Supporting Information

First-Principles Integrated Adsorption Modeling for Selective Capture of Uranium from Seawater by Polyamidoxime Sorbent Materials

Austin P. Ladshaw,[†]* Alexander S. Ivanov,[‡] Sadananda Das,[‡] Vyacheslav S. Bryantsev,[‡] Costas Tsouris,[†‡] Sotira Yiacoumi[†]*

[†]Georgia Institute of Technology, Atlanta, GA 30332, United States
[‡]Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States

*Corresponding authors: sotira.yiacoumi@ce.gatech.edu; aladshaw3@gatech.edu

Notations used in the Methods section.

Latin Symbols

A	specific surface area of the adsorbent
e	elementary electrical charge constant
F	Faraday's constant
g^C	combinatorial factor in UNIQUAC
g^R	residual factor in UNIQUAC
I	ionic strength of the solution
K	stability constant of a reaction
k_B	Boltzmann constant
$L_{\max}$	maximum surface concentration of ligands
m	number of sites involved in a surface reaction
N	net charge exchange term
n	ionic charge of a species
q	surface concentration of a species
R	gas law constant
$\mathbf{r}$	location vector
r	adsorbate volume factor
s	adsorbate area factor
T	system temperature
U	uranium
V	vanadium
y	adsorbed mole fraction
z	coordination constant

Greek Symbols

γ^{aq}	aqueous activity coefficient

γ^s	surface activity coefficient
ΔG_{aq}	change in free energy for an aqueous reaction
ε	dielectric constant of a medium
ε_0	permittivity of free space
η	Boltzmann factor
λ	adsorbate length factor
ρ	volumetric ion charge density
τ	binary interaction parameter
υ	stoichiometric constant
Φ	average volume factor
ψ	electric surface potential

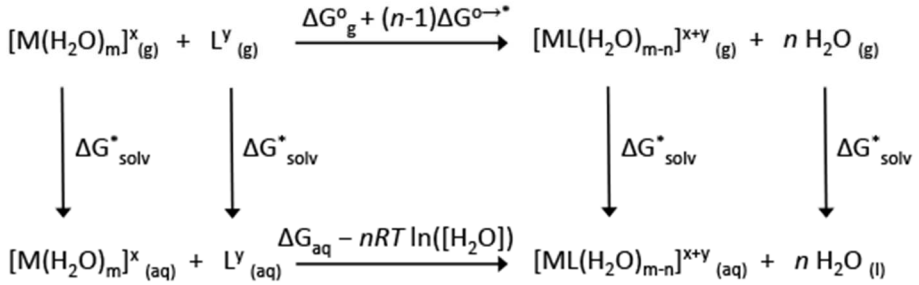
Sub/superscripts

i,j,k	indices for species
l,m,n	indices for ligands

Other Symbols

$[i]$	aqueous concentration of a species
$[L\phi]$	molar concentration of surface sites
$[U]_e$	equilibrium concentration of uranium
$\{i\}$	aqueous activity of a species
$\{q\}$	surface activity of a species
HAO	acyclic acetamidoxime
H_3IDO	cyclic glutarimidedioxime

Scheme S1. Thermodynamic cycle used to calculate ΔG_{aq}.



According to the thermodynamic cycle in **Scheme S1**, ΔG_{aq} is given by:

$$\Delta G_{aq} = \Delta G^{o}_{g} + \Delta\Delta G^{*}_{solv} + (n\text{-}1)\Delta G^{o\rightarrow *} + nRT\ln([H_2O])$$

where ΔG^{o}_{g} is the free energy of complexation in the gas phase, and $\Delta\Delta G^{*}_{solv}$ is the difference in the solvation free energies for a complexation reaction:

$$\Delta\Delta G^{*}_{solv} = \Delta G^{*}_{solv}([ML(H_2O)_{m-n}]^{x+y}) + n\Delta G^{*}_{solv}(H_2O) - \Delta G^{*}_{solv}([M(H_2O)_m]^{x}) - \Delta G^{*}_{solv}(L^{y})$$

where L^{y} denotes the ligand with a charge of y and M can be UO_2^{2+} or VO_2^{+}. The standard state correction terms must be introduced to connect ΔG^{o}_{g}, $\Delta\Delta G^{*}_{solv}$, and ΔG_{aq}, which are defined using different standard state conventions. The free energy change for the conversion of 1 mol of solute from the gas phase at a standard state of 1 atm (24.46 L/mol) to the aqueous phase at a standard state of 1 mol/L at 298.15 K is given by $\Delta G^{o\rightarrow *} = 1.89$ kcal/mol. Likewise, $RT\ln([H_2O]) = 2.38$ kcal/mol (T = 298.15 K) is the free energy change for the conversion of 1 mol of solvent from the aqueous phase at 1 mol/L to pure water at a standard state of 55.34 mol/L.

Table S1. Comparison of experimental and predicted log β values for the 1:2 uranyl complexes with an excess negative charge using the regression equation [$\log \beta^{expt} = 0.5693 \times \log \beta^{calc}$].

Ligand	expt. $\log\beta^{expt}$	calc. $\log\beta^{calc}$	pred.[e] $\log\beta$	abs. error
2carbonate	16.6[a]	35.1	20.0	3.4
2glutarimidedioximate ($2HIDO^{2-}$)	28.7[b]	57.8	32.9	4.2
2salicylamidoximate	25.5[c]	51.3	29.2	3.7
2oxalate	10.6[a]	28.1	16.0	5.4
2malonate	9.5[a]	28.7	16.3	6.8
2phthalate	7.73[a]	24.7	14.1	6.3
2dipicolinate	16.3[a]	36.1	20.6	4.3
phenanthroline dicarboxylate and hydroxide	21.7[d]	46.1	26.3	4.6
glutarimidedioximate ($HIDO^{2-}$) and H_2IDO^{-}	24.7[b]	47.8	27.2	2.5

[a]Taken from the Smith and Martell's compilation of Critical Stability Constants series.[S1,S2]
[b]Taken from ref. S3 and corrected to zero ionic strength with the Davies equation.[S4]
[c]Taken from ref. S5.
[d]Taken from ref. S6.
[e]Predicted using the regression equation [$\log \beta^{expt} = 0.5693 \times \log \beta^{calc}$] that was obtained from the correlations shown in Figure 3 of the main text.

Table S2. Comparison of experimental and predicted log β values for the 1:2 uranyl complexes with an excess negative charge using the regression equation [log β^{expt} = 0.6498×log β^{calc} – 7.7565].

Ligand	expt. logβ^{expt}	calc. logβ^{calc}	pred.[e] logβ	abs. error
2carbonate	16.6[a]	35.1	15.1	1.5
2glutarimidedioximate (2HIDO^{2-})	28.7[b]	57.8	29.8	1.1
2salicylamidoximate	25.5[c]	51.3	25.5	0.0
2oxalate	10.6[a]	28.1	10.5	0.1
2malonate	9.5[a]	28.7	10.9	1.4
2phthalate	7.73[a]	24.7	8.3	0.6
2dipicolinate	16.3[a]	36.1	15.7	0.6
phenanthroline dicarboxylate and hydroxide	21.7[d]	46.1	22.2	0.5
glutarimidedioximate (HIDO^{2-}) and H_2IDO^-	24.7[b]	47.8	23.3	1.4

[a]Taken from the Smith and Martell's compilation of Critical Stability Constants series.[S1,S2]
[b]Taken from ref. S3 and corrected to zero ionic strength with the Davies equation.[S4]
[c]Taken from ref. S5.
[d]Taken from ref. S6.
[e]Predicted using the regression equation [log β^{expt} = 0.6498×log β^{calc} – 7.7565] that was obtained from the correlations shown in Figure 3 of the main text.

Table S3. Equilibrium constants for the UO_2^{2+}/AO^- and UO_2^{2+}/IDO^{2-} complexes, all at 25 °C and zero ionic strength.

aqueous species, reactions	log β
acetamidoximate (AO^-):	
$UO_2^{2+} + AO^- \leftrightarrows [UO_2(AO)]^+$	13.6[a]
$UO_2^{2+} + 2AO^- \leftrightarrows [UO_2(AO)_2]$	23.7[a]
$UO_2^{2+} + 3AO^- \leftrightarrows [UO_2(AO)_3]^-$	27.9[b]
$UO_2^{2+} + AO^- + CO_3^{2-} \leftrightarrows [UO_2(AO)(CO_3)]^-$	15.8[b]
$UO_2^{2+} + 2AO^- + CO_3^{2-} \leftrightarrows [UO_2(AO)_2(CO_3)]^{2-}$	25.5[b]
glutarimide-dioximate (IDO^{2-}):	
$UO_2^{2+} + IDO^{2-} \leftrightarrows [UO_2(IDO)]$	19.2[a]
$UO_2^{2+} + H^+ + IDO^{2-} \leftrightarrows [UO_2(HIDO)]^+$	23.5[a]
$UO_2^{2+} + 2IDO^{2-} \leftrightarrows [UO_2(IDO)_2]^{2-}$	29.0[a]
$UO_2^{2+} + H^+ + 2IDO^{2-} \leftrightarrows [UO_2(HIDO)(IDO)]^-$	38.9[a]
$UO_2^{2+} + 2H^+ + 2IDO^{2-} \leftrightarrows [UO_2(HIDO)_2]$	44.2[a]
$UO_2^{2+} + IDO^{2-} + CO_3^{2-} \leftrightarrows [UO_2(IDO)(CO_3)]^{2-}$	25.2[b]
$UO_2^{2+} + H^+ + IDO^{2-} + CO_3^{2-} \leftrightarrows [UO_2(HIDO)(CO_3)]^-$	29.2[b]

[a]Taken from ref. S7, S3 and corrected to zero ionic strength with the Davies equation.[S4]
[b]Predicted from regression lines shown in Figure 3.

Table S4. Equilibrium constants for the VO_2^+/AO^- and VO_2^+/IDO^{2-} complexes, together with literature constants for the V(V) solution species, all at 25 °C and zero ionic strength.

aqueous species, reactions	log β
V(V) aqueous solution:	
$VO_4^{3-} + H^+ \leftrightarrows HVO_4^{2-}$	14.3[a]
$VO_4^{3-} + 2H^+ \leftrightarrows H_2VO_4^-$	22.9[a]
$VO_4^{3-} + 3H^+ \leftrightarrows H_3VO_4$	25.5[a]
$VO_4^{3-} + 4H^+ \leftrightarrows VO_2^+ + 2H_2O$	30.2[a]
acetamidoximate (AO^-) ligand:	
$VO_4^{3-} + 4H^+ + AO^- \leftrightarrows [VO_2(AO)] + 2H_2O$	40.6[b]
$VO_4^{3-} + 4H^+ + 2AO^- \leftrightarrows [VO_2(AO)_2]^- + 2H_2O$	48.4[b]
$VO_4^{3-} + 5H^+ + 2AO^- \leftrightarrows [VOOH(AO)_2] + 2H_2O$	51.4[b]
$VO_4^{3-} + 6H^+ + 3AO^- \leftrightarrows [V(AO)(H_{-1}AO)_2] + 4H_2O$	66.3[b]
$VO_4^{3-} + 8H^+ + 3AO^- \leftrightarrows [V(AO)_3]^{2+} + 4H_2O$	62.4[b]
glutarimidedioximate (IDO^{2-}) ligand:	
$VO_4^{3-} + 4H^+ + IDO^{2-} \leftrightarrows [VO_2(HIDO)]^- + 2H_2O$	48.5[b]
$VO_4^{3-} + 5H^+ + IDO^{2-} \leftrightarrows [VO_2(H_2IDO)] + 2H_2O$	51.9[b]
$VO_4^{3-} + 6H^+ + 2IDO^{2-} \leftrightarrows [V(IDO)_2]^- + 4H_2O$	76.4[b]
$VO_4^{3-} + 7H^+ + 2IDO^{2-} \leftrightarrows [V(HIDO)(IDO)] + 4H_2O$	77.8[b]
$VO_4^{3-} + 8H^+ + 2IDO^{2-} \leftrightarrows [V(HIDO)_2]^+ + 4H_2O$	74.6[b]

[a]Taken from ref. S8 and corrected to zero ionic strength with the Davies equation.[S4]
[b]Computationally predicted values from ref. S9.

As an example the reported log β for $[VO_2(AO)]$ was obtained through summation of the vanadium hydrolysis constant ($VO_4^{3-} + 4H^+ \leftrightarrows VO_2^+ + 2H_2O$, log β =30.2*)* and the computationaly predicted log β value for the reaction:

$VO_2^+ + AO^- \leftrightarrows [VO_2(AO)]$, log β =10.4

Note S1. Derivation of stability constants for the non-oxido 1:2 and 1:3 V(V) species.

