Density Functional Theory (DFT) Calculations of VI/V Reduction Potentials of Uranyl Coordination Complexes in Non-aqueous Solutions

Krishnamoorthy Arumugam*[1, 2] and Neil A. Burton[1]

[1]School of Chemistry, Brunswick Street, The University of Manchester, Manchester, UK, M13 9PL (UK)

[2]Current address: National Post Doctoral Fellow, Simulation Center for Atomic and Nanoscale MATerials (SCANMAT), Central University of Tamil Nadu, Thiruvarur, Tamil Nadu 610101, India.
Email: krish.odc@gmail.com
Phone: 00 91 97861 38099

Electronic Supplementary Information

1. Computational details

This section provides details about density functional theory (DFT) methods, basis sets and solvation method used to investigate the reduction free energies (RFEs) of uranyl complexes. The U-atom has been described by using a small-core effective-core potential (SC-ECP) (Stuttgart-Dresden-Dolg-SDD), which contains 60 core electrons, combined with a segmented contracted Gaussian basis set to describe the valence electrons[1,2,3] such as $5s^2 5p^6 5d^{10} 6s^2 6p^6 5f^3 6d^1 7s^2$. The non-metal C, O, N, S and H atoms have been described by using a 6-31G* basis set. This combination of basis sets is denoted as the B1 basis. The SC-ECP, on U and the 6-311+G** basis set on all the other atoms is collectively denoted as the B2 basis. The DFT functionals used in this study are the hybrid, B3LYP[4,5,6,7] and M06[8] functionals. The model complexes have been optimised in the gas-phase at the B3LYP/B1 level of theory and confirmed to be minima on the potential energy surface by calculations of their frequencies at the same level of theory. Single point energies were then calculated using the B2 basis with a Conductor-like Polarisable Continuum model (CPCM)[9,10] for description of bulk solvent at the B3LYP/B1 geometries. The level of theory here is referred to as the B3LYP/B2(CPCM)//B3LYP/B1 level. Moreover, the M06 functional has been used for single point energy calculations at the B3LYP/B1 geometries with the CPCM solvation model employing the B2 basis and this level of theory is referred to as the M06/B2(CPCM)//B3LYP/B1 level. In the CPCM model, the solute cavities have been described by using the United-Atom Kohn-Sham (UAKS) cavity, which has been used to predict accurate aqueous solvation free energies of a range of solutes within ~0.11 eV of experiment[11] and accurate RFEs of various actinyl complexes and redox-active mineral bound actinyl aqua complexes in aqueous solution[12,13]. The solvents used in this study and their dielectric constants (ε) are:

- Dimethylsulfoxide (DMSO)(ε= 46.826)
- Dimethylformamide (DMF) (ε= 37.219)
- Dichloromethane (DCM) (ε= 8.93)
- Acetonitrile (ACN) (ε=35.688)
- Pyridine (Py) (ε=12.978)

The free energy and Zero-point energy (ZPE) corrections obtained from the B3LYP/B1 frequency calculations have been added to the solvation energies obtained using the B2 basis. The systems with unpaired electrons have been treated with the un-restricted formalism thorough-out this study. Spin-orbit coupling effects were not considered explicitly; however, the RFE values have been corrected with a spin-orbit coupling correction, –0.31eV, for the penta-valent uranyl(V) ion as determined by Hay *et al*.[14].

All the calculations were carried out using the Gaussian 03[15] except the solvation calculations for the solvent pyridine, which were carried out with the Gaussian 09 package[16]. There are no solvent parameters available for DMF in G03; hence, the required parameters such as ε=36.71, radius of the solvent = 2.647Å, density =0.007780 and ε (infinity) =1.75 have been specified using the 'Solvent' keyword. Construction of the uranyl model complexes and visualisation of results have been carried out with the Gauss View and Molden[17] software packages.

1.1. Classical Molecular dynamics of uranyl ion in DMSO

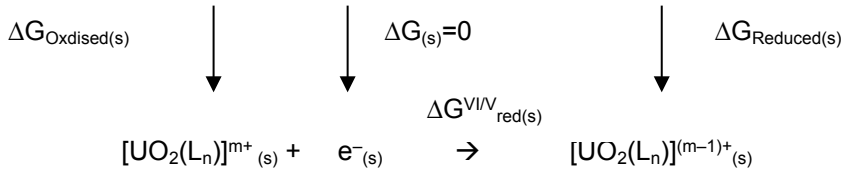
Classical molecular dynamics (MD) simulations were carried out to find the uranyl(VI) local coordination environment of DMSO molecules in the equatorial plane.. Classical MD simulations of the uranyl(VI) ion in a solvent box of DMSO have been carried out using the AMBER 10 molecular dynamics package[18]. The $[UO_2]^{2+}$ parameters[19] and DMSO solvent parameters[20] were obtained from the literature and pre-equilibrated DMSO solvent box was obtained from the Bryce's online amber parameter database[21].

A rectangular DMSO solvent box of size 20 Å was used for the simulation of the $[UO_2]^{2+}$ ion. The total number of DMSO molecules present was 531. Minimizations of $[UO_2]^{2+}$ in this DMSO box were carried out up to 9000 steps without any restraint on the uranyl ion. The systems were then heated up to 300 K using the Langevin dynamics with a collision frequency γ of 0.2 ps^{-1} for about 100 ps with a constant volume and a time step of 1 fs was used. Then the equilibrations of the system with a constant pressure of 1 bar for about 100 ps were performed and these were then followed by a final 1 *ns* production MD simulation. A non-bonded Ewald cut-off of 15 Å was used throughout these simulations. The coordinates were written to the 'mdcrd' file for every 0.1 ps and then these were used for the construction of the radial distribution function (RDF) of the $U\text{-}O_{DMSO}$ distances.

1.2. Reduction Free Energy prediction

With the help of a thermodynamic cycle, reduction free energies (RFE) in the gas and solution phase can be obtained. The thermodynamic cycle used for the determination of RFEs of oxidised and reduced uranyl complexes in the gas and solution phase are shown in Scheme. 1.

$$[UO_2(L_n)]^{m+}{}_{(g)} + e^-_{(g)} \xrightarrow{\Delta G^{VI/V}_{red(g)}} [UO_2(L_n)]^{(m-1)+}{}_{(g)}$$



Scheme 1. Thermodynamic cycle used for the RFE prediction of oxidised and reduced uranyl complexes in the gas and solution phase.

The predicted RFEs of the overall reduction process in solution are then referenced with respect to standard reference electrode free energies and directly compared with the available experimental RFEs. Two methods such as direct and isodesmic reaction methods are proposed for the determination of RFEs.

1.2.1 Direct method

The standard hydrogen electron (SHE) is used as the reference electrode for aqueous solution. For the non-aqueous solutions, the Fc/Fc^+ redox couple (eqn. 1) is widely employed as a reference electrode. The redox equation are provided below

$$Fc^+ + e^- \rightarrow Fc \quad (1)$$

$$[UO_2(L_n)]^{m+} + e^- \rightarrow [UO_2(L_n)]^{(m-1)+} \quad (2)$$

When the two redox equations (eqn. 1 and 2) are combined together, an overall redox equation is obtained (eqn.3); the RFE of the redox reaction (eqn.3) is computed using the thermodynamic cycle as discussed earlier (see Scheme. 1).

$$[UO_2(L_n)]^{m+} + Fc \rightarrow [UO_2(L_n)]^{(m-1)+} + Fc^+ \quad (3)$$

The following equations are used to determine the RFEs for VI/V reduction of uranyl complexes in non-aqueous solution.

$$\Delta G^{VI/V}_{red(s)} = \Delta G^{VI/V}_{red(g)} + \Delta\Delta G_{solv} \quad (4)$$

$$\Delta\Delta G_{solv} = \Delta G_{Reduced(s)} - \Delta G_{Oxdised(s)} \quad (5)$$

$$\Delta G_{red} = \Delta G^{VI/V}_{red(s)} - \Delta G_{red}^{ref.electrode} \quad (6)$$

where $\Delta G^{VI/V}_{red(g)}$ is the RFE of uranyl complexes in the gas-phase; $\Delta G_{Oxdised(s)}$ and $\Delta G_{Reduced(s)}$ are the solvation free energies of oxidised and reduced complexes, respectively; $\Delta\Delta G_{solv}$ is the difference between the solvation free energy of reduced and oxidised complexes ($\Delta G_{Reduced(s)}$ - $\Delta G_{Oxdised(s)}$). The absolute RFE for the uranyl(VI) to V reduction process, $\Delta G^{VI/V}_{red(s)}$ was determined by using the equation (4), then the equation (6) was utilized to obtain the RFE (ΔG_{red}) with respect to a reference electrode; $\Delta G_{red}^{ref.electrode}$ is the free energy of a reference electrode. The reference electrode for non-aqueous solutions is the Fc/Fc^+ electrode as recommended by the International Union of Pure and Applied Chemistry (IUPAC)[22].

1.2.2. Isodesmic models

Isodesmic reaction method is an alternative one and used to determine the RFEs of uranyl complexes in non-aqueous solutions. An example of isodesmic reaction is given below (see eqn. 7).

$$[UO_2(L_n)]^{m+} + [UO_2(L)_n]^{(m-1)+} \text{ (ref. complex)} \rightarrow$$

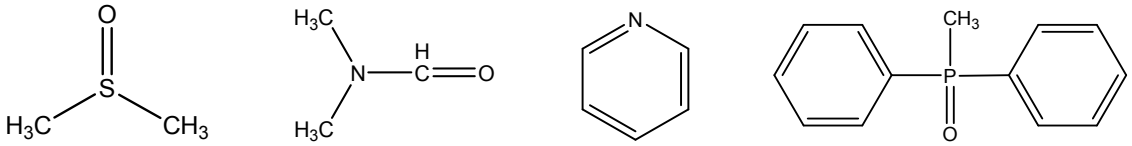
$$[UO_2(L)_n]^{m+} \text{ (ref. complex)} + [UO_2(L_n)]^{(m-1)+} \quad (7)$$

$$\Delta G_{red} = \Delta G^{VI/V}{}_{red(s)} + \Delta G_{red}{}^{ref.complex} \quad (8)$$

In the equation 8, the $\Delta G_{red}{}^{ref.complex}$ term represents the experimental RFE of the reference complex. The selection of a reference complex for the RFE determination under isodesmic reaction scheme and its consequences are discussed later. When two or more reference complexes are considered for the RFE prediction, employing the isodesmic reaction method, only the reference complex giving small mean un-signed error (MUE) of the predicted RFEs with respect to the experimental RFE are provided.

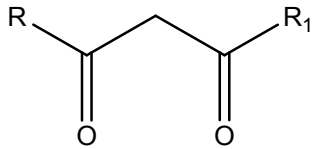
The advantage of the isodesmic reaction method over the other methods is the cancellation of errors. Other direct methods require the computation of reference electrode potentials; this procedure often ends up giving an imprecision value for the standard reference electrode. The isodesmic reaction method has been previously used to predict the reduction potentials of transition metal complexes[23,24] to within 0.08 eV of the experimental values. The important thing in this method is choosing a reference system which must have similar electronic and chemical properties to the other systems under consideration. If the reference system is not properly chosen, then, it may introduce systematic errors into the determination of reduction potentials. The experiments should typically have determined the reduction potentials of the reference complex and the other complexes in the same solvent and electrolyte conditions.

Figures

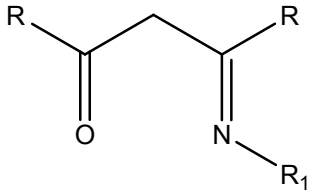


DMSO DMF Pyridine Ph_2MePO

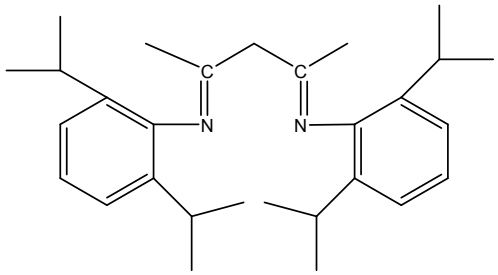
Figure S1. Mono-dentate ligand structures.



