

Electronic Supplementary Information

Assessing Ligand Selectivity for Uranium over Vanadium Ions to Aid in the Discovery of Superior Adsorbents for Extraction of UO_2^{2+} from Seawater

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Supplementary Information

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Sample Gaussian 09 input file

Cartesian coordinates for $[\text{VO}_2(\text{H}_2\text{O})_3]^+$, $E = -451.3142753$ Hartree {B3LYP/SSC/6-31+G(d) level of theory}

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

```
Vanadium(V)_complex
```

```
1 1
```

```
V      0.9076  -0.2464  -2.6297
O      1.1085   1.0827  -1.8001
O      0.4126  -1.4015  -1.6728
O     -0.9757   0.2409  -3.4153
H     -1.6857  -0.3600  -3.1172
H     -1.2651   1.1463  -3.1903
O      2.9272  -0.8134  -2.6694
H      3.1024  -1.6530  -2.2018
H      3.5226  -0.1466  -2.2756
O      1.2527  -0.4491  -4.7199
H      0.5912  -0.2976  -5.4178
H      2.0985  -0.7043  -5.1288
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```
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
```

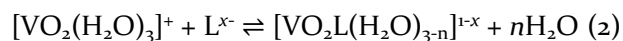
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F    1    1.00
      0.7700000      1.0000000
****