It is worth noting, however, that the developed regression approach[S10] for the estimation of stability constants for VO_2^+ complexes cannot be directly applied to assess log β of the non-oxido 1:2 and 1:3 V(V) species. Nevertheless, the log β values for these complexes can be obtained through a combination of the predicted log β for the VO_2^+ species with the vanadium hydrolysis reactions for which ΔG_{aq} is experimentally known and the additional reactions calculated at the CCSD(T)/aug-cc-pvDZ//M06/SSC/6-311++G(d,p) level.[S9] As an example, the complexation free energy, ΔG_{aq}, for the formation of the non-oxido $V(IDO)_2^-$ complex can be found by combination of the following reactions ($\Delta G_{aq} = 2\Delta G_{aq1} + 2G_{aq2} + \Delta G_{aq3}$):

$H_2VO_4^- + 2H^+ \leftrightarrows VO_2^+ + 2H_2O$, ΔG_{aq1} (1)
$VO_2^+ + HIDO^{2-} \leftrightarrows VO_2(HIDO)^-$, ΔG_{aq2} (2)
$VO_2(HIDO)^- + VO_2(HIDO)^- \leftrightarrows V(IDO)_2^- + H_2VO_4^-$, ΔG_{aq3} (3)

$H_2VO_4^- + 4H^+ + 2HIDO^{2-} \leftrightarrows V(IDO)_2^- + 4H_2O$

where ΔG_{aq1} is experimentally known value,[S8] ΔG_{aq2} was determined using our developed approach,[S10] and the free energy, ΔG_{aq12}, was determined using single-point coupled-cluster theory calculations, CCSD(T)/aug-cc-pvDZ (the valence electrons on C, O, H and the valence and subvalence electrons (3s, 3p) on V were correlated) at the M06/SSC/6-311++G(d,p) optimized geometries.[S9] Following similar analysis, the equilibrium constants (log β) of other non-oxido 1:2 and 1:3 V(V) species can be estimated. For the full description, including the free energy of the reactions, ΔG_{aq} (kcal/mol), assessed at the CCSD(T)/aug-cc-pvDZ//M06/SSC/6-311++G(d,p) level of theory and using the SMD solvation model, please refer to our previous work.[S9]

Table S5. Equilibrium constants for the protonation/deprotonation of the amidoxime ligands.[a]

Aqueous Reaction	log β
$HIDO^{2-} + H^+ \leftrightarrows H_2IDO^-$	12.9
$HIDO^{2-} + 2H^+ \leftrightarrows H_3IDO$	23.8
$HIDO^{2-} + 3H^+ \leftrightarrows H_4IDO^+$	26.0
$AO^- + H^+ \leftrightarrows HAO$	13.2
$AO^- + 2H^+ \leftrightarrows H_2AO^+$	19.0

[a]Taken from ref. S7 and S3, and corrected to zero ionic strength with the Davies equation.[S4]

Note S2. The adsorption reactions and binding constants input into the model are taken directly from the molecular modeling studies (Tables S3 and S4) with one minor modification. First, the ligands on the surface of the adsorbent, [$L\phi$] in equation 3, are considered as charge neutral in the formulation of the adsorption model, but the binding strengths from Tables S3 and S4 were calculated in terms of reactions with deprotonated ligands. To correct this, we combined the complexation reactions of the metal ions (Tables S3 and S4) with the deprotonation reactions of the HAO and H_3IDO ligands, for which experimental pK_a values are known (Table S5). The resulting reaction schemes and log β analyzed in this study for uranium and vanadium coordination with HAO and H_3IDO are summarized in Tables 3 and 4, respectively.

An example of the modifications applied to the metal complexation reactions is shown below:

	$H_3IDO \leftrightarrows 2H^+ + HIDO^{2-}$	log K = -23.8
(+)	$VO_4^{3-} + 4H^+ + HIDO^{2-} \leftrightarrows [VO_2(HIDO)]^- + 2H_2O$	log β = 48.4
(=)	$VO_4^{3-} + 2H^+ + H_3IDO \leftrightarrows [VO_2(HIDO)]^- + 2H_2O$	log K + log β = 24.6

Here, we add the deprotonation reaction for H_3IDO with the complexation reaction between VO_4^{3-} and $HIDO^{2-}$. The end result is the corrected adsorption reaction that will be input into the model with a binding constant that is formed from the known pK_a value of the deprotonation of H_3IDO with the calculated binding strength between metal and ligand from the molecular modeling studies.

Note S3. The equilibrium constants listed in Table S5 are not the same as the pK_as, since the definition of pK_a is for the dissociation of a single proton from an acid. The dissociation reactions in Table S5 do not only involve single proton dissociations. However, the pK_as can be formed from the information in Table S5 as noted below:

Example: Deprotonation of the first proton from H_3IDO (i.e., pK_{a1})

	$HIDO^{2-} + 2H^+ \leftrightarrows H_3IDO$	$\log \beta = 23.8$
(+)	$H_2IDO^- \leftrightarrows HIDO^{2-} + H^+$	$\log \beta = -12.9$
(=)	$H_2IDO^- + H^+ \leftrightarrows H_3IDO$	$\log \beta = 10.9$ (pK_{a1})

Table S6. Equilibrium constants for the aqueous reactions considered with the adsorption model. Constants are calculated at 20 °C and zero ionic strength using the standard formation energies and/or reaction energies.[a]

Aqueous Reaction	$\log \beta$
H_2O (l) $\leftrightarrows H^+ + OH^-$	-14.2
$H_2CO_3 \leftrightarrows H^+ + HCO_3^-$	-6.4
$HCO_3^- \leftrightarrows H^+ + CO_3^{2-}$	-10.4
$NaHCO_3$ (aq) $\leftrightarrows H^+ + CO_3^{2-} + Na^+$	-10.2
$NaCO_3^- \leftrightarrows CO_3^{2-} + Na^+$	-1.3
Na_2CO_3 (aq) $\leftrightarrows CO_3^{2-} + 2Na^+$	0.0
NaOH (aq) $\leftrightarrows OH^- + Na^+$	0.0
NaCl (aq) $\leftrightarrows Cl^- + Na^+$	0.0
$HCl \leftrightarrows Cl^- + H^+$	0.0
$HNO_3 \leftrightarrows H^+ + NO_3^-$	0.0
$NO_3^- + UO_2^{2+} \leftrightarrows UO_2NO_3^+$	0.3
$2NO_3^- + UO_2^{2+} \leftrightarrows UO_2(NO_3)_2$	-12.4
H_2O (l) + $UO_2^{2+} \leftrightarrows H^+ + UO_2OH^+$	-5.4
$2H_2O$ (l) + $UO_2^{2+} \leftrightarrows 2H^+ + UO_2(OH)$ (aq)	-12.4
$3H_2O$ (l) + $UO_2^{2+} \leftrightarrows 3H^+ + UO_2(OH)_3^-$	-20.9
$4H_2O$ (l) + $UO_2^{2+} \leftrightarrows 4H^+ + UO_2(OH)_4^{2-}$	-33.0
H_2O (l) + $2UO_2^{2+} \leftrightarrows H^+ + (UO_2)_2OH^{3+}$	-2.8
$2H_2O$ (l) + $2UO_2^{2+} \leftrightarrows 2H^+ + (UO_2)_2(OH)_2^{2+}$	-5.7
$4H_2O$ (l) + $3UO_2^{2+} \leftrightarrows 4H^+ + (UO_2)_3(OH)_4^{2+}$	-12.1
$5H_2O$ (l) + $3UO_2^{2+} \leftrightarrows 5H^+ + (UO_2)_3(OH)_5^+$	-15.8
$7H_2O$ (l) + $3UO_2^{2+} \leftrightarrows 7H^+ + (UO_2)_3(OH)_7^-$	-32.8
$7H_2O$ (l) + $4UO_2^{2+} \leftrightarrows 7H^+ + (UO_2)_4(OH)_7^+$	-22.3
$CO_3^{2-} + UO_2^{2+} \leftrightarrows UO_2CO_3$ (aq)	10.0
$2CO_3^{2-} + UO_2^{2+} \leftrightarrows UO_2(CO_3)_2^{2-}$	16.6
$3CO_3^{2-} + UO_2^{2+} \leftrightarrows UO_2(CO_3)_3^{4-}$	22.0
$Cl^- + UO_2^{2+} \leftrightarrows UO_2Cl^+$	0.2
$2Cl^- + UO_2^{2+} \leftrightarrows UO_2Cl_2$ (aq)	-1.1
$3Cl^- + UO_2^{2+} \leftrightarrows UO_2Cl_3^-$	-2.6
$2H_2O$ (l) + $VO_2^+ \leftrightarrows 4H^+ + VO_4^{3-}$	-28.9
$H_3VO_4 \leftrightarrows H^+ + H_2VO_4^-$	-3.6
$H_2VO_4^- \leftrightarrows H^+ + HVO_4^{2-}$	-8.0
$HVO_4^{2-} \leftrightarrows H^+ + VO_4^{3-}$	-13.5
$H^+ + CO_3^{2-} + H_2VO_4^- \leftrightarrows H_2O$ (l) + $VO_2OHCO_3^{2-}$	11.6
$2H^+ + 2CO_3^{2-} + H_2VO_4^- \leftrightarrows 2H_2O$ (l) + $VO_2(CO_3)_2^{3-}$	21.2

[a]Formation and reaction energies for the above come from ref. S11, S12, and S13. Constants were calculated as a function of temperature using the van't Hoff equation (ref. S11).

Note S4. Although the stability constants for vanadium-carbonate complexes in Table S6 are relatively high, vanadium does not complex favorably with carbonates in solution. In order to adequately compare binding constants for equilibrium reactions in aqueous systems, we have to consider what is happening in solution relative to the species involved with that particular reaction. In solution, vanadium (V) primarily acts as a triprotic acid with the following pK_as: pK_{a1} = 3.6, pK_{a2} = 8.0, and pK_{a3} = 13.5 (see Table S6). Based on these pK_as, it is clear to see that the primary vanadium species at pH 4-6 would be $H_2VO_4^-$ (i.e., the protonated form from the K_{a2} reaction). While this is the vanadium species used to describe the complexation with carbonates, the carbonates in those reactions (Table S6) are not the primary species at the given pH. At a pH of 4-6, the carbonate species would primarily be H_2CO_3, with almost no carbonate in the form of CO_3^{2-}. Thus, in order to make a fair comparison of binding strengths between the deprotonation reactions with $H_2VO_4^-$ and complexation with carbonates, we need to rewrite those complexation reactions in terms of H_2CO_3.

	$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$	log β = -6.4
(+)	$HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$	log β = -10.4
(+)	$H^+ + CO_3^{2-} + H_2VO_4^- \leftrightarrow H_2O + VO_2OHCO_3^{2-}$	log β = 11.6
(=)	$H_2CO_3 + H_2VO_4^- \leftrightarrow H^+ + H_2O + VO_2OHCO_3^{2-}$	sum = -5.2

	$2\times(H_2CO_3 \leftrightarrow H^+ + HCO_3^-$	log β = -6.4)
(+)	$2\times(HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$	log β = -10.4)
(+)	$2H^+ + 2CO_3^{2-} + H_2VO_4^- \leftrightarrow 2H_2O + VO_2(CO_3)_2^{3-}$	log β = 21.2
(=)	$2H_2CO_3 + H_2VO_4^- \leftrightarrow 2H^+ + 2H_2O + VO_2(CO_3)_2^{3-}$	sum = -12.4

From this, it is clear to see that the actual binding strengths for those complexation reactions under actual solution conditions are much less favorable than they first appear to be. Figure S1 below shows computationally the results of simulating vanadium speciation under seawater conditions using the aqueous reactions from Table S6.

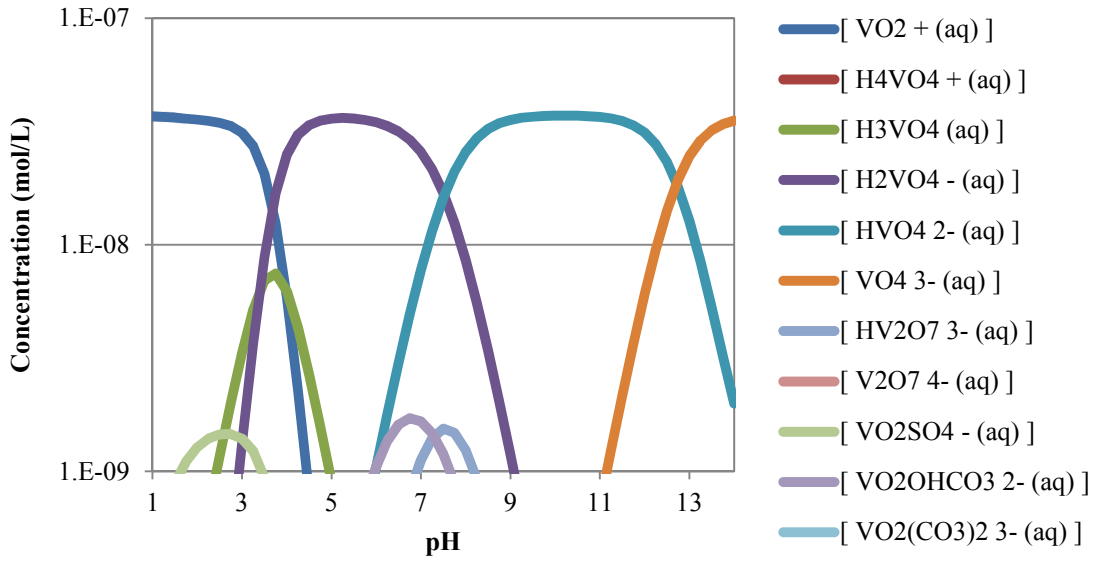


Figure S1. Simulated speciation of vanadium under seawater conditions. These results demonstrate that the vanadium-carbonate species are very minor species in solution, despite having apparently high binding constants from Table S6.

Adsorption Experimental Data

Table S7. Equilibrium data for the Uranium Adsorption pH Studies.

