Fig. S2a	1.95713 [79.863]	-----	3.10578	2.03819 [76.099]	2.09122 [104.524]	0.93341 0.94096	1.79105 [122.671]
Fig. S2b	2.20493 1.81416 [150.283]	2.52401 [64.969]	3.30659	1.78230 1.901 [87.739]	2.10954 [114.165]	0.93949 0.94333(b) 0.93461	1.76766 [----]
Fig. S2c	1.80238 [169.716]	2.70026 [62.337]	3.48842	1.82775 [99.747]	2.15741 [----]	0.3943 0.94137(b) 0.93501	1.75805 [----]
Fig. 1b (*)	1.78231 [164.588]	2.39322 [67.057]	3.46883	1.97978 [83.779]	-----	0.9339 0.94478(b)	1.79783 [117.789]

Table S3. Relative energies in kJ/mol for the four-hydroxide U(VI)-Fe(II) complex with four hydroxide ions in gas phase and in solution obtained at the SCF level.

Complex	Gas phase	In solvent
Fig. S1c	208	--- (*)
Fig. S1b	166	65
Fig.S1a	21	36
Fig. 1a	0.0	0.0

(*) This complex did not converge in solution.

Table S4. Relative energies in kJ/mol for the four-hydroxide U(V)-Fe(III) complex with four hydroxide ions in gas phase and in solution obtained at the SCF level.

Complex	Gas phase	In solvent
Fig.S2a	141	119
Fig.S2b	61	89
Fig.S2c	10	77
Fig. 1b	0.0	0.0

Table S5. Calculated structure of four-ligand complexes of Fe(II)/Fe(III) systems with two additional water molecules. The structures are obtained on the SCF level, bond distances are in Å. Label (b) marks the OH group of the bridge, while label (w) marks the OH groups of water molecule.

	U-Oyl [OUOangle]	U-O (bridge) [angle]	U-Fe	Fe-O (bridge) [angle]	U-O(lig) [angle]	O-H bonds	Fe-O (lig) [angle]	HOH angle
Fe(II)	1.79797 [167.439]	2.45779 [65.484]	3.51192	1.96318 [85.239]	2.62442 [128.509]	0.943081(b) 0.93323 0.94576(w) 0.94527(w)	1.80612 [115.705]	111.726
Fe(II)	1.76017 [173.725]	2.54258 [67.544]	3.40783	1.91647 [95.037]	2.16354 [114.769]	0.93884 0.94161(b) 0.94477(w) 0.94893(w)	2.13162 106.464	112.395

Table S6. Calculated structure of five-ligand complexes of Fe(II)/Fe(III) systems. The structures are obtained on the SCF level, bond distances are in Å. Label (w) marks the OH groups of water molecule.

	U-Oyl [OUOangle]	U-O (bridge) [angle]	U-Fe	Fe-O (bridge) [angle]	U-O(lig) [angle]	O-H bonds	Fe-O (lig) [angle]
Fe(II)	1.76075 [177.334]	2.4678 [65.548]	3.52839	1.97359 [85.285]	2.19226 [112.044]	0.93868 0.94198(b) 0.93531	1.86338 [---]
Fe(III)	1.81345 [176.885]	2.53447 [64.862]	3.52085	1.93814 [89.061]	2.21702 [---]	0.93963 0.94194(b) 0.93710	1.84173 [111.172]

Table S7. Calculated structure of six-ligand complexes of Fe(II)/Fe(III) systems. The structures are obtained on the SCF level, bond distances are in Å.

	U-Oyl [OUOangle]	U-O (bridge) [angle]	U-Fe	Fe-O (bridge) [angle]	U-O(lig) [angle]	O-H bonds	Fe-O (lig) [angle]
Fe(II)	1.76920 [179.396]	2.37258 [68.38]	3.62307	2.2953 [77.522]	2.23740 [105.335]	0.93926 0.94271(b) 0.94711	1.99295 [120.482]
Fe(III)	1.75789 [176.652]	2.49944 [62.667]	3.55491	1.92503 [84.937]	2.18060 [114.798]	0.93722 0.94134 0.93862	1.84424 [110.865]

(a)

(b)

(c)

FigS1. a,b,c : isomers of the precursor complex. Distances are in Å (see detailed information in Table S1). The U(VI) is on the left hand side and Fe(II) on the right hand side of the complex.

(a)

(b)

(c)

FigS2. a,b,c : isomers of the successor complex. Distances are in Å (see detailed information in Table S2). The U(V) is on the left hand side and Fe(III) on the right hand side of the complex.

(a)

(b)

Fig.S3a,b SCF optimized geometry of precursor (a) and successor (b) complexes with four OH groups and two additional water molecules. Bond distances are in Å (see detailed information in Table S5). The U(VI)/U(V) is on the left hand side and Fe(II)/Fe(III) on the right hand side of the precursor/ successor complexes