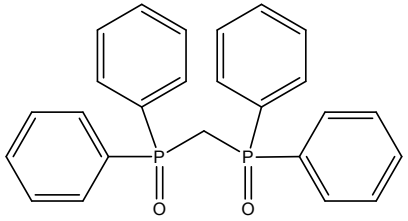
acac [R=R1=CH_3]
tfacac [R=CF_3, R1=CH_3]
hfacac [R=R1=CF_3]
dbm [R=R1=Ph]
btfacac [R=CF_3,R1=Ph]
ba [R=CH_3, R1=Ph]
dpm [R=R1=$C(CH_3)_3$]
ttfacac [R=CF_3, R1=C_4H_2S]
fod [R=$C(CH_3)_3$, R1= $(CF_2)_2CF_3$]



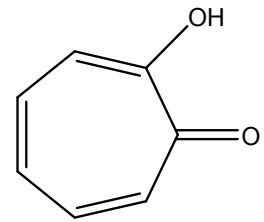
L2 [R=Ph, R1=Ph-(2,4,6-methyl)]
L3 [R=Ph, R1=Ph-(3,5-tert-butyl)]
L4 [R=Ph, R1=Ph-(2,6-isopropyl)]
L5 [R=Ph, R1=$C(CH_3)_3$]



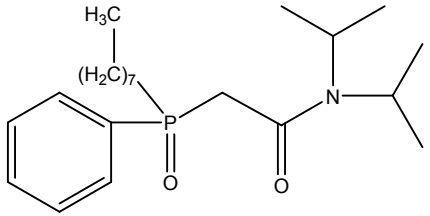
L1



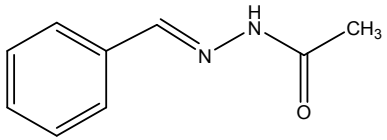
$DPPMO_2$



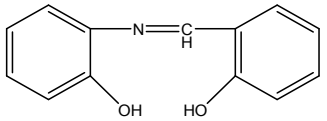
trop



CMPO

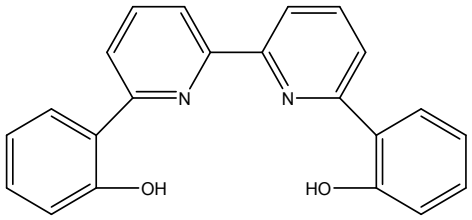


sldh

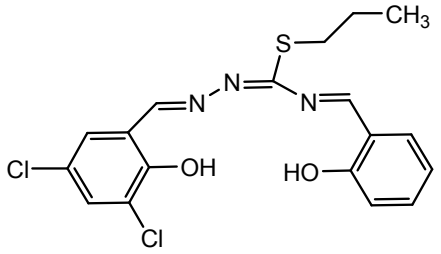


sap

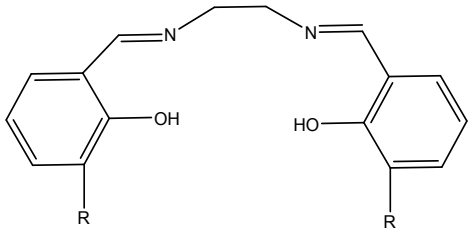
Figure S2. Bi-dentate ligands and tri-dentate ‘sap’ ligand structures.



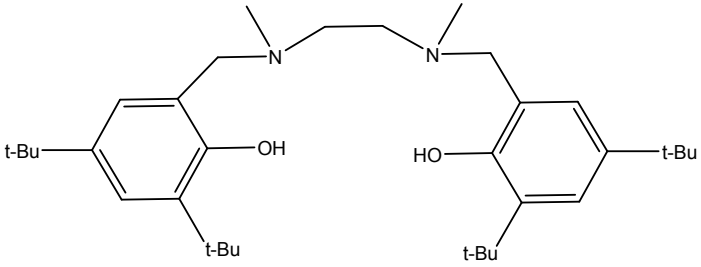
salbiby



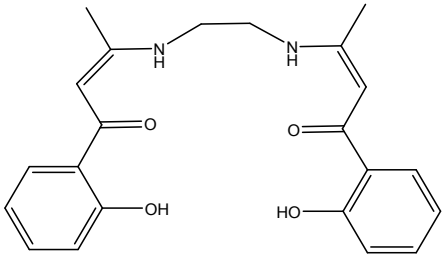
tsmc



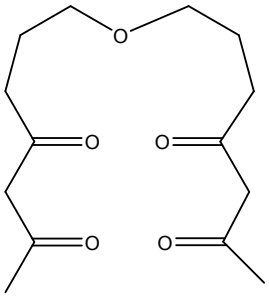
salen [R=H], salacen [R=COOH]



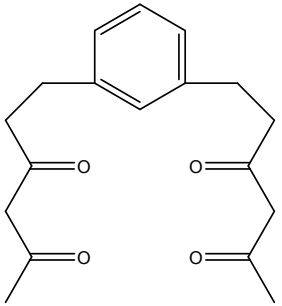
salan



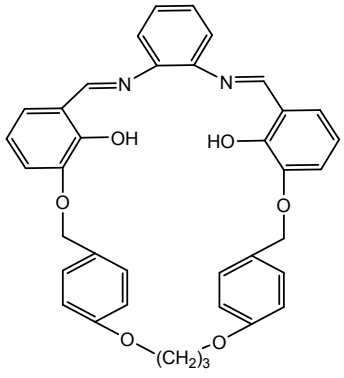
appn



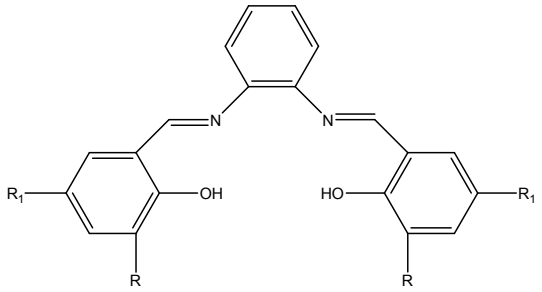
ac-o-ac



ac-ph-ac

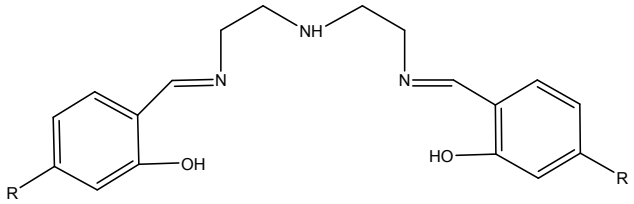


saloph2

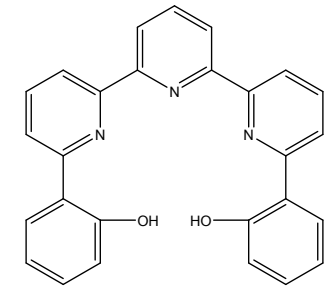


saloph	[R=R1=H]
saloph1	[R=O(CH2)-Ph, R1=H]
saloph3	[R=Ph, R1=H]
saloph4	[R=Ph-(2-OCH_3), R1=H]
saloph5	[R=OCH_3, R1=H]
saloph-tbu	[R=R1=$C(CH_3)_3$]

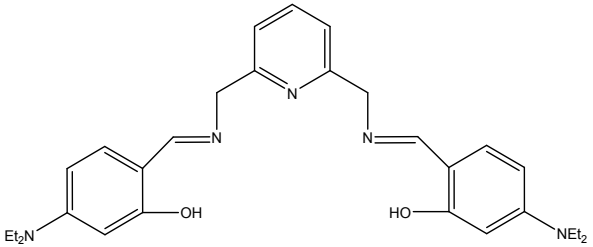
Figure S3. Tetra-dentate ligand structures.



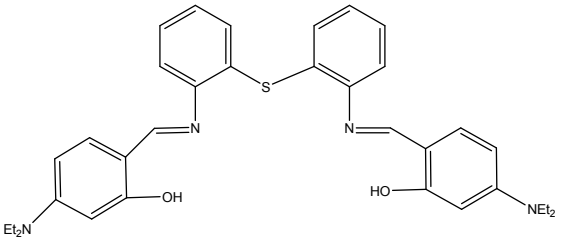
saldien [R=H], saldien-$(NEt_2)_2$ [R=NEt_2]



salterp

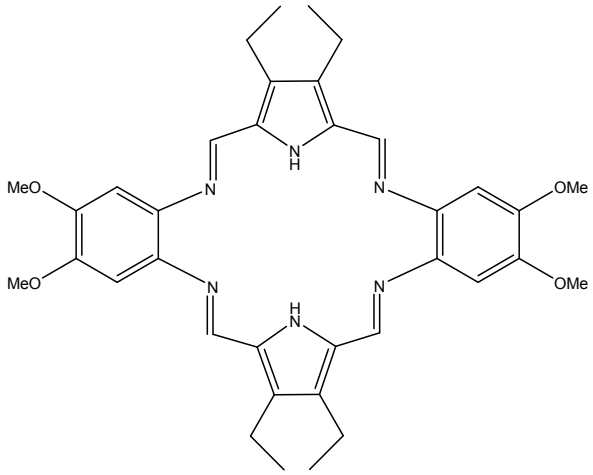


sal-ph-dien

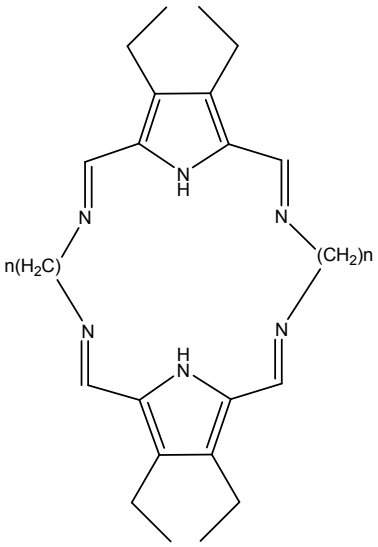


salddt

Figure S4. Penta-dentate ligand structures.



AP1



AP2 [n=2] and AP3 [n=3]

Figure S5. Hexa-dentate ligand structures.

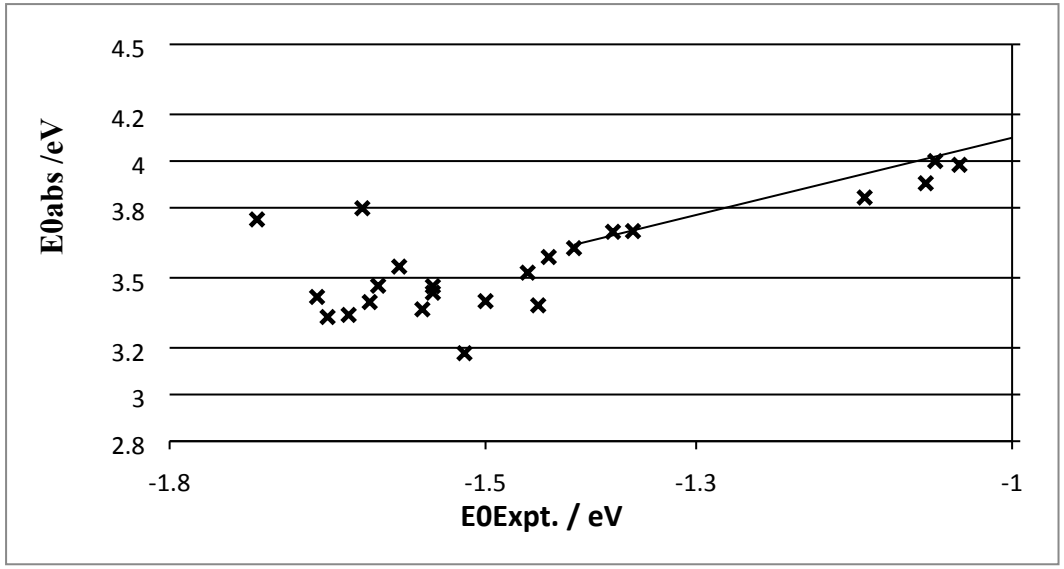


Figure S6. Absolute reduction potentials (E^0_{abs}) of the uranyl complexes computationally estimated in DMSO solution are plotted against the experimental reduction potentials ($E^0_{Expt.}$).