Run	pH	Measurement 1 U (g/kg)	Measurement 2 U (g/kg)
1	**2.03**	49.65	51.48
	3.97	216.27	217.17
	5.91	332.52	331.05
	6.52	269.92	271.89
	7.02	235.07	233.15
	7.48	181.19	178.89
	8.01	150.86	150.76
	8.51	138.15	139.98
2	**4.02**	244.63	244.88
	6.03	297.08	296.88
	6.99	217.73	216.83
	7.99	160.18	159.38
	8.99	129.67	133.69
	9.98	128.48	128.93
	10.99	175.89	176.23
	12.40	204.58	203.03

Table S8. Equilibrium data for the Vanadium Adsorption pH Studies.

pH	Measurement 1 V (g/kg)	Measurement 2 V (g/kg)
2.03	47.90	47.80
3.98	87.58	87.04
6.03	80.51	78.68
6.98	74.46	74.22
8.07	75.55	75.30
8.99	67.35	67.45
9.99	69.40	69.30
10.98	63.28	63.63
11.9	15.58	34.82

Table S9. Equilibrium data for the Uranium and Vanadium Adsorption pH Studies.

pH	Measurement 1 V (g/kg)	Measurement 1 U (g/kg)	Measurement 2 V (g/kg)	Measurement 2 U (g/kg)
2.02	47.16	32.58	48.32	28.26
3.99	64.07	89.57	71.32	106.66
6.03	88.16	183.99	89.30	182.10
6.54	82.25	145.29	80.84	140.60
7.00	63.40	94.56	63.45	92.29

7.65	59.41	107.47	59.95	107.81
8.00	53.58	93.45	54.02	94.18
8.49	50.03	66.43	49.39	66.48
8.98	51.34	66.81	51.49	65.96
10.00	43.95	75.57	45.90	77.82
11.00	45.90	140.87	45.60	139.77
12.48	25.80	217.02	25.10	218.82

Adsorption Model Details

The basics of the model are broken up into three parts: (i) aqueous reactions, (ii) mass balances, and (iii) electroneutrality. Aqueous reactions are represented in the model as shown in equations S1 and S2. In this representation, υ is the stoichiometric constant for each species involved in the reaction, γ^{aq} is the aqueous activity coefficient of those species, $[i]$ is the aqueous molar concentration of the i^{th} species, $\{i\}$ is the aqueous activity of the i^{th} species, and K is the equilibrium constant for that reaction. The aqueous activity coefficients can be determined using the Davies or Debye-Hückel equations or similar models.[S11]

$$\sum_{i}^{\text{reactants}} \upsilon_i \{i\} \Leftrightarrow \sum_{j}^{\text{products}} \upsilon_j \{j\} \tag{S1}$$

$$K = \frac{\prod_{j}^{\text{products}} \left(\gamma_j^{aq}[j]\right)^{\upsilon_j}}{\prod_{i}^{\text{reactants}} \left(\gamma_i^{aq}[i]\right)^{\upsilon_i}} \tag{S2}$$

Mass balances in the model are formed as the sums of the molar contributions and concentrations of each species in the system that contributes to a particular mass group. For instance, total carbonate in the system would be based on how much CO_3^{2-} was added to the system in total, and must equal the concentrations of each species containing CO_3^{2-} groups in their respective molar contributions (i.e., $UO_2(CO_3)_3^{4-}$ would contribute 3 moles of CO_3^{2-} to the carbonate mass balance). In addition, our model accounts for the mass removed from the aqueous phase via adsorption as shown in equation S3 below:[S14]

$$C_T - \frac{m_a}{V}\sum_j \delta_j q_j = \sum_i \delta_i [i] \tag{S3}$$

where C_T is the total concentration of a particular species group, m_a is the total mass of an adsorbent in the system, V is the total volume of the system, δ_i is the molar contribution of species i to the total concentration, and q_i is the adsorbed molar concentration of species i.

The pH of the system is determined using the condition of electroneutrality in the aqueous phase (equation S4). This condition looks at the ionic charge (n) of each species in solution and requires that the total concentrations of positive and negative ions cancel out each other, such that there is no net charge in the system.[S11,S14] Alternatively, our model can consider the system at a constant

pH by applying an equality constraint on the activity of the protons, $\{H^+\}$, in solution (equation S5).

$$0 = \sum_i n_i [i] \tag{S4}$$

$$\mathrm{pH} = -\log\left\{\mathrm{H}^+\right\} \tag{S5}$$

UNIQUAC Parameters

The parameters of UNIQUAC include structural information about the adsorbing species, as well as reaction energies for the bonding of the adsorbates with their respective ligands. Shape factors ($s_{i,l}$ and $r_{i,l}$) for each adsorbed species are determined as a ratio of the van der Waals areas and volumes ($a_{i,l}$ and $v_{i,l}$) of the adsorbates to a standard segment area and volume (A_w = 2.5 x 10^9 cm^2/mol and V_w = 15.17 cm^3/mol) defined by Abrams and Prausnitz[S15] (equations S6 and S7). The van der Waals areas and volumes themselves can be calculated from the atoms that make up each adsorbate.[S16]

$$r_{i,l} = v_{i,l} \Big/ V_w \tag{S6}$$

$$s_{i,l} = a_{i,l} \Big/ A_w \tag{S7}$$

After determining those shape factors, the remaining structural parameters of UNIQUAC are calculated as shown in equations S8 through S11.[S15] This gives information on the surface mole fractions ($y_{i,l}$), average area fractions ($\theta_{i,l}$), volume fractions ($\Phi_{i,l}$), and length factors ($\lambda_{i,l}$). Once this information is determined, the only missing parameters from UNIQUAC are the binary interaction terms ($\tau_{ij,lm}$).

$$y_{i,l} = \frac{q_{i,l}}{\sum_{\forall(j,m)} q_{j,m}} \tag{S8}$$

$$\theta_{i,l} = \frac{s_{i,l} y_{i,l}}{\sum_{\forall(j,m)} s_{j,m} y_{j,m}} \tag{S9}$$

$$\Phi_{i,l} = \frac{r_{i,l} y_{i,l}}{\sum_{\forall(j,m)} r_{j,m} y_{j,m}} \tag{S10}$$

$$\lambda_{i,l} = \left(\frac{z}{2}\right)\left(r_{i,l} - s_{i,l}\right) - \left(r_{i,l} - 1\right) \tag{S11}$$

In the original UNIQUAC model,[S14] the binary interaction terms were considered as adjustable parameters that needed to be obtained through optimization with adsorption data. It is possible, however, to provide approximations to those parameters from the binding energies of the individual adsorbing species. This can be accomplished by first considering the expansion of those binary parameters (equation S12) into a set of two energy terms: (i) a lateral interaction potential ($u_{ii,ll}$) and (ii) a cross-lateral interaction parameter ($u_{ji,ml}$).[S15,S17]

$$\tau_{ji,\,ml} = \exp\left[-\frac{u_{ji,\,ml} - u_{ii,\,ll}}{RT}\right] \tag{S12}$$

The physical meaning of the lateral ($u_{ii,ll}$) and cross-lateral ($u_{ji,ml}$) interaction parameters can be interpreted as the interaction energy between the i^{th} adsorbate with another i^{th} adsorbate and the interaction energy between the i^{th} adsorbate with the j^{th} adsorbate, respectively. Since the j^{th} and i^{th} adsorbates may be bonded to different ligands, the secondary subscripts of m and l are used to denote which ligand each is bound to (e.g., in equation S12 above, j and m are paired and i and l are paired). The lateral interaction parameter can be calculated from the heat of adsorption ($\Delta H_{i,l}$) and the area factor of the adsorbate ($s_{i,l}$) as shown in equation S13. It is then possible to provide an estimate to the cross-lateral term by taking the geometric average of each lateral interaction parameter (equation S14).[S15,S17]

$$u_{ii,\,ll} = -\frac{\Delta H_{i,\,l}}{s_{i,\,l}} \tag{S13}$$

$$u_{ji,\,ml} = u_{ij,\,lm} = \sqrt{u_{jj,\,mm}u_{ii,\,ll}} \tag{S14}$$

Computational Aspects

All of the model results and simulations were performed using software developed specifically for aqueous phase adsorption. That software is a module (called SHARK) of a larger programming project known as Ecosystem. Ecosystem is an open-source set of modeling tools for aqueous and gaseous physical/chemical processes developed by Dr. Austin Ladshaw as part of his PhD in Environmental Engineering. The software was developed entirely in C/C++ and has no external dependencies. Visit https://bitbucket.org/gitecosystem/ecosystem to download and/or view the source code.

Model Sensitivity

There are many different parameters and adsorption reactions involved with modeling the uptake of uranium and vanadium by amidoxime-functionalized fibers. From Figures 5b and 6b, it was shown that only a handful of all adsorption reactions considered contributes to the overall uptake capacities. For uranium, the major species were $UO_2(AO)_2$, $UO_2(H2IDO)_2$, and $UO_2(H_2IDO)(HIDO)^-$, while in the case of vanadium only two major species, $VO_2(HIDO)(IDO)$ and $V(IDO)_2^-$, showed major contributions to uptake. Therefore, the adsorption model will primarily be sensitive to the binding strengths ($\log \beta$) for reactions forming these species.

In addition, the electrical surface potential (ψ), and thus surface charging, also likely plays a key role in metal ion uptake. Figure 7 demonstrated that the addition of a counter-ion binding

mechanism with Na^+ in solution could account for major discrepancies between model predictions for vanadium adsorption and the experimental vanadium uptake. This counter-ion binding aids in the neutralization of the accumulated surface charge and allows for additional binding of negatively charged ions from solution. The electrical potential impacts the binding strength of metals through the Boltzmann factor (η), thus changing the electrical potential parameter will impact the binding affinities of all metal species for which there are adsorption reactions (Equations 5 and 6).

Figures S2 and S3 below show simulated results of a sensitivity analysis for modeling uranium and vanadium adsorption. In this analysis, only the major parameters that impact adsorption of each metal were examined for sensitivity. The baseline for each test represents the model as is, without variation of any parameters. Then, one parameter is varied by either +1 or -1 log unit (i.e., if log β is -2.7, then +1 log unit changes log β to -1.7) and the results are compared to those of the baseline. Electrical potential is changed such that the net effect to the binding affinities will be +1 or -1 log unit (i.e., the change in electrical potential applied corresponds to a +1 or -1 log unit change in the overall equilibrium constant).

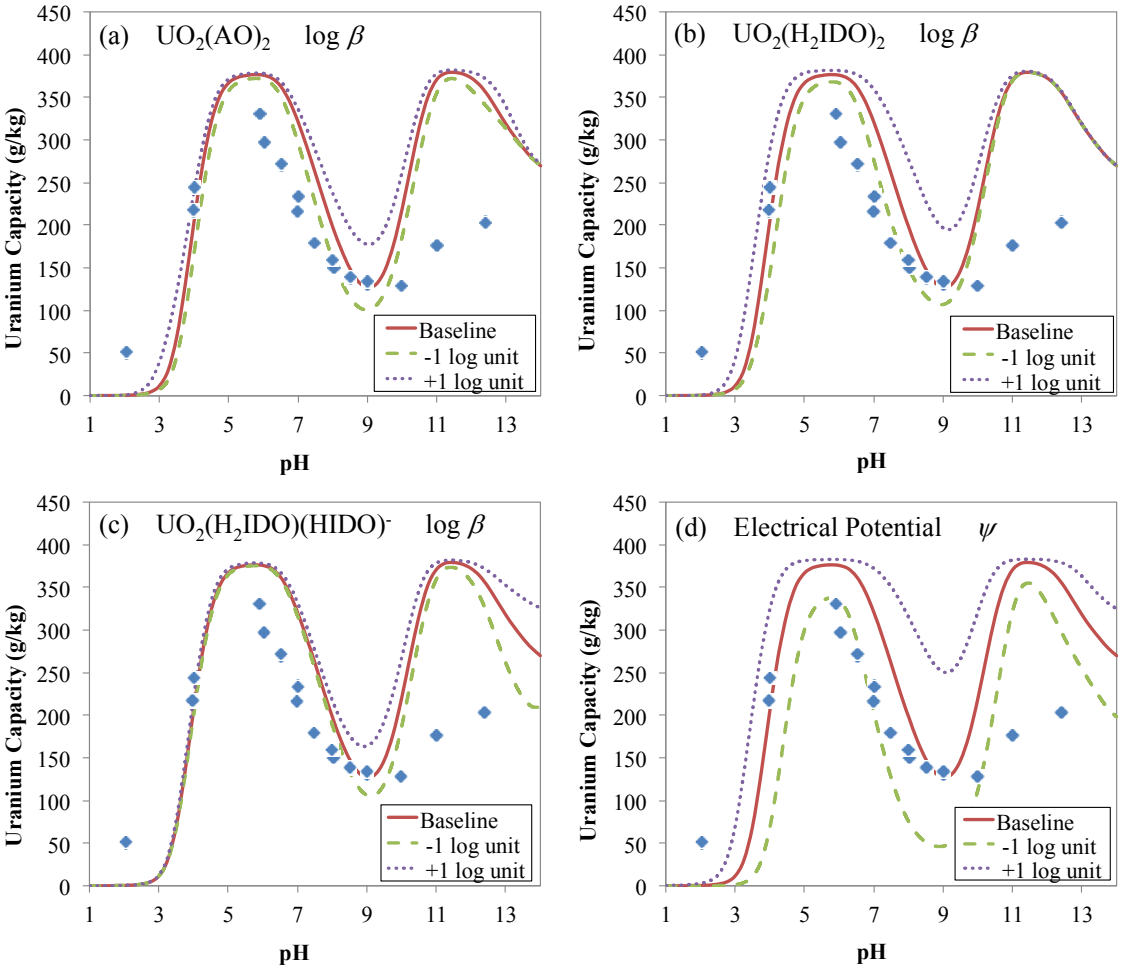


Figure S2. Adsorption model sensitivity to four major parameters associated with uranium uptake: (a) binding strength for formation of $UO_2(AO)_2$, (b) binding strength for formation of $UO_2(H_2IDO)_2$, (c) binding strength for formation of $UO_2(H_2IDO)(HIDO)^-$, and (d) electrical potential. Electrical surface potential has the greatest impact on the model results, which is due to the fact that changes in this parameter will affect all binding constants for all adsorption reactions on the same surface.