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

```

Table S1. Comparison of binding energies (E^{bind}), Gibbs free energies (ΔG_{aq}), and stability constant ($\log K_t$) values obtained at the CCSD(T)/aug-cc-pvDZ//B3LYP/aug-cc-pvDZ and M06/SSC/6-311++G(d,p)//B3LYP/SSC/6-311++G(d) levels of theory for VO^{2+} and VO_2^+ complexes with acetate and oxalate ligands.



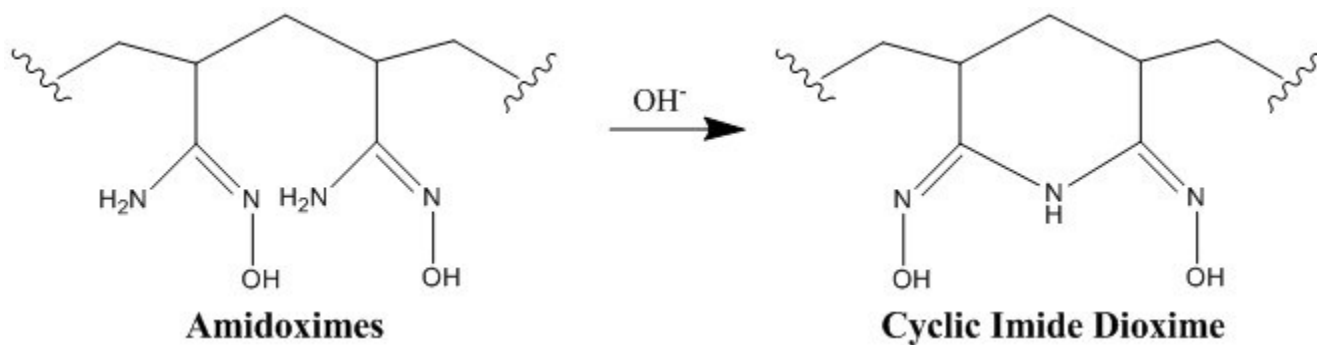
(1) VO^{2+} complexes

Method	L = acetate			L = oxalate		
	E^{bind}	ΔG_{aq}	$\log K_t$	E^{bind}	ΔG_{aq}	$\log K_t$
CCSD(T)/aug-cc-pvDZ	-226.2	-20.5	15.1	-427.9	-30.2	22.2
M06/SSC/6-311++G(d,p)	-222.9	-17.2	12.6	-427.8	-30.2	22.1

(2) VO_2^+ complexes

Method	L = acetate			L = oxalate		
	E^{bind}	ΔG_{aq}	$\log K_t$	E^{bind}	ΔG_{aq}	$\log K_t$
CCSD(T)/aug-cc-pvDZ	-136.1	-22.6	16.6	-258.3	-28.8	21.1
M06/SSC/6-311++G(d,p)	-128.7	-15.3	11.2	-254.5	-25.0	18.3

Scheme S1. Conversion of poly(acrylamidoximes) to poly(acrylimidedioximes) under basic conditions.



Cartesian coordinates (B₃LYP/SSC/6-31+G(d) level of theory) of [VO(H₂O)₄]²⁺ and [VO₂(H₂O)₃]⁺ complexes, as well as the corresponding complexes with different ligands discussed in the main text

[VO(H₂O)₄]²⁺

V	-0.000279000000	-0.000277000000	-0.532934000000
O	-2.051682000000	0.015407000000	-0.194438000000
H	-2.693543000000	0.019749000000	-0.934853000000
H	-2.557955000000	0.019992000000	0.643082000000
O	-0.000923000000	-0.001194000000	-2.066798000000
O	2.051408000000	-0.015538000000	-0.196145000000
H	2.558382000000	-0.019121000000	0.640956000000
H	2.692651000000	-0.020787000000	-0.937091000000
O	-0.014486000000	-1.914808000000	0.147554000000
H	0.769370000000	-2.501860000000	0.134776000000
H	-0.807203000000	-2.489864000000	0.135876000000
O	0.014504000000	1.915074000000	0.145235000000
H	0.807212000000	2.490113000000	0.132181000000
H	-0.769363000000	2.502112000000	0.132414000000

[VO₂(H₂O)₃]⁺

V	0.907617000000	-0.246359000000	-2.629741000000
O	1.108517000000	1.082685000000	-1.800140000000
O	0.412603000000	-1.401460000000	-1.672841000000
O	-0.975652000000	0.240915000000	-3.415301000000
H	-1.685742000000	-0.359998000000	-3.117218000000
H	-1.265146000000	1.146311000000	-3.190298000000
O	2.927188000000	-0.813405000000	-2.669358000000
H	3.102363000000	-1.652973000000	-2.201805000000
H	3.522606000000	-0.146590000000	-2.275640000000
O	1.252730000000	-0.449146000000	-4.719881000000
H	0.591172000000	-0.297637000000	-5.417848000000
H	2.098545000000	-0.704344000000	-5.128829000000

[VO(1a)(H₂O)₂]⁺

23	0.447041000	-0.310324000	-0.304404000
8	0.897924000	-0.587131000	-1.763226000
8	1.561647000	1.197812000	0.553658000
8	1.473315000	-1.739265000	0.827720000
6	-1.858374000	-0.046767000	0.124704000
8	-1.093778000	0.936435000	-0.203439000
8	-1.243795000	-1.180797000	0.225032000
1	0.896681000	-2.405266000	1.250339000
1	2.214035000	-2.225661000	0.419895000
1	2.518673000	1.209136000	0.733762000
1	1.261894000	2.116935000	0.419574000
6	-3.319373000	0.098120000	0.342983000
1	-3.828521000	-0.129855000	-0.603827000
1	-3.565264000	1.123480000	0.626926000
1	-3.666950000	-0.618206000	1.091445000

[VO(2a)(H₂O)₂]⁺

23	0.424285000	-0.319251000	-0.344719000
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8	0.964318000	-0.618611000	-1.766557000