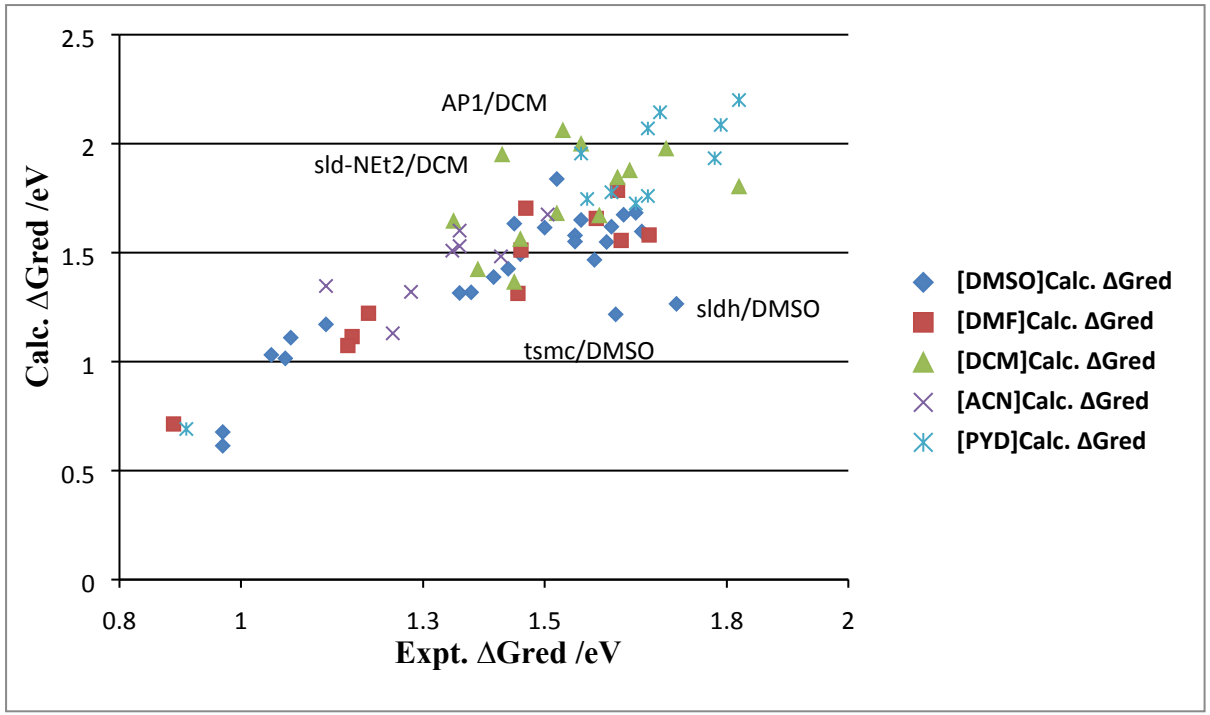


Figure S7. Plot of calculated uranyl(VI/V) REFs (Calc. ΔG_{red} includes the correction of Fc/Fc^{+} ref. 0.60 eV) at the B3LYP/B2(CPCM/UAKS)//B3LYP/B1 level of theory against the experimental RFEs (Expt. ΔG_{red}).

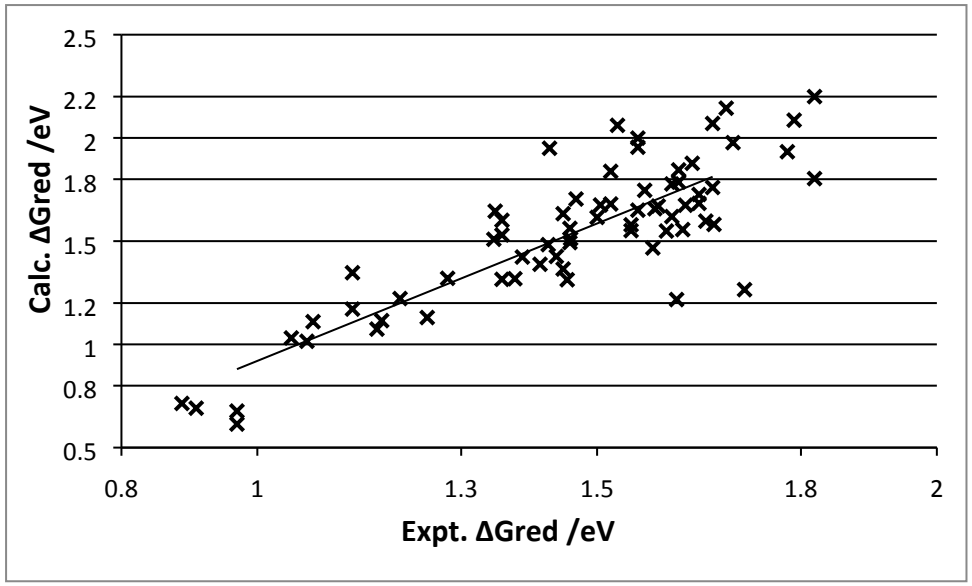


Figure S8. The plot of calculated uranyl(VI/V) REFs (Calc. ΔG_{red} includes the correction of Fc/Fc^{+} ref. 0.60 eV) at the B3LYP/B2(CPCM/UAKS)//B3LYP/B1 level of theory against the experimental RFEs (Expt. ΔG_{red}).

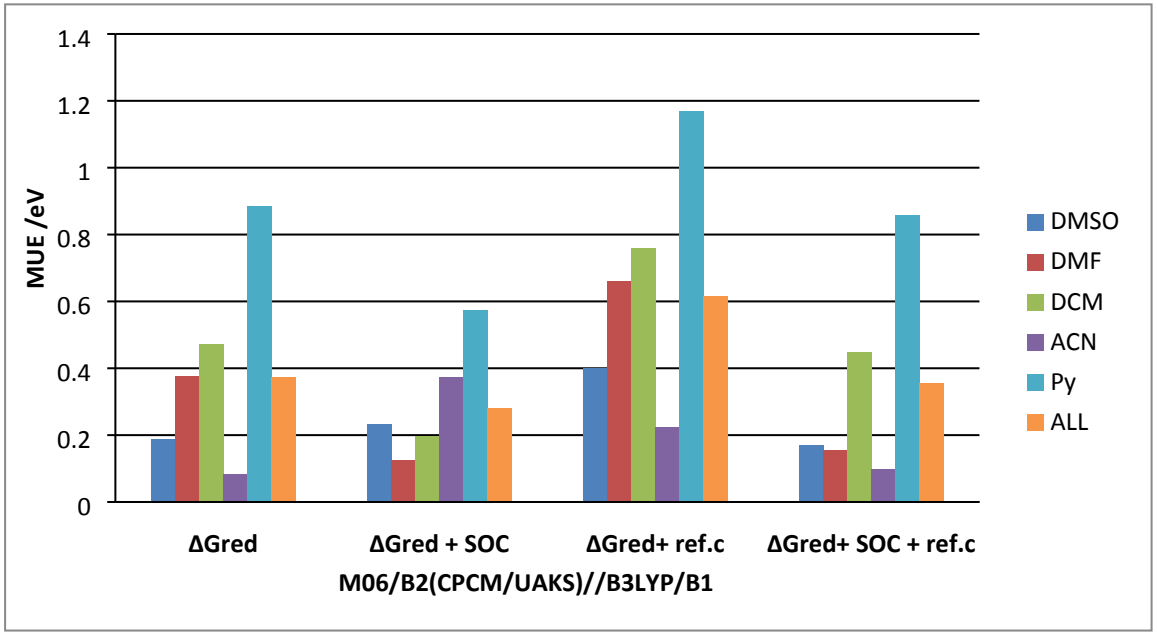


Figure S9. Mean unsigned errors (MUEs) for the predicted reduction free energies (RFEs) of investigated uranyl complexes at the M06/B2(CPCM/UAKS)//B3LYP/B1 level of theory.

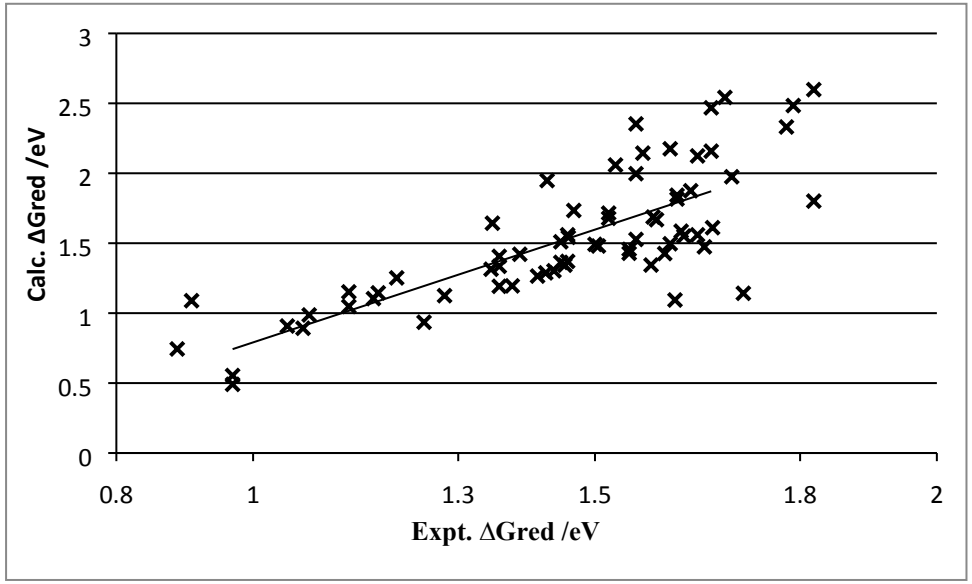


Figure S10. Plot of calculated uranyl(VI/V) REFs (Calc. ΔG_{red} are predicted using empirically estimated Fc/Fc^{+} couples) against the experimental RFEs (Expt. ΔG_{red}) at the B3LYP/B2(CPCM/UAKS)//B3LYP/B1 level of theory.

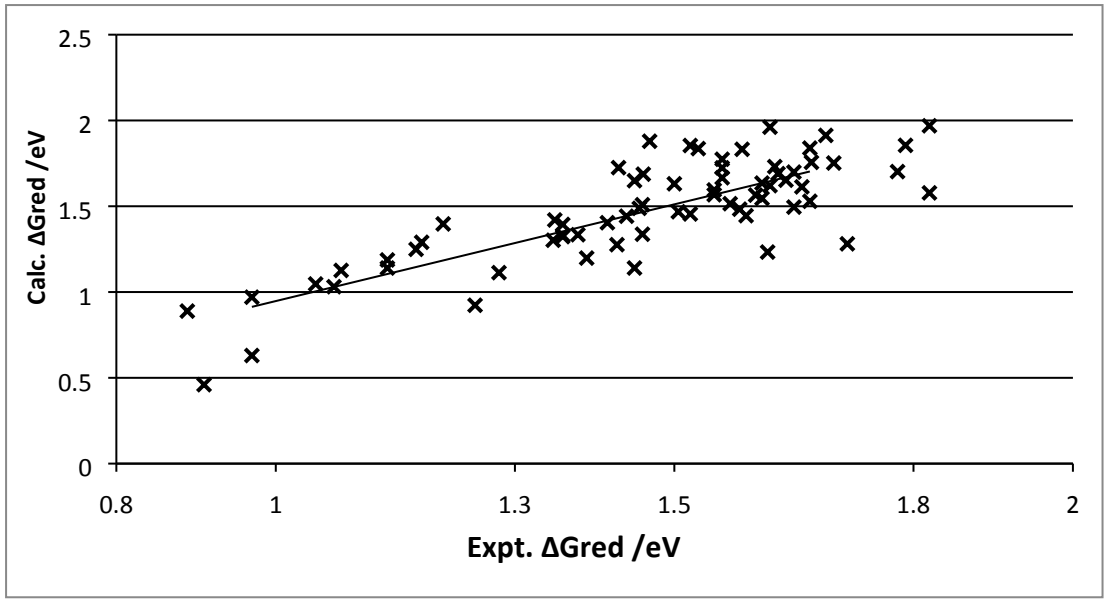


Figure S11. Plot of calculated uranyl(VI/V) REFs (Isodesmic model reference complexes: $[UO_2\text{-}(DMSO)_5.7DMSO]^{2+/+}$, $[UO_2\text{-}(DMF)_5]^{2+/+}$, $[UO_2\text{-salddt-NEt2}]^{0/-}$, $[UO_2\text{-(L4+DP)}]^{1+/0}$ and $[UO_2\text{-}(PY)_5]^{2+/+}$ (–0.46 eV)) against the experimental RFEs (Expt. ΔG_{red}).