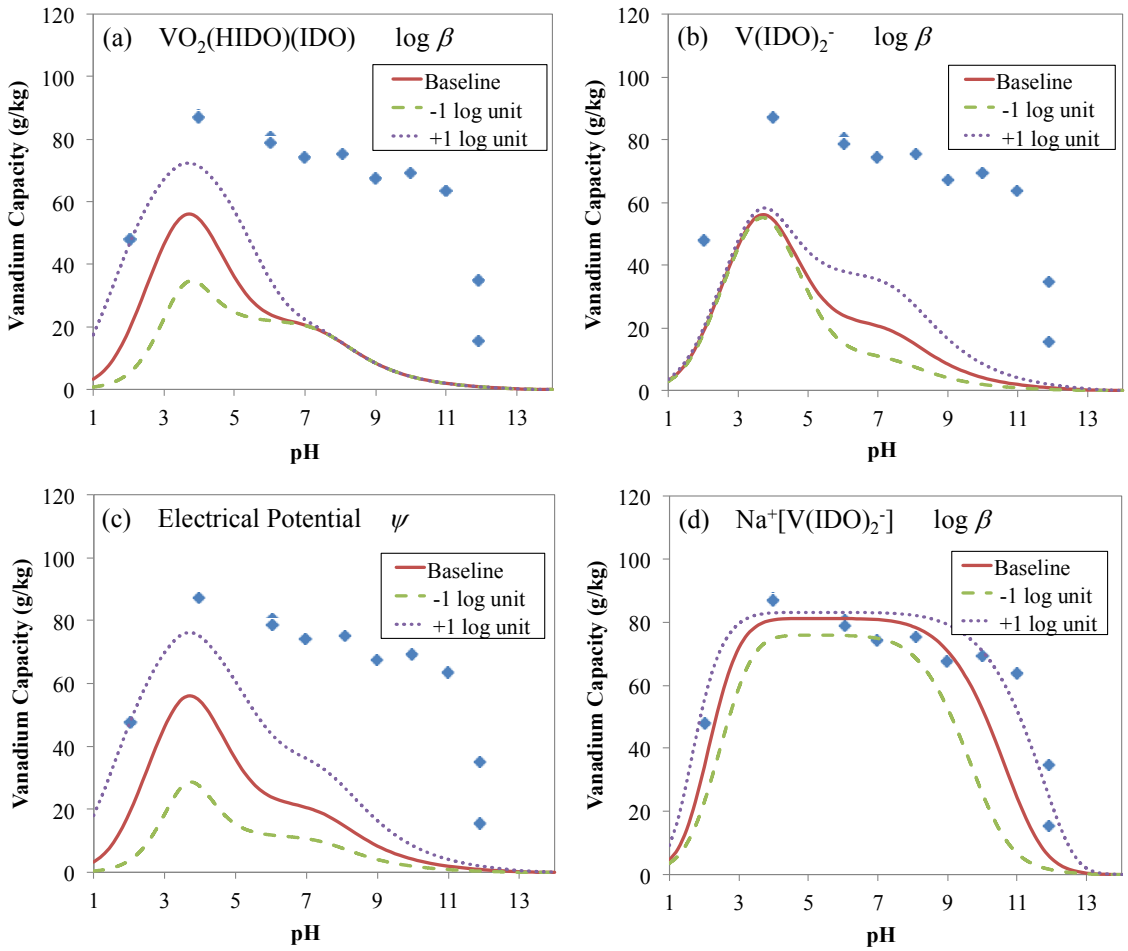


Figure S3. Adsorption model sensitivity to four major parameters associated with vanadium uptake: (a) binding strength for formation of $VO_2(HIDO)(IDO)$, (b) binding strength for formation of $V(IDO)_2^-$, (c) electrical potential, and (d) binding strength for formation of $Na^+[V(IDO)_2^-]$. Electrical surface potential has the greatest impact on the model results, but the data are best described by including the counter-ion binding mechanism to form $Na^+[V(IDO)_2^-]$.

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Free energy terms (kcal/mol) used to calculate log β^{calc} for the 1:2 uranyl complexes in Tables S1-S2.

ligand (L)	$\Delta G_{solv}^{*}(L)$	$\Delta G_{solv}^{*}(ML_2)$	$\Delta\Delta G_{solv}^{*}$	ΔG^{o}_{g}	ΔG_{aq}
carbonate	-258.30	-193.32	522.34	-570.26	-47.92
glutarimidedioximate ($HIDO^{2-}$)	-208.48	-216.23	394.69	-473.61	-78.93
salicylamidoximate	-194.43	-164.25	418.56	-488.49	-69.94
oxalate	-223.07	-176.15	469.06	-507.37	-38.31
malonate	-213.24	-172.07	453.47	-493.62	-39.15
phthalate	-200.95	-167.38	433.58	-467.26	-33.68
dipicolinate	-193.97	-176.93	404.98	-454.24	-49.26
phenanthroline dicarboxylate (PDA^{2-})	(PDA^{2-})	-78.27	379.25	-459.77	-62.95

and hydroxide (OH^-)	-185.28 (OH^-) -95.86				
glutarimidedioximate ($HIDO^{2-}$) and (H_2IDO^-)	($HIDO^{2-}$) -208.48 (H_2IDO^-) -58.63	-105.61	355.46	-420.67	-65.20

All values are calculated at 298.15 K. ΔG^*_{solv} for $[UO_2(H_2O)_5]^{2+}$ is -223.21 kcal/mol.

Sample Gaussian 09 input file

Cartesian coordinates for $UO_2(H_2O)_5^{2+}$, E = -1009.25500211 Hartree {B3LYP/SSC/6-31+G(d) level of theory}:

```
#N B3LYP/gen gfinput pseudo=read integral=(grid=199302) opt freq nosymm

Uranyl-water complex

2 1
U         0.000328430      0.000573500     -0.000680150
O        -0.000414280      0.002314290     -1.748420010
O         0.000789060      0.000047380      1.747059840
O        -2.086737240      1.375203180     -0.000490890
O        -1.951943970     -1.560025530     -0.001622770
O         0.879002380     -2.339364790     -0.002655720
H        -2.419181670      1.928579040     -0.732336010
H        -2.724806300      1.464176470      0.732518280
H        -2.230373280     -2.143732550      0.729197380
H        -2.584444310     -1.700603120     -0.731349310
H         0.816535500     -2.983665490     -0.732927750
H         1.350859080     -2.784432480      0.726443570
H         3.066061200      0.419173700      0.730261010
O         2.497157660      0.111245690     -0.000393400
H         3.090768610     -0.142205110     -0.732328440
H         1.087244070      2.897326550     -0.730970090
O         0.665487340      2.409506080      0.001492060
H         0.552119880      3.043933730      0.734288990

H, O 0
6-31+G(d)
********
U     0
S   7   1.00
   1534.9336000             0.0009200
    227.7483800             0.0036820
     30.6968310            -0.1502310
     18.1706260             0.9039950
     10.8135370            -1.4859220
      2.7332980             1.1244040
      1.4314980             0.3510760
S   7   1.00
```

```
   1534.9336000            -0.0006950
    227.7483800            -0.0022930
     30.6968310             0.0724440
     18.1706260            -0.4905590
     10.8135370             0.8898400
      2.7332980            -1.1157580
      1.4314980            -0.3336500
S   7   1.00
   1534.9336000             0.0002230
    227.7483800             0.0007220
     30.6968310            -0.0217020
     18.1706260             0.1497960
     10.8135370            -0.2761100
      2.7332980             0.3765790
      1.4314980             0.1244080
S   1   1.00
      0.6152980             1.0000000
S   1   1.00
      0.2866390             1.0000000
S   1   1.00
      0.0711700             1.0000000
S   1   1.00
      0.0305390             1.0000000
S   1   1.00
      0.0050000             1.0000000
P   6   1.00
    553.3452500            -0.0016100
    109.2550100            -0.0110870
     23.4760300            -0.0466190
      6.7944720             0.6441530
      5.4323190            -0.5204550
      2.7021690            -0.6311540
P   6   1.00
    553.3452500            -0.0010750
    109.2550100            -0.0080420
     23.4760300            -0.0279690
      6.7944720             0.4690490
      5.4323190            -0.4926390
      2.7021690            -0.3757660
P   1   1.00
      1.4938570             1.0000000
P   1   1.00
      0.7928170             1.0000000
P   1   1.00
      0.3515420             1.0000000
P   1   1.00
      0.1439620             1.0000000
P   1   1.00
      0.0050000             1.0000000
D   6   1.00
     81.2028580            -0.0016200
     18.3255750            -0.0251810
     10.4546990             0.0896320
      3.6663120            -0.4094290
      1.9233490            -0.4822600
      0.9896380            -0.2109030
D   6   1.00
     81.2028580            -0.0006390
     18.3255750            -0.0070210
     10.4546990             0.0266420
      3.6663120            -0.1571320
      1.9233490            -0.1575720
      0.9896380            -0.0011000
D   1   1.00
      0.4953460             1.0000000
D   1   1.00
      0.2044550             1.0000000
D   1   1.00
      0.0732730             1.0000000
D   1   1.00
      0.0050000             1.0000000
```

```
F   5   1.00
     55.3345250              0.0012940
     16.5886490              0.0098570
      4.7575180              0.1303860
      2.3875500              0.3180830
      1.1301950              0.3953140
F   1   1.00
      0.4895350              1.0000000
F   1   1.00
      0.1814200              1.0000000
****

U     0
U-ECP     5     60
h-ul potential
  1
2      1.000000000            0.000000000
s-ul potential
  1
2     16.414038690          536.516627780
p-ul potential
  1
2      9.060556060          169.544924650
d-ul potential
  1
2      8.831831980          142.615598370
f-ul potential
  1
2      7.018516290           60.393076020
g-ul potential
  1
2     12.804088440          -60.129989580
```

Cartesian coordinates for $VO_2(H_2O)_3^+$, E = -451.3142753 Hartree {B3LYP/SSC/6-31+G(d) level of theory}:

```
#N B3LYP/gen gfinput pseudo=read integral=(grid=199302) opt freq nosymm

Vanadium(V)-water complex

1 1
V         0.907600000     -0.246400000     -2.629700000
O         1.108500000      1.082700000     -1.800100000
O         0.412600000     -1.401500000     -1.672800000
O        -0.975700000      0.240900000     -3.415300000
H        -1.685700000     -0.360000000     -3.117200000
H        -1.265100000      1.146300000     -3.190300000
O         2.927200000     -0.813400000     -2.669400000
H         3.102400000     -1.653000000     -2.201800000
H         3.522600000     -0.146600000     -2.275600000
O         1.252700000     -0.449100000     -4.719900000
H         0.591200000     -0.297600000     -5.417800000
H         2.098500000     -0.704300000     -5.128800000

H, O 0
6-31+G(d)
********
V     0
S   3   1.00
     12.8432080              1.1406430
     11.3757530             -1.2188030
      5.4069740             -0.8929030
S   1   1.00
      1.4659270              1.0000000
```

```
S   1   1.00
      0.5980800              1.0000000
S   1   1.00
      0.0887900              1.0000000
S   1   1.00
      0.0353180              1.0000000
S   1   1.00
      0.0100000              1.0000000
P   2   1.00
     31.8898680              0.0394070
      8.2371780             -1.0226030
P   2   1.00
      4.3283730              0.1927560
      1.5405260              0.8511680
P   1   1.00
      0.5280810              1.0000000
P   1   1.00
      0.0899620              1.0000000
P   1   1.00
      0.0263930              1.0000000
D   4   1.00
     22.6804330              0.0362930
      6.8613120              0.1773010
      2.2754450              0.4304290
      0.7319220              0.5893030
D   1   1.00
      0.2007460              1.0000000
D   1   1.00
      0.0600000              1.0000000
F   1   1.00
      0.7700000              1.0000000
****

V     0
V-ECP     3     10
f-ul potential
  1
2      1.000000000            0.000000000
s-ul potential
  2
2     14.490000000          178.447971000
2      6.524000000           19.831375000
p-ul potential
  2
2     14.300000000          109.529763000
2      6.021000000           12.570310000
d-ul potential
  2
2     17.480000000          -19.219657000
2      5.709000000           -0.642775000
```

Cartesian coordinates ((B3LYP/SSC/6-31+G(d)) of ligands and metal−ligand complexes from Tables S1-S2 and Tables 3-4 in the main text.

```
Water (H2O), E= -76.4212209459 Hartree
H        0.000000000     -0.099169890     -0.896345770
O        0.000000000     -0.094651640      0.072628770
H        0.000000000      0.840136420      0.327782390
```

Ligands:

Carbonate (CO_3^{2-}), E= -263.694856752 Hartree

C	0.000001050	-0.000009330	-0.000002390
O	-1.141610560	-0.647283600	0.000106500
O	1.131376340	-0.665008700	0.000311620
O	0.010232300	1.312300080	-0.000416840

Glutarimidedioximate ($HIDO^{2-}$), E= -509.290313635 Hartree

C	0.033593610	0.081388280	1.233898680
N	-0.600013940	0.338758940	0.001045500
C	0.032730270	0.081363310	-1.232246840
N	-0.597910700	-0.141785330	2.358931790
N	-0.599574020	-0.141830380	-2.356827690
O	-1.943253890	-0.156723630	-2.311889000
C	1.531963090	0.206186120	-1.249754710
C	1.532842020	0.206204950	1.250342540
H	1.898139280	-0.239499460	-2.183364580
H	1.843320540	1.275072050	1.255102170
H	1.899662200	-0.239480830	2.183700590
O	-1.941622310	-0.156680700	2.314952660
H	1.842432840	1.275055650	-1.254727770
C	2.168071310	-0.432368870	0.000079210
H	3.264968860	-0.284505360	-0.000302690
H	1.975856130	-1.516737050	0.000153080
H	-1.602845830	0.153655290	0.001382760

Salicylamidoximate (Sal^{2-}), E= -474.861511766 Hartree

N	1.643621000	-2.522586000	-0.159491000
C	1.215980000	-1.266405000	-0.160317000
C	-2.695587000	0.543898000	0.057200000
C	-2.583249000	-0.853673000	0.080852000
C	-1.300953000	-1.437416000	0.009309000
C	-0.118924000	-0.675782000	-0.085674000
C	-0.214124000	0.799465000	-0.112690000
C	-1.547679000	1.339901000	-0.036385000
H	-3.681676000	1.019339000	0.111808000
H	-3.471213000	-1.486054000	0.153575000
H	-1.172634000	-2.515662000	0.025117000
O	0.810572000	1.570172000	-0.197633000
H	-1.628032000	2.429564000	-0.055484000
O	0.770796000	-3.520305000	-0.079063000
H	2.025891000	-0.542942000	-0.230649000

Oxalate ($Oxal^{2-}$), E= -377.107786808 Hartree

O	1.358812650	0.799385420	0.809322700
O	-1.356018320	0.804935580	-0.808504120
C	0.785753440	-0.001378310	0.004045640
C	-0.785753130	0.001360840	-0.004044450
O	1.364273070	-0.804142680	-0.795320580
O	-1.367067600	-0.800203270	0.794498920

Malonate ($Malon^{2-}$), E= -416.438288054 Hartree

O	-3.231235000	2.194978000	0.259168000
C	-2.646286000	2.934542000	-0.596794000
O	-2.917918000	3.013107000	-1.829785000
C	-1.558645000	3.913690000	-0.038608000
H	-1.968830000	4.929719000	-0.131402000
H	-1.441807000	3.693153000	1.032267000
C	-0.119171000	3.937257000	-0.655192000
O	0.317961000	5.075325000	-1.023210000
O	0.525468000	2.848757000	-0.661793000

Phthalate ($Phthal^{2-}$), E= -624.256746309 Hartree

O	-1.329876090	-1.854437560	1.167177280

C	-1.606800650	-1.097430380	0.201922270
O	-2.590321390	-1.165464840	-0.593823670
C	0.705742550	0.175296330	-0.043256140
C	-0.736313000	2.618487760	0.041171550
C	1.355709130	1.425114060	-0.074804920
C	-0.710523750	0.155241760	0.043478560
C	-1.395521550	1.386150320	0.076750150
C	0.661962520	2.638283570	-0.037418540
H	2.443477920	1.420937900	-0.115308950
H	-2.482730440	1.351112430	0.117122390
H	1.205759370	3.585078990	-0.067513920
H	-1.306619010	3.549509760	0.072623770
C	1.637145270	-1.051196510	-0.203593870
O	1.383424920	-1.812614380	-1.171788090
O	2.620721670	-1.093970720	0.593779800

Dipicolinate (Dip^{2-}), E= -624.256746309 Hartree

C	1.162005000	3.336873000	0.005835000
N	-0.000829000	2.656403000	0.055156000
C	-1.163175000	3.338684000	0.023384000
C	0.000059000	5.449566000	-0.110881000
C	1.199867000	4.743041000	-0.038489000
C	-1.200176000	4.740270000	-0.099263000
H	-2.165655000	5.230310000	-0.186520000
H	2.165782000	5.239019000	-0.010186000
C	-2.518360000	2.591676000	0.132163000
O	-2.610265000	1.689721000	1.000771000
C	2.517001000	2.581085000	-0.013162000
O	2.604258000	1.573717000	-0.757321000
O	-3.418328000	3.022700000	-0.652723000
O	3.421353000	3.109797000	0.704234000
H	0.000443000	6.540559000	-0.175842000

Phenanthroline dicarboxylate (PDA^{2-}), E= -947.6214293 Hartree

O	-0.819195000	2.746507000	12.574694000
O	-0.086613000	0.591413000	12.671031000
O	6.694383000	0.732147000	8.850749000
O	6.288172000	2.903528000	9.407945000
N	0.985879000	1.662906000	9.975731000
N	3.509495000	1.744525000	8.705192000
C	4.695184000	1.715938000	8.100239000
C	2.376947000	1.678503000	7.959660000
C	1.062508000	1.674475000	8.620422000
C	-0.107172000	1.669922000	7.795901000
C	-1.365436000	1.703475000	8.446539000
H	-2.274052000	1.711140000	7.841623000
C	-1.420588000	1.734520000	9.817081000
H	-2.364020000	1.790985000	10.353206000
C	-0.207688000	1.690669000	10.565033000
C	6.011386000	1.793315000	8.894461000
C	-0.355109000	1.673672000	12.097021000
C	-0.009649000	1.633074000	6.369165000
H	-0.930605000	1.625222000	5.784979000
C	1.210067000	1.603815000	5.756783000
H	1.290886000	1.567921000	4.669724000
C	2.413532000	1.624256000	6.530024000
C	3.687160000	1.591042000	5.910008000
H	3.744655000	1.539121000	4.821176000
C	4.820029000	1.615433000	6.683644000
H	5.814314000	1.561143000	6.248742000

Hydroxide (OH^{-}), E= -75.7953692872 Hartree

O	-0.108268380	0.000000000	0.000000000

H	0.866500980	0.000000000	0.000000000

Glutarimidedioximate (H_2IDO^-), E= -510.018368149 Hartree

C	0.036609000	0.266486000	1.182043000
N	-0.628178000	0.358553000	-0.006103000
C	0.051745000	0.308959000	-1.188188000
N	-0.572974000	0.216579000	2.338704000
N	-0.542840000	0.300368000	-2.353668000
O	-1.962690000	0.375436000	-2.232561000
C	1.570266000	0.269184000	-1.237419000
C	1.554291000	0.224173000	1.249292000
H	1.883790000	-0.201401000	-2.175877000
H	1.943288000	1.254231000	1.301920000
H	1.855648000	-0.280322000	2.174033000
O	-1.991158000	0.296654000	2.201923000
H	1.959328000	1.300525000	-1.247372000
C	2.128469000	-0.450006000	-0.003011000
H	3.227578000	-0.416987000	0.004678000
H	1.834720000	-1.509656000	-0.024046000
H	-2.117045000	0.399572000	-1.259618000
H	-2.132702000	0.355870000	1.228532000

Acetamidoximate (AO^-), E= -263.919290431 Hartree

N	-0.784947530	-0.721718310	0.004270350
C	-0.037524380	0.347054630	0.003684770
N	1.385690730	0.240443870	0.082817530
H	1.533665370	-0.778987800	-0.003852450
H	1.846693510	0.716269020	-0.695319380
C	-0.649183020	1.712453180	0.007462020
H	-0.337701590	2.323684230	-0.862432940
H	-0.373733280	2.294339700	0.905417730
H	-1.740736600	1.609639680	-0.025495060
O	-0.125154310	-1.892814570	-0.000792230

Complexes, Table S1-S2:

$UO_2(CO_3)_2(H_2O)^{2-}$, E= -1231.8429462 Hartree

U	0.139814000	-0.137228000	-0.181844000
O	-1.642135000	-0.384125000	0.071101000
O	1.928977000	-0.049353000	-0.399774000
O	0.242817000	1.195843000	1.735914000
C	0.412971000	0.249553000	2.652241000
O	0.491035000	0.464857000	3.873832000
O	0.494936000	-0.959688000	2.102983000
O	-0.109796000	-0.865110000	-2.421796000
C	-0.292549000	0.350210000	-2.918454000
O	-0.494642000	0.598481000	-4.120234000
O	-0.235217000	1.288143000	-1.967796000
O	-0.125538000	-2.848501000	0.420318000
H	-1.078470000	-2.714584000	0.283155000
H	0.051545000	-2.454313000	1.311854000

$UO_2(HIDO)_2^{2-}$, E= -1646.4397463 Hartree

C	3.276921000	1.249309000	-0.118582000
N	2.648014000	0.014995000	-0.207369000
C	3.348608000	-1.100998000	-0.165797000
N	2.555030000	2.323701000	-0.002461000
N	2.657693000	-2.239930000	-0.118772000
O	1.318636000	-2.253442000	-0.249251000
C	4.864539000	-1.157579000	-0.128383000
C	4.781922000	1.343518000	-0.177448000
H	5.199502000	-2.053850000	0.414781000

H	5.135111000	1.355431000	-1.227444000
H	5.101326000	2.287759000	0.279253000
O	-1.227709000	-2.103698000	0.009907000
H	5.260101000	-1.237811000	-1.154913000
C	5.419547000	0.125348000	0.515605000
H	6.517603000	0.149313000	0.434580000
H	5.165198000	0.136646000	1.585172000
U	0.000000000	0.000000000	0.000000000
O	0.197808000	-0.099502000	1.788252000
H	3.126890000	-3.136707000	-0.216503000

$UO_2(Sal)_2^{2-}$, E= -1577.61440002 Hartree

N	0.924879000	1.087099000	0.742898000
C	-0.169055000	1.202860000	0.068542000
H	-0.623741000	2.192634000	-0.060769000
C	-2.094705000	-2.189228000	-1.694363000
C	-2.649393000	-0.906759000	-1.841171000
C	-1.985914000	0.173077000	-1.248039000
C	-0.795045000	0.025590000	-0.516811000
C	-0.208605000	-1.296747000	-0.357067000
C	-0.915420000	-2.374617000	-0.976704000
H	-2.589039000	-3.051539000	-2.145325000
H	-3.571064000	-0.752859000	-2.400767000
H	-2.400436000	1.178345000	-1.349992000
O	0.881827000	-1.530124000	0.295825000
H	-0.481981000	-3.366066000	-0.860422000
O	1.610119000	2.034694000	1.328431000
U	2.605881000	-0.343365000	1.572866000
O	1.654254000	-0.587629000	3.084345000
O	3.557514000	-0.099166000	0.061384000
O	4.329729000	0.843615000	2.849869000
N	4.287113000	-1.773587000	2.402827000
O	3.602117000	-2.721314000	1.817230000
C	5.380988000	-1.889164000	3.077319000
C	6.006662000	-0.711823000	3.662856000
C	5.420017000	0.610409000	3.503064000
C	6.126475000	1.688372000	4.122942000
C	7.305625000	1.503155000	4.840868000
C	7.860530000	0.220783000	4.987704000
C	7.197397000	-0.859139000	4.394338000
H	5.835808000	-2.878870000	3.206683000
H	7.612085000	-1.864336000	4.496318000
H	8.782104000	0.067021000	5.547497000
H	7.799692000	2.365529000	5.292005000
H	5.692881000	2.679748000	4.006618000

$UO_2(Oxal)_2(H_2O)^{2-}$, E= -1458.5668265 Hartree

U	-0.344313000	0.540360000	-0.010464000
O	-0.074237000	0.589793000	-1.789626000
O	-0.504812000	0.490694000	1.776320000
O	2.315924000	0.943757000	0.123608000
O	1.203501000	-1.363248000	0.035646000
O	-1.361950000	-1.550004000	-0.198163000
C	0.804830000	-2.589798000	-0.134390000
C	-0.767243000	-2.705270000	-0.238837000
O	1.529378000	-3.580861000	-0.214202000
O	-1.314322000	-3.801308000	-0.347727000
H	2.406398000	-0.025378000	-0.040776000
H	2.450547000	1.399882000	-0.721614000
O	-2.272819000	1.810996000	-0.213093000
C	-2.309023000	3.112985000	-0.247784000
O	-3.316819000	3.806473000	-0.365110000
C	-0.871378000	3.759057000	-0.122360000

O	-0.715807000	4.979482000	-0.166217000
O	0.065024000	2.870111000	0.020721000

$UO_2(Malon)_2(H_2O)^{2-}$, E= -1537.209144 Hartree

U	-0.281533000	0.552336000	-0.097691000
O	0.019425000	0.152920000	-1.822030000
O	-0.523716000	0.959090000	1.631192000
O	2.293067000	1.164389000	0.353316000
O	1.353640000	-1.228174000	0.324340000
O	-1.443029000	-1.430101000	0.182627000
C	1.396257000	-2.477527000	-0.017101000
C	-1.223671000	-2.695652000	-0.007320000
O	2.396180000	-3.203141000	0.103638000
O	-2.027213000	-3.596886000	0.267756000
H	2.545849000	0.233191000	0.171266000
H	2.426319000	1.717664000	-0.434657000
C	0.123000000	-3.060023000	-0.658475000
H	0.216159000	-4.146043000	-0.712183000
H	0.091864000	-2.657662000	-1.682287000
O	-2.191763000	1.730733000	-0.643186000
C	-2.593877000	2.964571000	-0.611445000
O	-3.712803000	3.350328000	-0.974548000
C	-1.588892000	3.985260000	-0.042802000
H	-1.995187000	4.991381000	-0.158847000
H	-1.492586000	3.762591000	1.030587000
C	-0.164239000	3.939572000	-0.629442000
O	0.370897000	4.993673000	-1.008005000
O	0.402304000	2.776363000	-0.656337000