Tables

Table S1. Experimental uranyl(VI/V) reduction free energies (RFEs) of uranyl complexes reported in various non-aqueous solution (eV).

Sl. No.	Uranyl complexes	[ΔG_{red}]	Reference
	DMSO		
1	$[UO_2\text{-}(DMSO)_5]^{2+/+}$	0.970	ref [25]
2	$[UO_2\text{-}(salen)\text{-}DMSO]^{0/1-}$	1.602	ref [25]
3	$[UO_2\text{-}(saloph)\text{-}DMSO]^{0/1-}$	1.550	ref [26]
4	$[UO_2\text{-}saldien]^{0/1-}$	1.582	ref [27]
5	$[UO_2\text{-}(acac)_2\text{-}DMSO]^{0/1-}$	1.440	ref [25,28]
6	$[UO_2\text{-}(trop)_2\text{-}DMSO]^{0/1-}$	1.379	ref [25]
7	$[UO_2\text{-}(sap)\text{-}(DMSO)_2]^{0/1-}$	1.500	ref [25]
8	$[UO_2\text{-}(dbm)_2\text{-}DMSO]^{0/1-}$	1.360	ref [28]
9	$[UO_2\text{-}(hfacac)_2\text{-}DMSO]^{0/1-}$	0.970	ref [29,28]
10	$[UO_2\text{-}(dpm)_2\text{-}DMSO]^{0/1-}$	1.520	ref [29]
11	$[UO_2\text{-}(btfacac)_2\text{-}DMSO]^{0/1-}$	1.073	ref [25]
12	$[UO_2\text{-}(tfacac)_2\text{-}DMSO]^{0/1-}$	1.050	ref [28]
13	$[UO_2\text{-}(ttfacac)_2\text{-}DMSO]^{0/1-}$	1.082	ref [25]
14	$[UO_2\text{-}(tsmc)\text{-}(Nyl\text{-}OH)]^{0/1-}$	1.617[a]	ref [30]
15	$[UO_2\text{-}(sldh)(AcO)\text{-}DMSO]^{0/1-}$	1.717[a]	ref [31]
16	$[UO_2\text{-}salterp\ ]^{0/1-}$	1.560	ref [32]
17	$[UO_2\text{-}(salddt\text{-}NEt_2)]^{0/1-}$	1.550	ref [32]
18	$[UO_2\text{-}(salacen)\text{-}DMSO]^{0/1-}$	1.140	ref [33]
19	$[UO_2\text{-}(appen)\text{-}DMSO]^{0/1-}$	1.650	ref [33]
20	$[UO_2\text{-}(ac\text{-}o\text{-}ac)\text{-}DMSO]^{0/1-}$	1.450	ref [34]
21	$[UO_2\text{-}(ac\text{-}ph\text{-}ac)\text{-}DMSO]^{0/1-}$	1.460	ref [34]
22	$[UO_2\text{-}(salbiby)\text{-}DMSO]^{0/1-}$	1.610	ref [32]
23	$[UO_2\text{-}saldien\text{-}(NEt_2)_2]^{0/1-}$	1.660	ref [32]
24	$[UO_2\text{-}(sal\text{-}ph\text{-}dien)]^{0/1-}$	1.630	ref [32]

25	$[UO_2\text{-}(ba)_2\text{-}DMSO]^{0/1-}$	1.416	ref [25]
	DMF		
26	$[UO_2\text{-}salen\text{-}DMF]^{0/1-}$	1.672	ref [35, 36]
27	$[UO_2\text{-}saloph\text{-}DMF]^{0/1-}$	1.626	ref [26]
28	$[UO_2\text{-}(acac)_2\text{-}DMF]^{0/1-}$	1.469	ref [35, 36]
29	$[UO_2\text{-}(DMF)_5]^{2+/+}$	0.889	ref [35, 36]
30	$[UO_2\text{-}(trop)_2\text{-}DMF]^{0/1-}$	1.456	ref [35]
31	$[UO_2\text{-}sap\text{-}(DMF)_2]^{0/1-}$	1.585	ref [35]
32	$[UO_2\text{-}(dbm)_2\text{-}DMF]^{0/1-}$	1.461	ref [35]
33	$[UO_2\text{-}(btfacac)_2\text{-}DMF]^{0/1-}$	1.183	ref [35]
34	$[UO_2\text{-}(ttfacac)_2\text{-}DMF]^{0/1-}$	1.176	ref [35]
35	$[UO_2\text{-}(fod)2\text{-}DMF]^{0/1-}$	1.210	ref [29]
36	$[UO_2\text{-}salbiby\text{-}DMF]^{0/1-}$	1.620	ref [32]
	DCM		
37	$[UO_2(L1)\text{-}(acac)]^{0/1-}$	1.820	ref [37]
38	$[UO_2(L1)\text{-}(dbm)]^{0/1-}$	1.590	ref [37]
39	$[UO_2(L1)\text{-}(hfacac)]^{0/1-}$	1.390	ref [37]
40	$[UO_2\text{-}(L2)_2)]^{0/1-}$	1.520	ref [38]
41	$[UO_2\text{-}(L3)_2)]^{0/1-}$	1.350	ref [38]
42	$[UO_2\text{-}(L4+M)]^{+/0}$	1.450	ref [39]
43	$[UO_2\text{-}(L5)_2)]^{0/1-}$	1.460	ref [40]
44	$[UO_2\text{-}saldien\text{-}(NEt_2)_2]^{0/1-}$	1.430	ref [32]
45	$[UO_2\text{-}sal\text{-}ph\text{-}dien]^{0/1-}$	1.560	ref [32]
46	$[UO_2\text{-}AP1]^{0/1-}$	1.530	ref [41]
47	$[UO_2\text{-}AP2]^{0/1-}$	1.700	ref [41]
48	$[UO_2\text{-}AP3]^{0/1-}$	1.640	ref [41]
49	$[UO_2\text{-}salddt]^{0/1-}$	1.620	ref [32]
	Acetonitrile		
50	$[UO_2\text{-}(L4+DP)]^{1+/0}$	1.140	ref [39]
51	$[UO_2\text{-}tsmc\text{-}(Nyl\text{-}OH)]^{0/1-}$	1.280[b]	ref [30]

52	$[UO_2\text{-saloph1-}H_2O]^{0/1-}$	1.360[c]	ref [42]
53	$[UO_2\text{-saloph2-}H_2O]^{0/1-}$	1.428[c]	ref [42]
54	$[UO_2\text{-saloph3-}H_2O]^{0/1-}$	1.360[c]	ref [42]
55	$[UO_2\text{-saloph4-}H_2O]^{0/1-}$	1.505[c]	ref [42]
56	$[UO_2\text{-saloph5-}H_2O]^{0/1-}$	1.348[c]	ref [42]
57	$[UO_2\text{-(CMPO + 2}NO_3)]^{0/1-}$	1.250	ref [43]
	Pyridine		
58	$[UO_2\text{-(Py)}_5]^{2+/+}$	0.910	ref [44]
59	$[UO_2\text{-salen-Py}]^{0/1-}$	1.610	ref [32]
60	$[UO_2\text{-saloph-Py}]^{0/1-}$	1.570	ref [32]
61	$[UO_2\text{-salan-tBu}_2\text{-Py}]^{0/1-}$	1.820	ref [44]
62	$[UO_2\text{-saloph-tBu}_2\text{-Py}]^{0/1-}$	1.670	ref [44]
63	$[UO_2\text{-saloph-tBu}_2\text{-Py-K}]^{+/0}$	1.650	ref [44]
64	$[UO_2\text{-saldien-(NEt}_2)_2]^{0/1-}$	1.780	ref [32]
65	$[UO_2\text{-salterp}]^{0/1-}$	1.690	ref [32]
66	$[UO_2\text{-sal-ph-dien}]^{0/1-}$	1.790	ref [32]
67	$[UO_2\text{-salddt}]^{0/1-}$	1.560	ref [32]
68	$[UO_2\text{-salbiby-Py}]^{0/1-}$	1.670	ref [32]

[a] The uranyl(VI/V) reduction potentials were reported with respect the SCE reference electrode in DMSO; to convert the reported values with respect to the Fc/Fc^+ –0.575 eV has to be added. (Fc/Fc^+ [-0.53 eV] *vs* Ag/Ag^+ and Ag/Ag^+ [-0.047 eV] *vs* SCE).

[b] The uranyl(VI/V) reduction potentials were reported with respect to the SCE reference electrode in ACN solvent; to convert the reported values with respect to the Fc/Fc^+ –0.380 eV has to be added.

[c] The uranyl(VI/V) reduction potentials were reported with respect the Ag/Ag^+ reference electrode in ACN solvent; to convert the reported values with respect to the Fc/Fc^+ –0.420 eV has to be added.

Table S2. Abbreviations of the ligands investigated in this study.

Short name	Full name
acac	Acetylacetonate

ac-o-ac	8-oxo-2,4,12-tetraoxapenta decane
ac-ph-ac	m-bis(2,4-dioxo-1-pentyl)benzene
ba	benzoyl acetonate
btfacac	benzoyl trifluoroacetylacetonate
CMPO	n-Octyl(phenyl)-N,N-diisobutylcarbamoylmethylphosphine oxide
dbm	Dibenzoylmethanate
DPPMO2	Bis(diphenylphosphino)methanedioxide
DMSO	Dimethylsulfoxide
DMF	Dimethylformamide
dpm	Dipivalylmethanate
hfacac	Hexafluoroacetylacetonate
fod	Heptafluorobutanoyl-pivaloylmethanate
sap	salicylidine-2-aminophenol
salbipy	6,6'-Bis(2-hydroxyphenyl)-2,2'-bipyridine
salen	Bis(salicylidene)ethylenediamine
saloph	Bis(salicylidene)phenylenediamine
salterp	6,6-Bis(2-hydroxyphenyl)-2,2-6', 2'-terpyridine
saldien($Et_2N)_2$	N,N'-Bis((4-diethylamino)salicylidene) diethylenetriamine
saldien	N,N′-disalicylidenediethylenetriaminate
sal-ph-dien	N,N'-Bis((4-(diethylamino)salicylidene) diamino methyl pyridine
salddt	N,N'-Bis((4-diethylamino)salicylidene)2,2'-diaminodiphenyl thioether
sldh	salicylaldehyde-acetyl hydrazone
tsmc	N^1-3,5-dichlorosalicylidene-N^4-salicylidene-S-methylthiosemicarbazidate
tfacac	Trifluroacetylacetonate
ttfacac	Thoinyltrifluroacetylacetonate
trop	Tropolonate
TPPO	Tri phenyl phosphine oxide
salacen	see the reference [33] for the synthesis and name
appn	see the reference [33] for the synthesis and name

DIRECT METHOD

Table S3. The B3LYP/B2(CPCM/UAKS)//B3LYP/B1 level of theory predicted RFEs of uranyl complexes.