$UO_2(Phthal)_2(H_2O)^{2-}$, E= -1920.689575 Hartree

U	0.849188000	-1.490040000	0.962081000
O	-0.079911000	-1.263872000	-0.549126000
O	1.685489000	-1.738896000	2.518921000
O	-1.599480000	-2.027803000	1.857524000
O	-0.262697000	0.387575000	1.891986000
C	-1.156059000	1.025697000	1.222448000
O	-2.374206000	0.746467000	1.235625000
C	0.706528000	2.482248000	0.170153000
C	-1.300086000	4.092426000	-1.016182000
C	1.031779000	3.598307000	-0.624547000
C	-0.661591000	2.185846000	0.374117000
C	-1.640215000	3.000447000	-0.220768000
C	0.052361000	4.390225000	-1.221855000
H	2.083028000	3.838651000	-0.757303000
H	-2.678332000	2.737416000	-0.040536000
H	0.342938000	5.238781000	-1.840552000
H	-2.078195000	4.703559000	-1.471793000
C	1.924183000	1.726572000	0.730630000
O	2.040973000	0.478028000	0.435192000
O	2.764264000	2.413113000	1.328700000
H	-2.110165000	-1.215613000	1.644087000
H	-1.902178000	-2.765219000	1.282586000
O	3.696731000	-4.548661000	-0.293112000
C	2.680127000	-3.901970000	-0.581331000
O	2.465702000	-2.664331000	-0.294965000
C	1.659596000	-4.612341000	-1.487744000
C	2.206533000	-5.145559000	-2.670690000
H	3.274813000	-5.031964000	-2.833129000
H	1.879371000	-6.200065000	-4.521493000
C	1.422824000	-5.811828000	-3.611479000
C	0.053400000	-5.983243000	-3.376158000
H	-0.572440000	-6.505319000	-4.098857000
H	-1.560334000	-5.586282000	-1.988433000

C	-0.501795000	-5.474850000	-2.203917000
C	0.275303000	-4.788027000	-1.255464000
C	-0.442751000	-4.281118000	-0.015523000
O	0.300235000	-3.797238000	0.915890000
O	-1.688938000	-4.352121000	0.047843000

$UO_2(Dip)_2^{2-}$, E= -1876.3451932 Hartree

C	1.158258000	3.422052000	-0.008592000
N	-0.000015000	2.752170000	0.016245000
C	-1.158275000	3.422091000	-0.008140000
C	0.000005000	5.523676000	-0.112276000
C	1.204339000	4.817746000	-0.074765000
C	-1.204335000	4.817791000	-0.074143000
H	-2.175219000	5.302324000	-0.090444000
H	2.175235000	5.302237000	-0.091587000
U	0.000019000	-0.000030000	-0.000553000
C	-2.397227000	2.539141000	0.060880000
O	-2.122725000	1.296644000	0.112310000
C	2.397203000	2.539123000	0.060047000
O	2.122726000	1.296630000	0.112343000
O	-3.513961000	3.090814000	0.070409000
O	3.513984000	3.090715000	0.067797000
H	0.000012000	6.612066000	-0.165558000
O	0.000077000	-0.094494000	1.779150000
O	-0.000063000	0.094436000	-1.780261000
O	-2.122754000	-1.296725000	-0.113186000
C	-2.397236000	-2.539198000	-0.061102000
O	-3.513956000	-3.090904000	-0.070500000
C	-1.158279000	-3.422082000	0.008648000
N	-0.000018000	-2.752181000	-0.016306000
C	1.158257000	-3.422037000	0.009170000
C	2.397205000	-2.539175000	-0.060246000
O	2.122734000	-1.296724000	-0.113549000
O	3.513976000	-3.090793000	-0.067766000
C	1.204339000	-4.817674000	0.076526000
H	2.175229000	-5.302157000	0.093850000
C	0.000005000	-5.523578000	0.114533000
H	0.000013000	-6.611927000	0.168625000
C	-1.204337000	-4.817725000	0.075828000
H	-2.175214000	-5.302256000	0.092570000

$UO_2(PDA)(OH)^-$, E= -1651.2433212 Hartree

U	3.275387000	1.710285000	11.363023000
O	3.254729000	-0.085856000	11.301641000
O	1.136389000	1.684342000	12.490862000
O	-1.125656000	1.645815000	12.669921000
O	5.453046000	1.708921000	10.311309000
O	6.940233000	1.689597000	8.597222000
N	1.018458000	1.674832000	9.864424000
N	3.409612000	1.688128000	8.656979000
C	4.617088000	1.693629000	8.106547000
C	2.315297000	1.681347000	7.863244000
C	1.029417000	1.674210000	8.512578000
C	-0.155423000	1.666490000	7.735256000
C	-1.383436000	1.658946000	8.442346000
H	-2.320174000	1.653099000	7.887823000
C	-1.378361000	1.658594000	9.822652000
H	-2.287181000	1.652057000	10.414458000
C	-0.141325000	1.667286000	10.509367000
C	5.800386000	1.698214000	9.080616000
C	-0.060068000	1.665836000	12.039757000
C	-0.045876000	1.666555000	6.303210000
H	-0.959251000	1.661018000	5.712123000

C	1.175535000	1.673334000	5.686403000
H	1.242021000	1.673233000	4.600465000
C	2.393086000	1.680619000	6.448299000
C	3.691203000	1.687040000	5.879837000
H	3.801130000	1.687003000	4.796819000
C	4.798968000	1.692732000	6.703375000
H	5.814839000	1.696762000	6.323647000
O	3.210344000	3.500338000	11.254321000
O	4.247389000	1.716297000	13.288704000
H	4.473106000	0.882679000	13.727564000

$UO_2(HIDO)(H_2IDO)^-$, E= -1647.0942793 Hartree

C	-3.283726000	-1.236024000	0.098440000
N	-2.633073000	-0.090538000	0.171800000
C	-3.307638000	1.123080000	0.200856000
N	-2.529087000	-2.320472000	-0.038681000
N	-2.617921000	2.214664000	0.120009000
O	-1.277444000	1.982277000	0.048194000
C	-4.810909000	1.151488000	0.327366000
C	-4.792792000	-1.353758000	0.130245000
H	-5.188571000	2.100731000	-0.067500000
H	-5.124251000	-1.516851000	1.167815000
H	-5.120069000	-2.226107000	-0.451883000
O	-1.180261000	-2.233344000	0.021825000
H	-5.106512000	1.102279000	1.390057000
C	-5.427547000	-0.056089000	-0.402505000
H	-6.516922000	-0.084762000	-0.263356000
H	-5.235293000	0.028117000	-1.480853000
U	-0.096951000	0.015558000	-0.174568000
O	-0.368992000	-0.015159000	-1.946496000
O	0.266196000	-0.011585000	1.585355000
H	3.072056000	-3.095448000	-0.135117000
N	2.627256000	-2.186133000	-0.250691000
O	1.322806000	-2.201604000	-0.464561000
C	3.350052000	-1.083740000	-0.214651000
N	2.671874000	0.063967000	-0.352542000
H	5.349309000	-1.227645000	-0.998454000
C	4.847864000	-1.154674000	-0.020167000
H	5.122005000	-2.053374000	0.547702000
C	5.333996000	0.119050000	0.693809000
H	4.950889000	0.134118000	1.722278000
H	6.429682000	0.133945000	0.746938000
H	5.070257000	2.278559000	0.461106000
C	4.815148000	1.351420000	-0.068530000
H	5.311009000	1.395989000	-1.051463000
C	3.319385000	1.235660000	-0.249783000
N	2.563004000	2.313653000	-0.303893000
O	1.256796000	2.284819000	-0.484728000
H	2.981913000	3.238699000	-0.214787000
H	-2.916651000	-3.257471000	-0.015089000

Complexes, Tables S3-S4:

$UO_2(AO)^+$, E= -1120.69756022 Hartree

U	-0.000409640	0.546324980	0.000620690
O	-0.061103610	0.692054380	-1.771258400
O	-0.054842010	0.688504580	1.772997750
O	2.377196890	1.442877250	-0.002731850
H	2.929420550	1.247360210	0.774239960
H	2.926369180	1.249255740	-0.782337220
O	-0.450757060	3.060496420	0.004489280
H	-0.446711720	3.636781270	-0.778465470
H	-0.443735300	3.634336570	0.789218750

O	-2.533423190	0.385560250	0.004716820
H	-3.100799960	0.309674190	0.790217820
H	-3.103566270	0.311282630	-0.778931680
O	1.297938110	-1.245927910	-0.003515770
N	0.024389390	-1.797257270	-0.001751410
C	-0.049097000	-3.099316070	-0.003432480
N	1.059755720	-3.862102670	-0.006658310
H	1.968046760	-3.416120280	-0.007919780
H	1.006563430	-4.870007240	-0.007933980
C	-1.397054030	-3.758237520	-0.001631010
H	-1.514304660	-4.391878280	0.885094200
H	-1.517823680	-4.389541960	-0.889549880
H	-2.185777330	-3.003794770	0.000932870

$UO_2(AO)_2$, E= -1308.4117914 Hartree

U	0.000007000	0.000316000	0.001596000
O	-0.000089000	0.000405000	1.798700000
O	0.000081000	0.000285000	-1.782196000
O	-0.505617000	2.561652000	0.219713000
H	-0.687470000	2.718714000	1.160978000
H	0.420480000	2.839592000	0.084847000
O	1.905896000	1.370754000	0.011402000
N	2.421438000	0.100449000	-0.032567000
C	3.701837000	-0.025063000	-0.134307000
C	4.310720000	-1.394279000	-0.204622000
H	4.988444000	-1.571471000	0.641582000
H	3.523409000	-2.151355000	-0.188760000
H	4.890438000	-1.510441000	-1.128746000
N	4.520160000	1.074870000	-0.245778000
H	4.074768000	1.955655000	-0.013339000
H	5.484900000	0.976973000	0.039248000
N	-2.421431000	-0.099821000	-0.032790000
O	-1.905872000	-1.370114000	0.011324000
C	-3.701827000	0.025664000	-0.134610000
N	-4.520128000	-1.074291000	-0.246021000
H	-4.074737000	-1.955046000	-0.013466000
H	-5.484886000	-0.976378000	0.038939000
C	-4.310727000	1.394864000	-0.205087000
H	-3.523428000	2.151954000	-0.189255000
H	-4.988498000	1.572125000	0.641064000
H	-4.890397000	1.510931000	-1.129253000
O	0.505647000	-2.560942000	0.219871000
H	-0.420429000	-2.838929000	0.084957000
H	0.687412000	-2.717873000	1.161175000

$UO_2(AO)_3^-$, E= -1419.5414131 Hartree

O	-2.274203000	-0.755726000	0.109066000
N	-2.394416000	0.598912000	0.129552000
C	-3.575430000	1.104295000	0.056601000
N	-4.709585000	0.281558000	0.042858000
O	0.483441000	2.339956000	0.172183000
N	1.715948000	1.764854000	0.189256000
C	2.745570000	2.535178000	0.145008000
N	2.601888000	3.928803000	0.164785000
O	1.784054000	-1.595843000	0.147863000
N	0.669912000	-2.375954000	0.136629000
C	0.822729000	-3.651320000	0.061860000
N	2.101322000	-4.224122000	0.077480000
H	-4.428183000	-0.680102000	-0.145563000
H	-5.448471000	0.600663000	-0.575654000
H	2.799142000	-3.500197000	-0.091052000
H	2.208518000	-5.021821000	-0.540987000
H	1.630471000	4.172233000	-0.026347000

H	3.254107000	4.423798000	-0.435129000
U	-0.002736000	-0.003527000	0.160933000
O	0.018059000	0.014731000	-1.639309000
O	-0.023790000	-0.021682000	1.958040000
C	4.123442000	1.946432000	0.152389000
H	4.690972000	2.278330000	1.033309000
H	4.048972000	0.855858000	0.165826000
H	4.694633000	2.246882000	-0.740024000
C	-3.756714000	2.591640000	0.065964000
H	-4.279147000	2.939364000	-0.839052000
H	-4.351358000	2.912635000	0.932940000
H	-2.776435000	3.073755000	0.107463000
C	-0.376067000	-4.549936000	0.037532000
H	-0.395182000	-5.171404000	-0.871498000
H	-0.378469000	-5.230001000	0.901104000
H	-1.283321000	-3.940483000	0.060420000

$UO_2(AO)(CO_3)^-$, E= -1231.9543365 Hartree

N	0.622347000	0.956977000	-1.736582000
C	0.370499000	1.890428000	-2.586892000
O	0.602604000	-0.328965000	-2.199182000
U	1.291773000	-0.685764000	0.011432000
O	-0.435928000	-0.757456000	0.520590000
O	2.991421000	-0.406304000	-0.494529000
N	0.003641000	1.591311000	-3.897470000
H	0.212704000	0.619926000	-4.119073000
H	0.332933000	2.246076000	-4.597705000
O	1.360980000	1.161907000	1.907176000
H	1.738361000	0.433786000	2.460164000
H	0.421554000	1.188967000	2.152363000
O	2.357296000	-3.525296000	2.682457000
C	2.042834000	-2.640442000	1.891531000
O	1.689094000	-2.840741000	0.615610000
O	2.001614000	-1.334396000	2.179710000
C	0.392234000	3.326027000	-2.154903000
H	-0.593733000	3.792402000	-2.285967000
H	0.678646000	3.388110000	-1.101993000
H	1.115517000	3.908884000	-2.744334000

$UO_2(AO)_2(CO_3)^{2-}$, E= -1419.4078686 Hartree

N	-0.080934000	1.932341000	-1.436418000
C	-0.162340000	3.183312000	-1.721515000
O	-0.251639000	1.009571000	-2.401355000
U	-0.054727000	-0.207740000	-0.201687000
O	-1.856233000	-0.115590000	-0.075259000
O	1.730270000	-0.316312000	-0.470379000
N	-0.308659000	-2.180859000	-1.736533000
O	-0.206517000	-2.679839000	-0.491560000
C	-0.344847000	-2.997779000	-2.731185000
N	-0.361068000	-4.399381000	-2.513626000
N	-0.352816000	3.606299000	-3.061916000
H	0.327177000	-4.884942000	-3.087061000
H	-0.155426000	-4.536714000	-1.519657000
H	-0.608180000	2.774170000	-3.599705000
H	-1.077401000	4.317898000	-3.139236000
O	0.217597000	1.415567000	1.529173000
C	0.279682000	0.536832000	2.520238000
O	0.423710000	0.847943000	3.722129000
O	0.170751000	-0.713375000	2.086323000
C	-0.434766000	-2.473711000	-4.130396000
H	0.412258000	-2.816365000	-4.750505000
H	-1.357057000	-2.810188000	-4.630483000
H	-0.419831000	-1.380101000	-4.097762000