Spin-Orbit Coupling (SOC) = –0.31 eV; reference electrode (Fc/Fc^{+}) correction (ref.c) = 0.60 eV

	Complexes	Expt.	$\Delta G^{VI/V}_{red(s)}$	ΔG_{red}	ΔG_{red} + SOC	ΔG_{red} + ref.c	ΔG_{red} + SOC + ref.c
	DMSO						
1	$[UO_2\text{-}(DMSO)_5]^{2+/+}$	0.970	-4.338	0.077	-0.233	0.677	0.367
2	$[UO_2\text{-salen-DMSO}]^{0/1-}$	1.602	-3.466	0.949	0.639	1.549	1.239
3	$[UO_2\text{-saloph-DMSO}]^{0/1-}$	1.550	-3.436	0.979	0.669	1.579	1.269
4	$[UO_2\text{-saldien}]^{0/1-}$	1.582	-3.548	0.867	0.557	1.467	1.157
5	$[UO_2\text{-}(acac)_2\text{-DMSO}]^{0/1-}$	1.440	-3.589	0.826	0.516	1.426	1.116
6	$[UO_2\text{-}(trop)_2\text{-DMSO}]^{0/1-}$	1.379	-3.697	0.718	0.408	1.318	1.008
7	$[UO_2\text{-sap-}(DMSO)_2]^{0/1-}$	1.500	-3.400	1.015	0.705	1.615	1.305
8	$[UO_2\text{-}(dbm)_2\text{-DMSO}]^{0/1-}$	1.360	-3.700	0.715	0.405	1.315	1.005
9	$[UO_2\text{-}(hfacac)_2\text{-DMSO}]^{0/1-}$	0.970	-4.401	0.014	-0.296	0.614	0.304
10	$[UO_2\text{-}(dpm)_2\text{-DMSO}]^{0/1-}$	1.520	-3.177	1.238	0.928	1.838	1.528
11	$[UO_2\text{-}(btfacac)_2\text{-DMSO}]^{0/1-}$	1.073	-4.000	0.415	0.105	1.015	0.705
12	$[UO_2\text{-}(ttfacac)_2\text{-DMSO}]^{0/1-}$	1.050	-3.984	0.431	0.121	1.031	0.721
13	$[UO_2\text{-}(tfacac)_2\text{-DMSO}]^{0/1-}$	1.082	-3.905	0.510	0.200	1.110	0.800
14	$[UO_2\text{-(tsmc)-(Nyl-OH)}]^{0/1-}$	1.617	-3.798	0.617	0.307	1.217	0.907
15	$[UO_2\text{-(sldh)(AcO)-DMSO}]^{0/1-}$	1.717	-3.750	0.665	0.355	1.265	0.955
16	$[UO_2\text{-salterp }]^{0/1-}$	1.560	-3.365	1.050	0.740	1.650	1.340
17	$[UO_2\text{-(salddt-}NEt_2)]^{0/1-}$	1.550	-3.464	0.951	0.641	1.551	1.241
18	$[UO_2\text{-(salacen)-DMSO}]^{0/1-}$	1.140	-3.844	0.571	0.261	1.171	0.861
19	$[UO_2\text{-appen-DMSO}]^{0/1-}$	1.650	-3.332	1.083	0.773	1.683	1.373
20	$[UO_2\text{-(ac-o-ac)-DMSO}]^{0/1-}$	1.450	-3.382	1.033	0.723	1.633	1.323
21	$[UO_2\text{-(ac-ph-ac)-DMSO}]^{0/1-}$	1.460	-3.522	0.893	0.583	1.493	1.183
22	$[UO_2\text{-salbiby-DMSO}]^{0/1-}$	1.610	-3.396	1.019	0.709	1.619	1.309
23	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.660	-3.418	0.997	0.687	1.597	1.287
24	$[UO_2\text{-(sal-ph-dien)}]^{0/1-}$	1.630	-3.341	1.074	0.764	1.674	1.364

25	$[UO_2\text{-}(ba)_2\text{-}DMSO]^{0/1-}$	1.416	-3.627	0.788	0.478	1.388	1.078
	DMF						
26	$[UO_2\text{-}salen\text{-}DMF]^{0/1-}$	1.672	-3.469	0.981	0.671	1.581	1.271
27	$[UO_2\text{-}saloph\text{-}DMF]^{0/1-}$	1.626	-3.494	0.956	0.646	1.556	1.246
28	$[UO_2\text{-}(acac)_2\text{-}DMF]^{0/1-}$	1.469	-3.346	1.104	0.794	1.704	1.394
29	$[UO_2\text{-}(DMF)_5]^{2+/+}$	0.889	-4.336	0.114	-0.196	0.714	0.404
30	$[UO_2\text{-}(trop)_2\text{-}DMF]^{0/1-}$	1.456	-3.737	0.713	0.403	1.313	1.003
31	$[UO_2\text{-}sap\text{-}(DMF)_2]^{0/1-}$	1.585	-3.393	1.057	0.747	1.657	1.347
32	$[UO_2\text{-}(dbm)_2\text{-}DMF]^{0/1-}$	1.461	-3.538	0.912	0.602	1.512	1.202
33	$[UO_2\text{-}(btfacac)_2\text{-}DMF]^{0/1-}$	1.183	-3.935	0.515	0.205	1.115	0.805
34	$[UO_2\text{-}(ttfacac)_2\text{-}DMF]^{0/1-}$	1.176	-3.976	0.474	0.164	1.074	0.764
35	$[UO_2\text{-}(fod)2\text{-}DMF]^{0/1-}$	1.210	-3.828	0.622	0.312	1.222	0.912
36	$[UO_2\text{-}salbiby\text{-}DMF]^{0/1-}$	1.620	-3.264	1.186	0.876	1.786	1.476
	DCM						
37	$[UO_2(L1)\text{-}(acac)]^{0/1-}$	1.820	-3.380	1.203	0.893	1.803	1.493
38	$[UO_2(L1)\text{-}(dbm)]^{0/1-}$	1.590	-3.513	1.070	0.760	1.670	1.360
39	$[UO_2(L1)\text{-}(hfacac)]^{0/1-}$	1.390	-3.760	0.823	0.513	1.423	1.113
40	$[UO_2\text{-}(L2)_2)]^{0/1-}$	1.520	-3.503	1.080	0.770	1.680	1.370
41	$[UO_2\text{-}(L3)_2)]^{0/1-}$	1.350	-3.538	1.045	0.735	1.645	1.335
42	$[UO_2\text{-}(L4+M)]^{+/0}$	1.450	-3.818	0.765	0.455	1.365	1.055
43	$[UO_2\text{-}(L5)_2)]^{0/1-}$	1.460	-3.621	0.962	0.652	1.562	1.252
44	$[UO_2\text{-}saldien\text{-}(NEt_2)_2]^{0/1-}$	1.430	-3.233	1.350	1.040	1.950	1.640
45	$[UO_2\text{-}sal\text{-}ph\text{-}dien]^{0/1-}$	1.560	-3.184	1.399	1.089	1.999	1.689
46	$[UO_2\text{-}AP1]^{0/1-}$	1.530	-3.122	1.461	1.151	2.061	1.751
47	$[UO_2\text{-}AP2]^{0/1-}$	1.700	-3.206	1.377	1.067	1.977	1.667
48	$[UO_2\text{-}AP3]^{0/1-}$	1.640	-3.306	1.277	0.967	1.877	1.567
49	$[UO_2\text{-}salddt]^{0/1-}$	1.620	-3.338	1.245	0.935	1.845	1.535
	ACN						
50	$[UO_2\text{-}(L4+DP)]^{1+/0}$	1.140	-3.777	0.747	0.437	1.347	1.037
51	$[UO_2\text{-}tsmc\text{-}(Nyl\text{-}OH)]^{0/1-}$	1.280	-3.804	0.720	0.410	1.320	1.010
52	$[UO_2\text{-}saloph1\text{-}H_2O]^{0/1-}$	1.360	-3.523	1.001	0.691	1.601	1.291

53	$[UO_2$-saloph2-$H_2O]^{0/1-}$	1.428	-3.641	0.883	0.573	1.483	1.173
54	$[UO_2$-saloph3-$H_2O]^{0/1-}$	1.360	-3.594	0.930	0.620	1.530	1.220
55	$[UO_2$-saloph4-$H_2O]^{0/1-}$	1.505	-3.449	1.075	0.765	1.675	1.365
56	$[UO_2$-saloph5-$H_2O]^{0/1-}$	1.348	-3.615	0.909	0.599	1.509	1.199
57	$[UO_2$-(CMPO + $2NO_3)]^{0/1-}$	1.250	-3.994	0.530	0.220	1.130	0.820
	Py						
58	$[UO_2$-$(Py)_5]^{2+/+}$	0.910	-4.888	0.091	-0.219	0.691	0.381
59	$[UO_2$-salen-Py$]^{0/1-}$	1.610	-3.802	1.177	0.867	1.777	1.467
60	$[UO_2$-saloph-Py$]^{0/1-}$	1.570	-3.833	1.146	0.836	1.746	1.436
61	$[UO_2$-salan-tBu_2-Py$]^{0/1-}$	1.820	-3.379	1.600	1.290	2.200	1.890
62	$[UO_2$-saloph-tBu_2-Py$]^{0/1-}$	1.670	-3.819	1.160	0.850	1.760	1.450
63	$[UO_2$-saloph-tBu_2-Py-K$]^{+/0}$	1.650	-3.853	1.126	0.816	1.726	1.416
64	$[UO_2$-saldien-$(NEt_2)_2]^{0/1-}$	1.780	-3.646	1.333	1.023	1.933	1.623
65	$[UO_2$-salterp$]^{0/1-}$	1.690	-3.435	1.544	1.234	2.144	1.834
66	$[UO_2$-sal-ph-dien$]^{0/1-}$	1.790	-3.493	1.486	1.176	2.086	1.776
67	$[UO_2$-salddt$]^{0/1-}$	1.560	-3.624	1.355	1.045	1.955	1.645
68	$[UO_2$-salbiby-Py$]^{0/1-}$	1.670	-3.509	1.470	1.160	2.070	1.760
	MUE	-	-	**0.527**	**0.837**	**0.162**	**0.266**

Table S4. The M06/B2(CPCM/UAKS)//B3LYP/B1 level of theory predicted RFEs of uranyl complexes.

Spin-Orbit Coupling (SOC) = –0.31 eV; reference electrode (Fc/Fc^+) correction (ref.c) = 0.285 eV

	Complexes	Expt.	$\Delta G^{VI/V}_{red(s)}$	ΔG_{red}	ΔG_{red} + SOC	ΔG_{red} + ref.c	ΔG_{red} + SOC + ref.c
	DMSO						
1	$[UO_2$-$(DMSO)_5]^{2+/+}$	0.970	-4.830	-0.096	-0.406	0.189	-0.121
2	$[UO_2$-salen-DMSO$]^{0/1-}$	1.602	-3.825	0.909	0.599	1.194	0.884
3	$[UO_2$-saloph-DMSO$]^{0/1-}$	1.550	-3.812	0.922	0.612	1.207	0.897
4	$[UO_2$-saldien$]^{0/1-}$	1.582	-3.882	0.852	0.542	1.137	0.827
5	$[UO_2$-$(acac)_2$-DMSO$]^{0/1-}$	1.440	-3.912	0.822	0.512	1.107	0.797
6	$[UO_2$-$(trop)_2$-DMSO$]^{0/1-}$	1.379	-4.036	0.698	0.388	0.983	0.673

7	$[UO_2\text{-sap-}(DMSO)_2]^{0/1-}$	1.500	-3.840	0.894	0.584	1.179	0.869
8	$[UO_2\text{-}(dbm)_2\text{-DMSO}]^{0/1-}$	1.360	-3.988	0.746	0.436	1.031	0.721
9	$[UO_2\text{-}(hfacac)_2\text{-DMSO}]^{0/1-}$	0.970	-4.607	0.127	-0.183	0.412	0.102
10	$[UO_2\text{-}(dpm)_2\text{-DMSO}]^{0/1-}$	1.520	-3.467	1.267	0.957	1.552	1.242
11	$[UO_2\text{-}(btfacac)_2\text{-DMSO}]^{0/1-}$	1.073	-4.275	0.459	0.149	0.744	0.434
12	$[UO_2\text{-}(ttfacac)_2\text{-DMSO}]^{0/1-}$	1.050	-4.265	0.469	0.159	0.754	0.444
13	$[UO_2\text{-}(tfacac)_2\text{-DMSO}]^{0/1-}$	1.082	-4.200	0.534	0.224	0.819	0.509
14	$[UO_2\text{-(tsmc)-(Nyl-OH)}]^{0/1-}$	1.617	-4.120	0.614	0.304	0.899	0.589
15	$[UO_2\text{-(sldh)(AcO)-DMSO}]^{0/1-}$	1.717	-4.092	0.642	0.332	0.927	0.617
16	$[UO_2\text{-salterp }]^{0/1-}$	1.560	-3.398	1.336	1.026	1.621	1.311
17	$[UO_2\text{-(salddt-}NEt_2)]^{0/1-}$	1.550	-3.827	0.907	0.597	1.192	0.882
18	$[UO_2\text{-(salacen)-DMSO}]^{0/1-}$	1.140	-4.210	0.524	0.214	0.809	0.499
19	$[UO_2\text{-appen-DMSO}]^{0/1-}$	1.650	-3.693	1.041	0.731	1.326	1.016
20	$[UO_2\text{-(ac-o-ac)-DMSO}]^{0/1-}$	1.450	-3.738	0.996	0.686	1.281	0.971
21	$[UO_2\text{-(ac-ph-ac)-DMSO}]^{0/1-}$	1.460	-3.855	0.879	0.569	1.164	0.854
22	$[UO_2\text{-salbiby-DMSO}]^{0/1-}$	1.610	-3.760	0.974	0.664	1.259	0.949
23	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.660	-3.765	0.969	0.659	1.254	0.944
24	$[UO_2\text{-(sal-ph-dien)}]^{0/1-}$	1.630	-3.710	1.024	0.714	1.309	0.999
25	$[UO_2\text{-}(ba)_2\text{-DMSO}]^{0/1-}$	1.416	-3.933	0.801	0.491	1.086	0.776
	DMF						
26	$[UO_2\text{-salen-DMF}]^{0/1-}$	1.672	-3.822	0.929	0.619	1.214	0.904
27	$[UO_2\text{-saloph-DMF}]^{0/1-}$	1.626	-3.834	0.917	0.607	1.202	0.892
28	$[UO_2\text{-}(acac)_2\text{-DMF}]^{0/1-}$	1.469	-3.773	0.978	0.668	1.263	0.953
29	$[UO_2\text{-}(DMF)_5]^{2+/+}$	0.889	-4.807	-0.056	-0.366	0.229	-0.081
30	$[UO_2\text{-}(trop)_2\text{-DMF}]^{0/1-}$	1.456	-4.072	0.679	0.369	0.964	0.654
31	$[UO_2\text{-sap-}(DMF)_2]^{0/1-}$	1.585	-3.773	0.978	0.668	1.263	0.953
32	$[UO_2\text{-}(dbm)_2\text{-DMF}]^{0/1-}$	1.461	-3.929	0.822	0.512	1.107	0.797
33	$[UO_2\text{-}(btfacac)_2\text{-DMF}]^{0/1-}$	1.183	-4.201	0.550	0.240	0.835	0.525
34	$[UO_2\text{-}(ttfacac)_2\text{-DMF}]^{0/1-}$	1.176	-4.236	0.515	0.205	0.800	0.490
35	$[UO_2\text{-(fod)2-DMF}]^{0/1-}$	1.210	-4.107	0.644	0.334	0.929	0.619
36	$[UO_2\text{-salbiby-DMF}]^{0/1-}$	1.620	-3.518	1.233	0.923	1.518	1.208