C	0.000091000	4.200512000	-0.635255000
H	-0.886685000	4.853501000	-0.557005000
H	0.134596000	3.674899000	0.316391000
H	0.867916000	4.853031000	-0.821249000

$UO_2(HIDO)$, E= -1289.93007127 Hartree

C	1.044488850	-2.214052610	0.000911730
N	-0.056767990	-1.497392560	0.148675680
C	-1.322221600	-2.085004080	0.208458040
N	2.174487460	-1.526784340	-0.131683850
N	-2.364402670	-1.323704950	0.209682500
O	-2.011139670	0.016079190	0.170814610
C	-1.443987840	-3.585514210	0.272731650
C	1.055735950	-3.724177180	-0.042922470
H	-2.428818990	-3.884091350	-0.097428510
H	1.253927040	-4.102179530	0.970642510
H	1.871182580	-4.079716850	-0.684083990
O	2.162577990	-0.169148750	0.021956600
H	3.089336900	-1.961465310	-0.142739120
H	-1.379419330	-3.912880460	1.321924080
C	-0.308877720	-4.245188130	-0.530921930
H	-0.346673620	-5.334890020	-0.424458160
H	-0.428112050	-4.017649910	-1.598019470
U	0.021604890	0.951804540	0.014747670
O	0.124059940	1.227691110	1.777374760
O	0.017950990	0.905071980	-1.772295500
H	-2.617299930	1.853807650	-0.037568190
O	-2.006834580	2.607468990	-0.213112040
H	-2.191661130	2.887997080	-1.124141240
H	2.425646240	2.751861230	0.801061320
O	2.174420250	2.443708940	-0.085279590
H	2.762828540	1.680510630	-0.273489560

$UO_2(H_2IDO)^+$, E= -1290.3383448 Hartree

C	1.039680000	-2.377554000	0.071088000
N	-0.098160000	-1.655102000	0.073287000
C	-1.303048000	-2.259267000	0.075225000
N	2.134181000	-1.655157000	0.025322000
N	-2.319249000	-1.430199000	0.031420000
O	-2.132656000	-0.096837000	0.019276000
C	-1.470977000	-3.754778000	0.129038000
C	1.056241000	-3.882686000	0.123914000
H	-2.392319000	-4.058216000	-0.379464000
H	1.127678000	-4.194872000	1.175744000
H	1.940161000	-4.277219000	-0.388479000
O	2.082311000	-0.309826000	0.015310000
H	3.067945000	-2.056686000	0.014010000
H	-1.569139000	-4.058062000	1.181309000
C	-0.239882000	-4.436909000	-0.498431000
H	-0.294199000	-5.517035000	-0.336994000
H	-0.233665000	-4.269808000	-1.582019000
U	0.028853000	0.854294000	-0.029120000
O	0.039576000	1.037449000	1.734942000
O	0.027802000	0.863978000	-1.802837000
H	-2.080878000	3.086222000	0.667843000
O	-1.553399000	2.835784000	-0.109782000
H	-2.102508000	3.010403000	-0.893137000
H	2.345548000	2.873812000	0.664761000
O	1.796423000	2.672363000	-0.112129000
H	2.357835000	2.796015000	-0.896410000
H	-3.288719000	-1.735747000	0.022543000

$UO_2(HIDO)_2^{2-}$, E= -1646.4397463 Hartree

C	3.276921000	1.249309000	-0.118582000
N	2.648014000	0.014995000	-0.207369000
C	3.348608000	-1.100998000	-0.165797000
N	2.555030000	2.323701000	-0.002461000
N	2.657693000	-2.239930000	-0.118772000
O	1.318636000	-2.253442000	-0.249251000
C	4.864539000	-1.157579000	-0.128383000
C	4.781922000	1.343518000	-0.177448000
H	5.199502000	-2.053850000	0.414781000
H	5.135111000	1.355431000	-1.227444000
H	5.101326000	2.287759000	0.279253000
O	-1.227709000	-2.103698000	0.009907000
H	5.260101000	-1.237811000	-1.154913000
C	5.419547000	0.125348000	0.515605000
H	6.517603000	0.149313000	0.434580000
H	5.165198000	0.136646000	1.585172000
U	0.000000000	0.000000000	0.000000000
O	0.197808000	-0.099502000	1.788252000
H	3.126890000	-3.136707000	-0.216503000

$UO_2(H_2IDO)(HIDO)^-$, E= -1647.0942793 Hartree

C	-3.283726000	-1.236024000	0.098440000
N	-2.633073000	-0.090538000	0.171800000
C	-3.307638000	1.123080000	0.200856000
N	-2.529087000	-2.320472000	-0.038681000
N	-2.617921000	2.214664000	0.120009000
O	-1.277444000	1.982277000	0.048194000
C	-4.810909000	1.151488000	0.327366000
C	-4.792792000	-1.353758000	0.130245000
H	-5.188571000	2.100731000	-0.067500000
H	-5.124251000	-1.516851000	1.167815000
H	-5.120069000	-2.226107000	-0.451883000
O	-1.180261000	-2.233344000	0.021825000
H	-5.106512000	1.102279000	1.390057000
C	-5.427547000	-0.056089000	-0.402505000
H	-6.516922000	-0.084762000	-0.263356000
H	-5.235293000	0.028117000	-1.480853000
U	-0.096951000	0.015558000	-0.174568000
O	-0.368992000	-0.015159000	-1.946496000
O	0.266196000	-0.011585000	1.585355000
H	3.072056000	-3.095448000	-0.135117000
N	2.627256000	-2.186133000	-0.250691000
O	1.322806000	-2.201604000	-0.464561000
C	3.350052000	-1.083740000	-0.214651000
N	2.671874000	0.063967000	-0.352542000
H	5.349309000	-1.227645000	-0.998454000
C	4.847864000	-1.154674000	-0.020167000
H	5.122005000	-2.053374000	0.547702000
C	5.333996000	0.119050000	0.693809000
H	4.950889000	0.134118000	1.722278000
H	6.429682000	0.133945000	0.746938000
H	5.070257000	2.278559000	0.461106000
C	4.815148000	1.351420000	-0.068530000
H	5.311009000	1.395989000	-1.051463000
C	3.319385000	1.235660000	-0.249783000
N	2.563004000	2.313653000	-0.303893000
O	1.256796000	2.284819000	-0.484728000
H	2.981913000	3.238699000	-0.214787000
H	-2.916651000	-3.257471000	-0.015089000

$UO_2(H_2IDO)_2$, E= -1647.6473781 Hartree

C	-5.586147000	9.886636000	-1.189472000
N	-6.080071000	8.872792000	-0.458546000

C	-7.171073000	9.065610000	0.302062000
N	-4.558105000	9.571015000	-1.943578000
N	-7.603002000	7.993726000	0.926148000
C	-7.864763000	10.398333000	0.445153000
C	-6.149976000	11.286107000	-1.164451000
H	-5.629617000	11.874832000	-0.394109000
O	-4.013598000	8.358066000	-1.943401000
H	-7.441288000	10.938866000	1.304946000
C	-7.651915000	11.230790000	-0.832077000
H	-8.046244000	12.243205000	-0.693798000
H	-8.199231000	10.775087000	-1.666673000
O	-6.978539000	6.822055000	0.856184000
H	-8.932701000	10.257046000	0.650017000
H	-5.976722000	11.788782000	-2.123466000
C	-3.079765000	3.774427000	-1.886473000
N	-4.170520000	3.967332000	-1.125556000
C	-4.663972000	2.953514000	-0.394144000
N	-2.647853000	4.846221000	-2.510754000
N	-5.691869000	3.269015000	0.360164000
C	-4.099914000	1.554129000	-0.419032000
C	-2.386222000	2.441674000	-2.029806000
H	-2.810424000	1.900967000	-2.889137000
O	-3.272247000	6.017961000	-2.440783000
H	-4.620589000	0.965078000	-1.188915000
C	-2.598168000	1.609494000	-0.752243000
H	-2.203831000	0.597080000	-0.890510000
H	-2.050389000	2.065462000	0.081905000
O	-6.236935000	4.481626000	0.359979000
U	-5.125181000	6.420118000	-0.792016000
O	-6.304230000	6.272818000	-2.118360000
O	-3.946273000	6.567189000	0.534475000
H	-4.272595000	1.051721000	0.540229000
H	-1.318448000	2.582882000	-2.235564000
H	-1.822963000	4.822111000	-3.105416000
H	-8.428292000	8.017594000	1.520273000
H	-6.140888000	2.585105000	0.964644000
H	-4.108406000	10.254857000	-2.547592000

$UO_2(HIDO)(CO_3)^{2-}$, E= -1400.9343642 Hartree

C	-3.071040000	3.814938000	-1.946605000
N	-4.167489000	4.067725000	-1.272393000
C	-4.736727000	3.145322000	-0.404755000
N	-2.499997000	4.841226000	-2.595979000
N	-5.690144000	3.517257000	0.398102000
C	-4.233709000	1.722231000	-0.406187000
C	-2.393517000	2.457218000	-1.964061000
H	-2.764903000	1.869107000	-2.819497000
O	-3.129033000	6.037954000	-2.703735000
H	-4.721266000	1.135517000	-1.207574000
C	-2.712901000	1.701760000	-0.659332000
H	-2.336256000	0.669294000	-0.718801000
H	-2.198433000	2.193634000	0.177995000
O	-6.047765000	4.816177000	0.269803000
U	-4.961333000	6.514304000	-1.010702000
O	-6.185805000	6.277176000	-2.320286000
O	-3.679635000	6.615471000	0.262484000
H	-4.490956000	1.243699000	0.545893000
H	-1.308141000	2.570915000	-2.098451000
H	-1.784256000	4.661707000	-3.295389000
C	-5.597340000	9.257079000	-0.767726000
O	-5.886221000	10.465661000	-0.653066000
O	-4.675796000	8.786515000	-1.597624000
O	-6.179018000	8.285818000	-0.069652000

$UO_2(H_2IDO)(CO_3)^-$, E= -1401.5651603 Hartree

C	-3.083590000	3.780568000	-2.008629000
N	-4.216092000	4.040635000	-1.343415000
C	-4.735699000	3.150806000	-0.488380000
N	-2.561517000	4.790726000	-2.679822000
N	-5.743879000	3.577209000	0.249941000
C	-4.197908000	1.747264000	-0.337632000
C	-2.409989000	2.428624000	-1.983117000
H	-2.814109000	1.799738000	-2.791247000
O	-3.117210000	5.993741000	-2.754675000
H	-4.702319000	1.079375000	-1.052774000
C	-2.684197000	1.748827000	-0.627534000
H	-2.298757000	0.722483000	-0.634122000
H	-2.160207000	2.294200000	0.167491000
O	-6.271160000	4.791046000	0.150703000
U	-4.965410000	6.577493000	-1.105049000
O	-6.139746000	6.393691000	-2.452680000
O	-3.730626000	6.507536000	0.206380000
H	-4.402404000	1.356976000	0.667112000
H	-1.331545000	2.526127000	-2.159481000
H	-1.699590000	4.669537000	-3.207651000
H	-6.187987000	2.957346000	0.924326000
C	-5.577379000	9.242284000	-0.656395000
O	-5.845919000	10.426285000	-0.453716000
O	-4.633588000	8.804405000	-1.497991000
O	-6.186062000	8.207115000	-0.066312000

$VO_2(AO)$, E= -562.6397782 Hartree

V	-0.249349000	0.564376000	-0.602389000
O	-1.019130000	0.254534000	-1.978457000
O	-1.917636000	-0.118120000	0.570717000
N	1.767861000	-1.163738000	0.481136000
C	2.429467000	-0.496639000	-0.458587000
N	1.700968000	0.357961000	-1.144606000
H	2.163807000	0.859570000	-1.893911000
O	-0.325792000	2.122419000	-0.261048000
H	2.190278000	-1.744086000	1.193261000
O	0.451158000	-0.850103000	0.663946000
H	-2.597933000	-0.393660000	-0.067008000
H	-1.583942000	-0.922367000	1.012009000
C	3.892172000	-0.768617000	-0.673714000
H	4.266898000	-1.532664000	0.014269000
H	4.064970000	-1.117039000	-1.697819000
H	4.472640000	0.147892000	-0.522189000

$VO_2(AO)_2^-$, E= -562.6397782 Hartree

V	0.508047000	3.097873000	1.024485000
O	0.441335000	4.476623000	1.866214000
N	2.473997000	1.024458000	1.003629000
C	2.079482000	-0.134949000	1.419069000
N	1.183846000	-0.353205000	2.457830000
H	0.643969000	-1.206308000	2.369667000
O	1.869442000	2.065650000	1.718953000
C	2.692720000	-1.347933000	0.773540000
H	3.406664000	-1.029781000	0.009733000
H	3.212917000	-1.968682000	1.516570000
H	1.924952000	-1.974387000	0.295519000
N	-3.467288000	2.454514000	2.099747000
H	-4.416604000	2.106586000	2.153725000
C	-2.535434000	1.823097000	2.913542000
C	-2.976803000	1.382874000	4.279648000
N	-1.298224000	1.660368000	2.576320000

O	-1.062432000	2.071599000	1.258164000
H	-3.360157000	2.234473000	4.857309000
H	-2.127604000	0.946535000	4.811819000
H	-3.779294000	0.631601000	4.222518000
O	0.618273000	3.366659000	-0.563645000
H	-3.112065000	2.570324000	1.153154000
H	0.589887000	0.447665000	2.678951000