	DCM						
37	$[UO_2(L1)\text{-}(acac)]^{0/1-}$	1.820	-3.510	1.394	1.084	1.679	1.369
38	$[UO_2(L1)\text{-}(dbm)]^{0/1-}$	1.590	-3.637	1.267	0.957	1.552	1.242
39	$[UO_2(L1)\text{-}(hfacac)]^{0/1-}$	1.390	-3.802	1.102	0.792	1.387	1.077
40	$[UO_2\text{-}(L2)_2)]^{0/1-}$	1.520	-3.713	1.191	0.881	1.476	1.166
41	$[UO_2\text{-}(L3)_2)]^{0/1-}$	1.350	-3.764	1.140	0.830	1.425	1.115
42	$[UO_2\text{-}(L4+M)]^{+/0}$	1.450	-4.118	0.786	0.476	1.071	0.761
43	$[UO_2\text{-}(L5)_2)]^{0/1-}$	1.460	-3.906	0.998	0.688	1.283	0.973
44	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.430	-3.589	1.315	1.005	1.600	1.290
45	$[UO_2\text{-sal-ph-dien}]^{0/1-}$	1.560	-3.482	1.422	1.112	1.707	1.397
46	$[UO_2\text{-AP1}]^{0/1-}$	1.530	-3.156	1.748	1.438	2.033	1.723
47	$[UO_2\text{-AP2}]^{0/1-}$	1.700	-3.414	1.490	1.180	1.775	1.465
48	$[UO_2\text{-AP3}]^{0/1-}$	1.640	-3.638	1.266	0.956	1.551	1.241
49	$[UO_2\text{-salddt}]^{0/1-}$	1.620	-3.698	1.206	0.896	1.491	1.181
	ACN						
50	$[UO_2\text{-}(L4+DP)]^{1+/0}$	1.140	-4.035	0.714	0.404	0.999	0.689
51	$[UO_2\text{-tsmc-}(Nyl\text{-}OH)]^{0/1-}$	1.280	-4.127	0.622	0.312	0.907	0.597
52	$[UO_2\text{-saloph1-}H_2O]^{0/1-}$	1.360	-3.926	0.823	0.513	1.108	0.798
53	$[UO_2\text{-saloph2-}H_2O]^{0/1-}$	1.428	-3.953	0.796	0.486	1.081	0.771
54	$[UO_2\text{-saloph3-}H_2O]^{0/1-}$	1.360	-3.873	0.876	0.566	1.161	0.851
55	$[UO_2\text{-saloph4-}H_2O]^{0/1-}$	1.505	-3.743	1.006	0.696	1.291	0.981
56	$[UO_2\text{-saloph5-}H_2O]^{0/1-}$	1.348	-3.954	0.795	0.485	1.080	0.770
57	$[UO_2\text{-}(CMPO + 2NO_3)]^{0/1-}$	1.250	-4.182	0.567	0.257	0.852	0.542
	Py						
58	$[UO_2\text{-}(Py)_5]^{2+/+}$	0.910	-5.157	-0.647	-0.957	-0.362	-0.672
59	$[UO_2\text{-salen-Py}]^{0/1-}$	1.610	-4.168	0.342	0.032	0.627	0.317
60	$[UO_2\text{-saloph-Py}]^{0/1-}$	1.570	-4.234	0.276	-0.034	0.561	0.251
61	$[UO_2\text{-salan-}tBu_2\text{-Py}]^{0/1-}$	1.820	-3.810	0.700	0.390	0.985	0.675
62	$[UO_2\text{-saloph-}tBu_2\text{-Py}]^{0/1-}$	1.670	-4.186	0.324	0.014	0.609	0.299
63	$[UO_2\text{-saloph-}tBu_2\text{-Py-K}]^{+/0}$	1.650	-4.272	0.238	-0.072	0.523	0.213
64	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.780	-4.000	0.510	0.200	0.795	0.485

65	[UO_2-salterp] $^{0/1-}$	1.690	-3.214	1.296	0.986	1.581	1.271
66	[UO_2-sal-ph-dien] $^{0/1-}$	1.790	-3.764	0.746	0.436	1.031	0.721
67	[UO_2-salddt] $^{0/1-}$	1.560	-3.918	0.592	0.282	0.877	0.567
68	[UO_2-salbiby-Py] $^{0/1-}$	1.670	-3.785	0.725	0.415	1.010	0.700
	MUE	-	-	**0.656**	**0.960**	**0.396**	**0.681**

Isodesmic models

Table S5. The predicted RFEs of uranyl complexes using the Isodesmic models.

	Complexes		B3LYP/B2(CPCM/UAKS)//B3LYP/B1		M06/B2(CPCM/UAKS)//B3LYP/B1	
		Expt.				
	DMSO		ref: $[UO_2(DMSO)_5]^{2+/+}$	ref: $[UO_2(DMSO)_5]^{2+/+}$.7DMSO	ref: $[UO_2(DMSO)_5]^{2+/+}$	ref: $[UO_2(DMSO)_5]^{2+/+}$.7DMSO
1	[UO_2-$(DMSO)_5$]$^{2+/+}$	0.970	0.970	0.970	0.970	0.970
2	[UO_2-salen-DMSO]$^{0/1-}$	1.602	1.842	1.565	1.975	1.740
3	[UO_2-saloph-DMSO]$^{0/1-}$	1.550	1.872	1.595	1.988	1.753
4	[UO_2-saldien]$^{0/1-}$	1.582	1.760	1.483	1.918	1.683
5	[UO_2-$(acac)_2$-DMSO]$^{0/1-}$	1.440	1.719	1.442	1.888	1.653
6	[UO_2-$(trop)_2$-DMSO]$^{0/1-}$	1.379	1.611	1.334	1.764	1.529
7	[UO_2-sap-$(DMSO)_2$]$^{0/1-}$	1.500	1.908	1.631	1.960	1.725
8	[UO_2-$(dbm)_2$-DMSO]$^{0/1-}$	1.360	1.608	1.331	1.812	1.577
9	[UO_2-$(hfacac)_2$-DMSO]$^{0/1-}$	0.970	0.907	0.630	1.193	0.958
10	[UO_2-$(dpm)_2$-DMSO]$^{0/1-}$	1.520	2.131	1.854	2.333	2.098
11	[UO_2-$(btfacac)_2$-DMSO]$^{0/1-}$	1.073	1.308	1.031	1.525	1.290
12	[UO_2-$(ttfacac)_2$-DMSO]$^{0/1-}$	1.050	1.324	1.047	1.535	1.300
13	[UO_2-$(tfacac)_2$-DMSO]$^{0/1-}$	1.082	1.403	1.126	1.600	1.365
14	[UO_2-(tsmc)-(Nyl-OH)]$^{0/1-}$	1.617	1.510	1.233	1.680	1.445
15	[UO_2-(sldh)(AcO)-DMSO] $^{0/1-}$	1.717	1.558	1.281	1.708	1.473
16	[UO_2-salterp]$^{0/1-}$	1.560	1.943	1.666	2.402	2.167

17	$[UO_2$-(salddt-$NEt_2)]^{0/1-}$	1.550	1.844	1.567	1.973	1.738
18	$[UO_2$-(salacen)-DMSO$]^{0/1-}$	1.140	1.464	1.187	1.590	1.355
19	$[UO_2$-appen-DMSO$]^{0/1-}$	1.650	1.976	1.699	2.107	1.872
20	$[UO_2$-(ac-o-ac)-DMSO$]^{0/1-}$	1.450	1.926	1.649	2.062	1.827
21	$[UO_2$-(ac-ph-ac)-DMSO$]^{0/1-}$	1.460	1.786	1.509	1.945	1.710
22	$[UO_2$-salbiby-DMSO$]^{0/1-}$	1.610	1.912	1.635	2.040	1.805
23	$[UO_2$-saldien-$(NEt_2)_2]^{0/1-}$	1.660	1.890	1.613	2.035	1.800
24	$[UO_2$-(sal-ph-dien)$]^{0/1-}$	1.630	1.967	1.690	2.090	1.855
25	$[UO_2$-$(ba)_2$-DMSO$]^{0/1-}$	1.416	1.681	1.404	1.867	1.632
	DMF		ref : $[UO_2(DMF)_5]^{2+/+}$			
26	$[UO_2$-salen-DMF$]^{0/1-}$	1.672	1.756	1.756	1.874	1.874
27	$[UO_2$-saloph-DMF$]^{0/1-}$	1.626	1.731	1.731	1.862	1.862
28	$[UO_2$-$(acac)_2$-DMF$]^{0/1-}$	1.469	1.879	1.879	1.923	1.923
29	$[UO_2$-$(DMF)_5]^{2+/+}$	0.889	0.889	0.889	0.889	0.889
30	$[UO_2$-$(trop)_2$-DMF$]^{0/1-}$	1.456	1.488	1.488	1.624	1.624
31	$[UO_2$-sap-$(DMF)_2]^{0/1-}$	1.585	1.832	1.832	1.923	1.923
32	$[UO_2$-$(dbm)_2$-DMF$]^{0/1-}$	1.461	1.687	1.687	1.767	1.767
33	$[UO_2$-$(btfacac)_2$-DMF$]^{0/1-}$	1.183	1.290	1.290	1.495	1.495
34	$[UO_2$-$(ttfacac)_2$-DMF$]^{0/1-}$	1.176	1.249	1.249	1.460	1.460
35	$[UO_2$-(fod)2-DMF$]^{0/1-}$	1.210	1.397	1.397	1.589	1.589
36	$[UO_2$-salbiby-DMF$]^{0/1-}$	1.620	1.961	1.961	2.178	2.178
	DCM		ref: $[UO_2$-salddt$]^{0/1-}$			
37	$[UO_2$(L1)-(acac)$]^{0/1-}$	1.820	1.578	1.578	1.808	1.808
38	$[UO_2$(L1)-(dbm)$]^{0/1-}$	1.590	1.445	1.445	1.681	1.681
39	$[UO_2$(L1)-(hfacac)$]^{0/1-}$	1.390	1.198	1.198	1.516	1.516
40	$[UO_2$-$(L2)_2)]^{0/1-}$	1.520	1.455	1.455	1.605	1.605
41	$[UO_2$-$(L3)_2)]^{0/1-}$	1.350	1.420	1.420	1.554	1.554
42	$[UO_2$-(L4+M)$]^{+/0}$	1.450	1.140	1.140	1.200	1.200
43	$[UO_2$-$(L5)_2)]^{0/1-}$	1.460	1.337	1.337	1.412	1.412
44	$[UO_2$-saldien-$(NEt_2)_2]^{0/1-}$	1.430	1.725	1.725	1.729	1.729
45	$[UO_2$-sal-ph-dien$]^{0/1-}$	1.560	1.774	1.774	1.836	1.836

46	$[UO_2\text{-AP1}]^{0/1-}$	1.530	1.836	1.836	2.162	2.162
47	$[UO_2\text{-AP2}]^{0/1-}$	1.700	1.752	1.752	1.904	1.904
48	$[UO_2\text{-AP3}]^{0/1-}$	1.640	1.652	1.652	1.680	1.680
49	$[UO_2\text{-salddt}]^{0/1-}$	1.620	1.620	1.620	1.620	1.620
	ACN		ref: $[UO_2\text{-(L4+DP)}]^{1+/0}$			
50	$[UO_2\text{-(L4+DP)}]^{1+/0}$	1.140	1.140	1.140	1.140	1.140
51	$[UO_2\text{-tsmc-(Nyl-OH)}]^{0/1-}$	1.280	1.113	1.113	1.048	1.048
52	$[UO_2\text{-saloph1-}H_2O]^{0/1-}$	1.360	1.394	1.394	1.249	1.249
53	$[UO_2\text{-saloph2-}H_2O]^{0/1-}$	1.428	1.276	1.276	1.222	1.222
54	$[UO_2\text{-saloph3-}H_2O]^{0/1-}$	1.360	1.323	1.323	1.302	1.302
55	$[UO_2\text{-saloph4-}H_2O]^{0/1-}$	1.505	1.468	1.468	1.432	1.432
56	$[UO_2\text{-saloph5-}H_2O]^{0/1-}$	1.348	1.302	1.302	1.221	1.221
57	$[UO_2\text{-(CMPO + 2NO}_3)]^{0/1-}$	1.250	0.923	0.923	0.993	0.993
	Py		ref: $[UO_2\text{-(Py)}_5]^{2+/+}$	ref : $[UO_2\text{-(Py)}_5]^{2+/+}$ **[–0.46 eV]**	ref:$[UO_2(Py)_5]^{2+/+}$	ref: $[UO_2\text{-(Py)}_5]^{2+/+}$ **[–0.46 eV]**
58	$[UO_2\text{-(Py)}_5]^{2+/+}$	0.910	0.910	0.460	0.910	0.460
59	$[UO_2\text{-salen-Py}]^{0/1-}$	1.610	1.996	1.546	1.899	1.449
60	$[UO_2\text{-saloph-Py}]^{0/1-}$	1.570	1.965	1.515	1.833	1.383
61	$[UO_2\text{-salan-tBu}_2\text{-Py}]^{0/1-}$	1.820	2.419	1.969	2.257	1.807
62	$[UO_2\text{-saloph-tBu}_2\text{-Py}]^{0/1-}$	1.670	1.979	1.529	1.881	1.431
63	$[UO_2\text{-saloph-tBu}_2\text{-Py-K}]^{+/0}$	1.650	1.945	1.495	1.795	1.345
64	$[UO_2\text{-saldien-(NEt}_2)_2]^{0/1-}$	1.780	2.152	1.702	2.067	1.617
65	$[UO_2\text{-salterp}]^{0/1-}$	1.690	2.363	1.913	2.853	2.403
66	$[UO_2\text{-sal-ph-dien}]^{0/1-}$	1.790	2.305	1.855	2.303	1.853
67	$[UO_2\text{-salddt}]^{0/1-}$	1.560	2.174	1.724	2.149	1.699
68	$[UO_2\text{-salbiby-Py}]^{0/1-}$	1.670	2.289	1.839	2.282	1.832
	MUE	-	**0.240**	**0.125**	**0.316**	**0.211**

RFEs using empirical Fc/Fc^+ potentials

Table S6. The B3LYP/B2(CPCM/UAKS)//B3LYP/B1 level of theory predicted RFEs of uranyl complexes.

Spin-Orbit Coupling (SOC) = –0.31 eV; reference electrode (Fc/Fc^+) correction (ref.c) = 0.60 eV

	Complexes	Expt.	$\Delta G^{VI/V}_{red(s)}$	ΔG_{red}	ΔG_{red} + SOC	ΔG_{red} + ref.c	ΔG_{red} + SOC + ref.c
	DMSO						
1	$[UO_2\text{-}(DMSO)_5]^{2+/+}$	0.970	-4.338	0.864	0.554	1.464	1.154
2	$[UO_2\text{-salen-DMSO}]^{0/1-}$	1.602	-3.466	1.736	1.426	2.336	2.026
3	$[UO_2\text{-saloph-DMSO}]^{0/1-}$	1.550	-3.436	1.766	1.456	2.366	2.056
4	$[UO_2\text{-saldien}]^{0/1-}$	1.582	-3.548	1.654	1.344	2.254	1.944
5	$[UO_2\text{-}(acac)_2\text{-DMSO}]^{0/1-}$	1.440	-3.589	1.613	1.303	2.213	1.903
6	$[UO_2\text{-}(trop)_2\text{-DMSO}]^{0/1-}$	1.379	-3.697	1.505	1.195	2.105	1.795
7	$[UO_2\text{-sap-}(DMSO)_2]^{0/1-}$	1.500	-3.400	1.802	1.492	2.402	2.092
8	$[UO_2\text{-}(dbm)_2\text{-DMSO}]^{0/1-}$	1.360	-3.700	1.502	1.192	2.102	1.792
9	$[UO_2\text{-}(hfacac)_2\text{-DMSO}]^{0/1-}$	0.970	-4.401	0.801	0.491	1.401	1.091
10	$[UO_2\text{-}(dpm)_2\text{-DMSO}]^{0/1-}$	1.520	-3.177	2.025	1.715	2.625	2.315
11	$[UO_2\text{-}(btfacac)_2\text{-DMSO}]^{0/1-}$	1.073	-4.000	1.202	0.892	1.802	1.492
12	$[UO_2\text{-}(ttfacac)_2\text{-DMSO}]^{0/1-}$	1.050	-3.984	1.218	0.908	1.818	1.508
13	$[UO_2\text{-}(tfacac)_2\text{-DMSO}]^{0/1-}$	1.082	-3.905	1.297	0.987	1.897	1.587
14	$[UO_2\text{-(tsmc)-(Nyl-OH)}]^{0/1-}$	1.617	-3.798	1.404	1.094	2.004	1.694
15	$[UO_2\text{-(sldh)(AcO)-DMSO}]^{0/1-}$	1.717	-3.750	1.452	1.142	2.052	1.742
16	$[UO_2\text{-salterp }]^{0/1-}$	1.560	-3.365	1.837	1.527	2.437	2.127
17	$[UO_2\text{-(salddt-}NEt_2)]^{0/1-}$	1.550	-3.464	1.738	1.428	2.338	2.028
18	$[UO_2\text{-(salacen)-DMSO}]^{0/1-}$	1.140	-3.844	1.358	1.048	1.958	1.648
19	$[UO_2\text{-appen-DMSO}]^{0/1-}$	1.650	-3.332	1.870	1.560	2.47	2.16
20	$[UO_2\text{-(ac-o-ac)-DMSO}]^{0/1-}$	1.450	-3.382	1.820	1.510	2.42	2.11
21	$[UO_2\text{-(ac-ph-ac)-DMSO}]^{0/1-}$	1.460	-3.522	1.680	1.370	2.28	1.97
22	$[UO_2\text{-salbiby-DMSO}]^{0/1-}$	1.610	-3.396	1.806	1.496	2.406	2.096
23	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.660	-3.418	1.784	1.474	2.384	2.074
24	$[UO_2\text{-(sal-ph-dien)}]^{0/1-}$	1.630	-3.341	1.861	1.551	2.461	2.151

25	$[UO_2\text{-}(ba)_2\text{-}DMSO]^{0/1-}$	1.416	-3.627	1.575	1.265	2.175	1.865
	DMF						
26	$[UO_2\text{-}salen\text{-}DMF]^{0/1-}$	1.672	-3.469	1.921	1.611	2.521	2.211
27	$[UO_2\text{-}saloph\text{-}DMF]^{0/1-}$	1.626	-3.494	1.896	1.586	2.496	2.186
28	$[UO_2\text{-}(acac)_2\text{-}DMF]^{0/1-}$	1.469	-3.346	2.044	1.734	2.644	2.334
29	$[UO_2\text{-}(DMF)_5]^{2+/+}$	0.889	-4.336	1.054	0.744	1.654	1.344
30	$[UO_2\text{-}(trop)_2\text{-}DMF]^{0/1-}$	1.456	-3.737	1.653	1.343	2.253	1.943
31	$[UO_2\text{-}sap\text{-}(DMF)_2]^{0/1-}$	1.585	-3.393	1.997	1.687	2.597	2.287
32	$[UO_2\text{-}(dbm)_2\text{-}DMF]^{0/1-}$	1.461	-3.538	1.852	1.542	2.452	2.142
33	$[UO_2\text{-}(btfacac)_2\text{-}DMF]^{0/1-}$	1.183	-3.935	1.455	1.145	2.055	1.745
34	$[UO_2\text{-}(ttfacac)_2\text{-}DMF]^{0/1-}$	1.176	-3.976	1.414	1.104	2.014	1.704
35	$[UO_2\text{-}(fod)2\text{-}DMF]^{0/1-}$	1.210	-3.828	1.562	1.252	2.162	1.852
36	$[UO_2\text{-}salbiby\text{-}DMF]^{0/1-}$	1.620	-3.264	2.126	1.816	2.726	2.416
	DCM						
37	$[UO_2(L1)\text{-}(acac)]^{0/1-}$	1.820	-3.380	2.111	1.801	2.711	2.401
38	$[UO_2(L1)\text{-}(dbm)]^{0/1-}$	1.590	-3.513	1.978	1.668	2.578	2.268
39	$[UO_2(L1)\text{-}(hfacac)]^{0/1-}$	1.390	-3.760	1.731	1.421	2.331	2.021
40	$[UO_2\text{-}(L2)_2)]^{0/1-}$	1.520	-3.503	1.988	1.678	2.588	2.278
41	$[UO_2\text{-}(L3)_2)]^{0/1-}$	1.350	-3.538	1.953	1.643	2.553	2.243
42	$[UO_2\text{-}(L4+M)]^{+/0}$	1.450	-3.818	1.673	1.363	2.273	1.963
43	$[UO_2\text{-}(L5)_2)]^{0/1-}$	1.460	-3.621	1.870	1.560	2.47	2.16
44	$[UO_2\text{-}saldien\text{-}(NEt_2)_2]^{0/1-}$	1.430	-3.233	2.258	1.948	2.858	2.548
45	$[UO_2\text{-}sal\text{-}ph\text{-}dien]^{0/1-}$	1.560	-3.184	2.307	1.997	2.907	2.597
46	$[UO_2\text{-}AP1]^{0/1-}$	1.530	-3.122	2.369	2.059	2.969	2.659
47	$[UO_2\text{-}AP2]^{0/1-}$	1.700	-3.206	2.285	1.975	2.885	2.575
48	$[UO_2\text{-}AP3]^{0/1-}$	1.640	-3.306	2.185	1.875	2.785	2.475
49	$[UO_2\text{-}salddt]^{0/1-}$	1.620	-3.338	2.153	1.843	2.753	2.443
	ACN						
50	$[UO_2\text{-}(L4+DP)]^{1+/0}$	1.140	-3.777	1.462	1.152	2.062	1.752
51	$[UO_2\text{-}tsmc\text{-}(Nyl\text{-}OH)]^{0/1-}$	1.280	-3.804	1.435	1.125	2.035	1.725
52	$[UO_2\text{-}saloph1\text{-}H_2O]^{0/1-}$	1.360	-3.523	1.716	1.406	2.316	2.006