$VOOH(AO)_2$, E= -750.7429484 Hartree

V	0.076570000	2.066442000	1.394088000
O	0.882617000	3.190569000	2.138860000
N	1.296081000	0.480468000	1.619829000
C	2.101842000	-0.519391000	1.586145000
N	1.908736000	-1.615036000	2.392816000
H	2.343400000	-2.484579000	2.116955000
O	0.162068000	0.444941000	2.395081000
C	3.311534000	-0.452382000	0.702430000
H	3.300769000	0.482980000	0.139522000
H	4.229327000	-0.505191000	1.300404000
H	3.318604000	-1.288896000	-0.008055000
N	-3.908970000	3.180671000	2.166929000
H	-4.844297000	2.991507000	2.498296000
C	-2.871344000	2.457304000	2.695897000
C	-3.008561000	1.842243000	4.056181000
N	-1.760800000	2.345478000	2.054691000
O	-1.583550000	2.897844000	0.820423000
H	-3.228957000	2.613656000	4.803743000
H	-2.079220000	1.337938000	4.328607000
H	-3.825147000	1.108926000	4.073282000
O	0.518961000	2.025939000	-0.389991000
H	-0.047852000	2.616598000	-0.912720000
H	-3.822960000	3.440506000	1.191161000
H	0.992922000	-1.696282000	2.819167000

$V(AO)(H_{-1}AO)_2$, E= -862.3634972 Hartree

V	5.886342000	6.424321000	6.133566000
N	8.359209000	5.066216000	6.121825000
N	7.671426000	7.017584000	5.361193000
N	5.320547000	5.323131000	4.602545000
N	4.957087000	7.383019000	3.708546000
N	4.530908000	5.410726000	7.173483000
N	4.946012000	6.990979000	8.732410000
C	8.665379000	6.170026000	5.465715000
C	4.313550000	5.888727000	8.407818000
C	5.021160000	6.083784000	3.536082000
O	7.140980000	4.984569000	6.676031000
O	5.132871000	7.627144000	5.036963000
O	5.717300000	7.285085000	7.661214000
H	9.024536000	4.353741000	6.392595000
H	7.826325000	7.843741000	4.795529000
H	4.046586000	4.557507000	6.922979000
H	5.261767000	4.317588000	4.492343000
C	4.753401000	5.519896000	2.185612000
H	5.611578000	4.944561000	1.823838000
H	3.889022000	4.848121000	2.215040000
H	4.544861000	6.327637000	1.482506000
C	3.385561000	5.261955000	9.385343000
H	2.377763000	5.184750000	8.965017000
H	3.721059000	4.252358000	9.643351000
H	3.342941000	5.862431000	10.295128000
C	10.030631000	6.353774000	4.907013000
H	10.500992000	7.233077000	5.355857000
H	10.666611000	5.485614000	5.095060000

H	9.976542000	6.515405000	3.826969000

$V(AO)_3^{2+}$, E= -863.0299318 Hartree

V	0.007131000	-0.046144000	0.137688000
N	2.471933000	-1.273852000	0.170796000
C	2.786795000	-0.040000000	-0.149183000
N	1.733782000	0.727288000	-0.348464000
H	1.907802000	1.694442000	-0.615191000
H	3.099406000	-2.068768000	0.286754000
O	1.173497000	-1.524864000	0.233765000
N	-0.856858000	-1.006417000	-1.403721000
H	-0.802956000	-1.996721000	-1.630563000
C	-1.471538000	-0.231413000	-2.251848000
N	-1.512218000	1.040152000	-1.880705000
H	-1.972308000	1.821687000	-2.343034000
O	-0.978533000	1.276480000	-0.687765000
H	-1.713087000	-1.867240000	1.374343000
N	-1.280178000	-0.948613000	1.421132000
C	-1.632914000	-0.178434000	2.406386000
H	-0.950317000	1.638185000	3.239123000
N	-0.943864000	0.957416000	2.482169000
O	0.068500000	1.035383000	1.623191000
C	-2.113557597	-0.661700441	-3.583862848
H	-1.359364932	-0.781741851	-4.369923875
H	-2.639891396	-1.617652784	-3.482692729
H	-2.840465921	0.079826815	-3.934362902
C	4.262795265	0.373513733	-0.297606753
H	4.749736142	0.472076858	0.679267009
H	4.828370842	-0.366535283	-0.875152651
H	4.357590802	1.336429644	-0.812306107
C	-2.717255450	-0.473846094	3.459256037
H	-3.708019952	-0.559130106	2.998581758
H	-2.516283187	-1.413546441	3.986210446
H	-2.770334631	0.321511975	4.211384228

$VO_2(IDO)^{2-}$, E= -731.0813909 Hartree

C	-2.283421000	1.098859000	-0.182207000
N	-1.626821000	-0.075296000	0.015349000
C	-2.233858000	-1.261424000	0.286273000
N	-1.573831000	2.179085000	-0.251506000
N	-1.480231000	-2.257490000	0.625577000
O	-0.166563000	-1.892910000	0.608760000
C	-3.724306000	-1.363961000	0.173531000
C	-3.775320000	1.090094000	-0.316803000
H	-4.082192000	-2.187729000	0.803157000
H	-4.063354000	0.896036000	-1.367045000
H	-4.171766000	2.077431000	-0.050271000
O	-0.246752000	1.890414000	-0.135189000
H	-4.013025000	-1.601370000	-0.867597000
C	-4.367510000	-0.026343000	0.545975000
H	-5.460993000	-0.073561000	0.425719000
H	-4.162435000	0.189781000	1.604962000
V	0.345616000	0.058673000	0.483552000
O	0.717091000	0.372128000	2.033717000
O	1.670019000	-0.095464000	-0.449850000

$VO_2(HIDO)^{-}$, E= -731.763265 Hartree

C	-1.114957190	1.107573350	-0.511823130
N	-0.453411190	-0.059393650	-0.251884130
C	-1.073796190	-1.256607650	-0.032100130
N	-0.416361190	2.189744350	-0.408770130
N	-0.340429190	-2.189304650	0.479582870
O	0.926225810	-1.689527650	0.672862870

C	-2.526744190	-1.399065650	-0.355046130
C	-2.569527190	1.064965350	-0.855118130
H	-2.950185190	-2.226348650	0.231755870
H	-2.685820190	0.885866350	-1.940142130
H	-3.024167190	2.040963350	-0.634266130
O	0.864320810	1.847753350	-0.043704130
H	-2.641190190	-1.661039650	-1.423242130
C	-3.248180190	-0.075193650	-0.092933130
H	-4.307662190	-0.152809650	-0.384260130
H	-3.222229190	0.144431350	0.987859870
V	1.463733810	0.063371350	0.188796870
O	2.497103810	0.381907350	1.661838870
O	2.386821810	-0.177167650	-1.079735130
H	3.440239810	0.370320350	1.479490870

$VO_2(H_2IDO)$, E= -732.2779095 Hartree

C	-1.142572000	1.072559000	-0.477592000
N	-0.498585000	-0.034087000	-0.176092000
C	-1.103243000	-1.264782000	0.002669000
N	-0.361206000	2.125454000	-0.377511000
N	-0.350180000	-2.157504000	0.528475000
O	0.879718000	-1.639421000	0.784596000
C	-2.533638000	-1.416094000	-0.383636000
C	-2.585697000	1.069723000	-0.846881000
H	-2.980053000	-2.243627000	0.172640000
H	-2.663814000	0.941184000	-1.935202000
H	-3.053048000	2.028005000	-0.599099000
O	0.886108000	1.912700000	0.075813000
H	-2.594611000	-1.671738000	-1.451422000
C	-3.276086000	-0.100145000	-0.136146000
H	-4.310506000	-0.177480000	-0.481399000
H	-3.312467000	0.103443000	0.941261000
V	1.471446000	0.039652000	0.238730000
O	2.621539000	0.408295000	1.537749000
O	2.206928000	-0.222654000	-1.112807000
H	3.568260000	0.469396000	1.384015000
H	-0.615136000	3.086294000	-0.566647000

$V(IDO)_2^-$, E= -1089.478638 Hartree

C	2.474329000	0.174933000	1.228907000
N	1.944390000	-0.346714000	0.090003000
C	2.591159000	-0.421141000	-1.102959000
N	1.646748000	0.316690000	2.210133000
N	1.862559000	-0.782030000	-2.106919000
O	0.591318000	-1.006112000	-1.662052000
C	4.043581000	-0.081189000	-1.171542000
C	3.920994000	0.542902000	1.262114000
H	4.296494000	0.236644000	-2.187338000
H	4.514957000	-0.335086000	1.560491000
H	4.083420000	1.316120000	2.018834000
O	0.419942000	-0.130560000	1.816357000
H	4.640308000	-0.980559000	-0.953284000
C	4.362810000	0.994796000	-0.131372000
H	5.434712000	1.223642000	-0.136122000
H	3.829720000	1.918194000	-0.394902000
V	-0.008224000	-0.447575000	0.017595000
C	-2.209373000	1.311352000	-0.429732000
N	-1.894597000	0.009308000	-0.160344000
C	-2.802981000	-0.962598000	0.121845000
N	-1.207086000	2.104376000	-0.574394000
N	-2.306149000	-2.110954000	0.441968000
O	-0.941242000	-2.005735000	0.388065000
C	-4.262743000	-0.653674000	0.052062000

C	-3.644445000	1.711142000	-0.532386000
H	-4.810261000	-1.318578000	0.726580000
H	-3.981365000	1.581991000	-1.572785000
H	-3.746881000	2.772937000	-0.289697000
O	-0.046735000	1.395384000	-0.427695000
H	-4.624643000	-0.857370000	-0.967427000
C	-4.495588000	0.822758000	0.376222000
H	-5.557089000	1.072614000	0.266232000
H	-4.225684000	1.011082000	1.424000000

V(HIDO)(IDO), E= -1089.9868583 Hartree

C	2.192349000	0.385988000	1.030609000
N	1.867305000	-0.097824000	-0.210137000
C	2.782969000	-0.402181000	-1.175143000
N	1.187741000	0.755175000	1.743335000
N	2.269891000	-0.702221000	-2.322957000
O	0.914275000	-0.636438000	-2.178119000
C	4.238515000	-0.352750000	-0.862630000
C	3.623542000	0.456633000	1.439552000
H	4.801703000	-0.163672000	-1.779937000
H	3.903519000	-0.501228000	1.901715000
H	3.746649000	1.229519000	2.202370000
O	0.043657000	0.522905000	1.027293000
H	4.548880000	-1.340064000	-0.491173000
C	4.503362000	0.701465000	0.212605000
H	5.558919000	0.687831000	0.498772000
H	4.295241000	1.699449000	-0.194404000
V	0.005130000	-0.118554000	-0.708719000
C	-2.460248000	1.335334000	-0.685530000
N	-1.988286000	0.109916000	-0.603540000
C	-2.640896000	-0.932479000	0.014376000
N	-1.549690000	2.170629000	-1.140975000
N	-1.923438000	-1.981577000	0.199417000
O	-0.676446000	-1.794608000	-0.309800000
C	-4.060350000	-0.743397000	0.423713000
C	-3.845741000	1.680710000	-0.262185000
H	-4.305599000	-1.439911000	1.228754000
H	-4.512121000	1.576644000	-1.129809000
H	-3.900594000	2.723750000	0.065447000
O	-0.358378000	1.653132000	-1.471216000
H	-4.718760000	-0.980933000	-0.424616000
C	-4.273498000	0.712598000	0.847010000
H	-5.322262000	0.887127000	1.101547000
H	-3.681897000	0.918112000	1.748010000
H	-1.671241000	3.163708000	-1.294622000

V$(HIDO)_2^+$, E= -1090.3703173 Hartree

C	2.563994000	0.202683000	1.210133000
N	1.966402000	-0.237538000	0.114756000
C	2.588167000	-0.346817000	-1.113039000
N	1.694235000	0.324576000	2.187988000
N	1.792658000	-0.676509000	-2.067058000
O	0.550596000	-0.884088000	-1.555567000
C	4.050725000	-0.095380000	-1.209529000
C	4.017430000	0.509752000	1.248413000
H	4.301257000	0.231473000	-2.221056000
H	4.545504000	-0.401216000	1.563805000
H	4.230729000	1.278568000	1.996877000
O	0.440589000	-0.063763000	1.913376000
H	4.577333000	-1.045734000	-1.042657000
C	4.474533000	0.928533000	-0.154013000
H	5.560057000	1.046611000	-0.160400000
H	4.046129000	1.908370000	-0.396501000

V	-0.012494000	-0.365870000	0.080300000
C	-2.302019000	1.312673000	-0.401465000
N	-1.931706000	0.072925000	-0.102540000
C	-2.825524000	-0.951167000	0.159501000
N	-1.256472000	2.090611000	-0.523961000
N	-2.259451000	-2.053919000	0.496913000
O	-0.911127000	-1.868218000	0.452760000
C	-4.285292000	-0.700487000	0.029505000
C	-3.729752000	1.695449000	-0.554316000
H	-4.833211000	-1.369491000	0.696513000
H	-3.994291000	1.573941000	-1.614495000
H	-3.876784000	2.750419000	-0.305546000
O	-0.053144000	1.514750000	-0.345128000
H	-4.588206000	-0.955703000	-0.995972000
C	-4.592368000	0.771128000	0.312016000
H	-5.647306000	0.977281000	0.120123000
H	-4.413305000	0.992551000	1.370903000
H	-1.251729000	3.077376000	-0.757951000
H	1.877509000	0.614556000	3.142549000