53	$[UO_2\text{-saloph2-}H_2O]^{0/1-}$	1.428	-3.641	1.598	1.288	2.198	1.888
54	$[UO_2\text{-saloph3-}H_2O]^{0/1-}$	1.360	-3.594	1.645	1.335	2.245	1.935
55	$[UO_2\text{-saloph4-}H_2O]^{0/1-}$	1.505	-3.449	1.790	1.480	2.39	2.08
56	$[UO_2\text{-saloph5-}H_2O]^{0/1-}$	1.348	-3.615	1.624	1.314	2.224	1.914
57	$[UO_2\text{-(CMPO + 2}NO_3)]^{0/1-}$	1.250	-3.994	1.245	0.935	1.845	1.535
	Py						
58	$[UO_2\text{-(Py)}_5]^{2+/+}$	0.910	-4.888	1.399	1.089	1.999	1.689
59	$[UO_2\text{-salen-Py}]^{0/1-}$	1.610	-3.802	2.485	2.175	3.085	2.775
60	$[UO_2\text{-saloph-Py}]^{0/1-}$	1.570	-3.833	2.454	2.144	3.054	2.744
61	$[UO_2\text{-salan-t}Bu_2\text{-Py}]^{0/1-}$	1.820	-3.379	2.908	2.598	3.508	3.198
62	$[UO_2\text{-saloph-t}Bu_2\text{-Py}]^{0/1-}$	1.670	-3.819	2.468	2.158	3.068	2.758
63	$[UO_2\text{-saloph-t}Bu_2\text{-Py-K}]^{+/0}$	1.650	-3.853	2.434	2.124	3.034	2.724
64	$[UO_2\text{-saldien-(NEt}_2)_2]^{0/1-}$	1.780	-3.646	2.641	2.331	3.241	2.931
65	$[UO_2\text{-salterp}]^{0/1-}$	1.690	-3.435	2.852	2.542	3.452	3.142
66	$[UO_2\text{-sal-ph-dien}]^{0/1-}$	1.790	-3.493	2.794	2.484	3.394	3.084
67	$[UO_2\text{-salddt}]^{0/1-}$	1.560	-3.624	2.663	2.353	3.263	2.953
68	$[UO_2\text{-salbiby-Py}]^{0/1-}$	1.670	-3.509	2.778	2.468	3.378	3.068
	MUE	-	-	**0.406**	0.239	0.983	0.673

Table S7. The M06/B2(CPCM/UAKS)//B3LYP/B1 level of theory predicted RFEs of uranyl complexes.

Spin-Orbit Coupling (SOC) = –0.31 eV; reference electrode (Fc/Fc^{+}) correction (ref.c) = 0.285 eV

	Complexes	Expt.	$\Delta G^{VI/V}_{red(s)}$	ΔG_{red}	ΔG_{red} + SOC	ΔG_{red} + ref.c	ΔG_{red} + SOC + ref.c
	DMSO						
1	$[UO_2\text{-}(DMSO)_5]^{2+/+}$	0.970	-4.830	0.664	0.354	0.949	0.639
2	$[UO_2\text{-salen-DMSO}]^{0/1-}$	1.602	-3.825	1.669	1.359	1.954	1.644
3	$[UO_2\text{-saloph-DMSO}]^{0/1-}$	1.550	-3.812	1.682	1.372	1.967	1.657
4	$[UO_2\text{-saldien}]^{0/1-}$	1.582	-3.882	1.612	1.302	1.897	1.587
5	$[UO_2\text{-}(acac)_2\text{-DMSO}]^{0/1-}$	1.440	-3.912	1.582	1.272	1.867	1.557
6	$[UO_2\text{-}(trop)_2\text{-DMSO}]^{0/1-}$	1.379	-4.036	1.458	1.148	1.743	1.433
7	$[UO_2\text{-sap-}(DMSO)_2]^{0/1-}$	1.500	-3.840	1.654	1.344	1.939	1.629
8	$[UO_2\text{-}(dbm)_2\text{-DMSO}]^{0/1-}$	1.360	-3.988	1.506	1.196	1.791	1.481
9	$[UO_2\text{-}(hfacac)_2\text{-DMSO}]^{0/1-}$	0.970	-4.607	0.887	0.577	1.172	0.862
10	$[UO_2\text{-}(dpm)_2\text{-DMSO}]^{0/1-}$	1.520	-3.467	2.027	1.717	2.312	2.002
11	$[UO_2\text{-}(btfacac)_2\text{-DMSO}]^{0/1-}$	1.073	-4.275	1.219	0.909	1.504	1.194
12	$[UO_2\text{-}(ttfacac)_2\text{-DMSO}]^{0/1-}$	1.050	-4.265	1.229	0.919	1.514	1.204
13	$[UO_2\text{-}(tfacac)_2\text{-DMSO}]^{0/1-}$	1.082	-4.200	1.294	0.984	1.579	1.269
14	$[UO_2\text{-}(tsmc)\text{-}(Nyl\text{-}OH)]^{0/1-}$	1.617	-4.120	1.374	1.064	1.659	1.349
15	$[UO_2\text{-}(sldh)(AcO)\text{-DMSO}]^{0/1-}$	1.717	-4.092	1.402	1.092	1.687	1.377
16	$[UO_2\text{-salterp }]^{0/1-}$	1.560	-3.398	2.096	1.786	2.381	2.071
17	$[UO_2\text{-}(salddt\text{-}NEt_2)]^{0/1-}$	1.550	-3.827	1.667	1.357	1.952	1.642
18	$[UO_2\text{-}(salacen)\text{-DMSO}]^{0/1-}$	1.140	-4.210	1.284	0.974	1.569	1.259
19	$[UO_2\text{-appen-DMSO}]^{0/1-}$	1.650	-3.693	1.801	1.491	2.086	1.776
20	$[UO_2\text{-}(ac\text{-}o\text{-}ac)\text{-DMSO}]^{0/1-}$	1.450	-3.738	1.756	1.446	2.041	1.731
21	$[UO_2\text{-}(ac\text{-}ph\text{-}ac)\text{-DMSO}]^{0/1-}$	1.460	-3.855	1.639	1.329	1.924	1.614
22	$[UO_2\text{-salbiby-DMSO}]^{0/1-}$	1.610	-3.760	1.734	1.424	2.019	1.709
23	$[UO_2\text{-saldien-}(NEt_2)_2]^{0/1-}$	1.660	-3.765	1.729	1.419	2.014	1.704
24	$[UO_2\text{-}(sal\text{-}ph\text{-}dien)]^{0/1-}$	1.630	-3.710	1.784	1.474	2.069	1.759
25	$[UO_2\text{-}(ba)_2\text{-DMSO}]^{0/1-}$	1.416	-3.933	1.561	1.251	1.846	1.536

	DMF						
26	$[UO_2$-salen-DMF$]^{0/1-}$	1.672	-3.822	1.956	1.646	2.241	1.931
27	$[UO_2$-saloph-DMF$]^{0/1-}$	1.626	-3.834	1.944	1.634	2.229	1.919
28	$[UO_2$-$(acac)_2$-DMF$]^{0/1-}$	1.469	-3.773	2.005	1.695	2.290	1.980
29	$[UO_2$-$(DMF)_5]^{2+/+}$	0.889	-4.807	0.971	0.661	1.256	0.946
30	$[UO_2$-$(trop)_2$-DMF$]^{0/1-}$	1.456	-4.072	1.706	1.396	1.991	1.681
31	$[UO_2$-sap-$(DMF)_2]^{0/1-}$	1.585	-3.773	2.005	1.695	2.290	1.980
32	$[UO_2$-$(dbm)_2$-DMF$]^{0/1-}$	1.461	-3.929	1.849	1.539	2.134	1.824
33	$[UO_2$-$(btfacac)_2$-DMF$]^{0/1-}$	1.183	-4.201	1.577	1.267	1.862	1.552
34	$[UO_2$-$(ttfacac)_2$-DMF$]^{0/1-}$	1.176	-4.236	1.542	1.232	1.827	1.517
35	$[UO_2$-(fod)2-DMF$]^{0/1-}$	1.210	-4.107	1.671	1.361	1.956	1.646
36	$[UO_2$-salbiby-DMF$]^{0/1-}$	1.620	-3.518	2.260	1.950	2.545	2.235
	DCM						
37	$[UO_2$(L1)-(acac)$]^{0/1-}$	1.820	-3.510	2.153	1.843	2.438	2.128
38	$[UO_2$(L1)-(dbm)$]^{0/1-}$	1.590	-3.637	2.026	1.716	2.311	2.001
39	$[UO_2$(L1)-(hfacac)$]^{0/1-}$	1.390	-3.802	1.861	1.551	2.146	1.836
40	$[UO_2$-$(L2)_2)]^{0/1-}$	1.520	-3.713	1.950	1.640	2.235	1.925
41	$[UO_2$-$(L3)_2)]^{0/1-}$	1.350	-3.764	1.899	1.589	2.184	1.874
42	$[UO_2$-(L4+M)$]^{+/0}$	1.450	-4.118	1.545	1.235	1.830	1.520
43	$[UO_2$-$(L5)_2)]^{0/1-}$	1.460	-3.906	1.757	1.447	2.042	1.732
44	$[UO_2$-saldien-$(NEt_2)_2]^{0/1-}$	1.430	-3.589	2.074	1.764	2.359	2.049
45	$[UO_2$-sal-ph-dien$]^{0/1-}$	1.560	-3.482	2.181	1.871	2.466	2.156
46	$[UO_2$-AP1$]^{0/1-}$	1.530	-3.156	2.507	2.197	2.792	2.482
47	$[UO_2$-AP2$]^{0/1-}$	1.700	-3.414	2.249	1.939	2.534	2.224
48	$[UO_2$-AP3$]^{0/1-}$	1.640	-3.638	2.025	1.715	2.310	2.000
49	$[UO_2$-salddt$]^{0/1-}$	1.620	-3.698	1.965	1.655	2.250	1.940
	ACN						
50	$[UO_2$-(L4+DP)$]^{1+/0}$	1.140	-4.035	1.211	0.901	1.496	1.186
51	$[UO_2$-tsmc-(Nyl-OH)$]^{0/1-}$	1.280	-4.127	1.119	0.809	1.404	1.094
52	$[UO_2$-saloph1-$H_2O]^{0/1-}$	1.360	-3.926	1.320	1.010	1.605	1.295
53	$[UO_2$-saloph2-$H_2O]^{0/1-}$	1.428	-3.953	1.293	0.983	1.578	1.268

54	$[UO_2\text{-saloph3-}H_2O]^{0/1-}$	1.360	-3.873	1.373	1.063	1.658	1.348
55	$[UO_2\text{-saloph4-}H_2O]^{0/1-}$	1.505	-3.743	1.503	1.193	1.788	1.478
56	$[UO_2\text{-saloph5-}H_2O]^{0/1-}$	1.348	-3.954	1.292	0.982	1.577	1.267
57	$[UO_2\text{-(CMPO + 2}NO_3)]^{0/1-}$	1.250	-4.182	1.064	0.754	1.349	1.039
	Py						
58	$[UO_2\text{-(Py)}_5]^{2+/+}$	0.910	-5.157	1.383	1.073	1.668	1.358
59	$[UO_2\text{-salen-Py}]^{0/1-}$	1.610	-4.168	2.372	2.062	2.657	2.347
60	$[UO_2\text{-saloph-Py}]^{0/1-}$	1.570	-4.234	2.306	1.996	2.591	2.281
61	$[UO_2\text{-salan-tBu}_2\text{-Py}]^{0/1-}$	1.820	-3.810	2.730	2.420	3.015	2.705
62	$[UO_2\text{-saloph-tBu}_2\text{-Py}]^{0/1-}$	1.670	-4.186	2.354	2.044	2.639	2.329
63	$[UO_2\text{-saloph-tBu}_2\text{-Py-K}]^{+/0}$	1.650	-4.272	2.268	1.958	2.553	2.243
64	$[UO_2\text{-saldien-(NEt}_2)_2]^{0/1-}$	1.780	-4.000	2.540	2.230	2.825	2.515
65	$[UO_2\text{-salterp}]^{0/1-}$	1.690	-3.214	3.326	3.016	3.611	3.301
66	$[UO_2\text{-sal-ph-dien}]^{0/1-}$	1.790	-3.764	2.776	2.466	3.061	2.751
67	$[UO_2\text{-salddt}]^{0/1-}$	1.560	-3.918	2.622	2.312	2.907	2.597
68	$[UO_2\text{-salbiby-Py}]^{0/1-}$	1.670	-3.785	2.755	2.445	3.040	2.730
	MUE	-	-	0.372	0.280	0.614	0.355

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