8	1.460480000	1.203247000	0.568400000
8	1.422027000	-1.702382000	0.864942000
6	-1.893040000	-0.066879000	-0.013465000
8	-1.142782000	0.913063000	-0.362751000
8	-1.291651000	-1.199633000	0.108257000
1	0.846852000	-2.334176000	1.339347000
1	2.150590000	-2.221783000	0.475439000
1	2.384319000	1.203904000	0.877112000
1	1.179051000	2.126229000	0.421598000
6	-3.354022000	0.101114000	0.282170000
17	-3.505714000	0.445611000	2.046907000
1	-3.759015000	0.947953000	-0.272464000
1	-3.895836000	-0.819291000	0.061840000

[VO(3a)(H₂O)₂]⁺

23	0.368740000	-0.392897000	-0.269193000
8	0.780762000	-1.043481000	-1.615794000
8	1.555409000	1.234699000	0.167712000
8	1.349009000	-1.529160000	1.184093000
6	-1.905455000	0.044409000	0.133032000
8	-1.138329000	0.893232000	-0.459209000
8	-1.332532000	-1.046441000	0.493898000
1	0.740196000	-2.036587000	1.756666000
1	2.062050000	-2.139506000	0.918436000
1	2.513754000	1.248560000	0.340744000
1	1.293522000	2.103954000	-0.190370000
6	-3.360458000	0.334386000	0.362170000
1	-3.428267000	1.345743000	0.793223000
1	-3.826591000	0.375492000	-0.636991000
8	-3.893643000	-0.665594000	1.187338000
1	-4.853237000	-0.547799000	1.268502000

[VO(4a)(H₂O)₂]⁺

23	0.465343000	-0.289988000	-0.293360000
8	0.948187000	-0.921794000	-1.659716000
8	1.679388000	1.406640000	0.160440000
8	1.746797000	-1.407909000	1.029494000
6	-2.042356000	1.169979000	-0.202242000
8	-2.742737000	2.158051000	-0.296101000
8	-0.739347000	1.170324000	-0.498745000
1	1.217619000	-1.735607000	1.781138000
1	2.068714000	-2.193405000	0.552624000
1	2.535035000	1.517043000	-0.285278000
1	1.078897000	2.122718000	-0.136037000
6	-2.606693000	-0.174030000	0.263691000
1	-3.255432000	-0.003041000	1.126398000
1	-3.229529000	-0.579567000	-0.541026000
16	-1.302384000	-1.406054000	0.695832000

[VO(5a)(H₂O)₂]

23	-0.220326000	-0.455567000	-0.529334000
8	-1.025265000	-0.688435000	-1.859614000
8	-1.414533000	0.956633000	0.534284000
1	-2.217836000	1.236687000	0.061415000
1	-0.818407000	1.732320000	0.574298000

8	1.032627000	0.980142000	-0.467070000
8	1.501527000	-1.307485000	-0.410800000
16	2.361457000	0.054131000	-0.331194000
8	3.226891000	0.210894000	-1.488015000
8	2.917196000	0.204938000	1.012522000
8	-0.663678000	-1.843310000	0.979987000
1	-1.091448000	-1.591299000	1.815291000
1	0.194900000	-2.264870000	1.185232000

[VO(6a)(H₂O)₂]

6	-3.377556000	-4.865456000	-2.021235000
6	-3.275054000	-5.641090000	-0.664763000
8	-0.106666000	-6.763167000	-2.425582000
8	-2.160623000	-4.682341000	-2.563394000
8	0.408886000	-5.095929000	0.060561000
8	-2.000542000	-5.928778000	-0.369589000
8	-4.410626000	-4.461602000	-2.489992000
8	-4.228078000	-5.900965000	0.026077000
23	-0.694913000	-5.503813000	-1.687376000
1	-0.206744000	-5.277141000	0.798596000
1	0.882718000	-4.268021000	0.242043000
8	0.295033000	-3.869781000	-2.649022000
1	-0.443653000	-3.509218000	-3.183242000
1	0.991739000	-4.140460000	-3.272180000

[VO(7a)(H₂O)₂]

8	4.197717000	2.164538000	23.689363000
6	4.918377000	2.953366000	23.115427000
8	5.892823000	4.927608000	19.975702000
23	5.293892000	5.291754000	21.384755000
8	6.620036000	5.349242000	22.735486000
8	4.435361000	3.837394000	22.226627000
6	7.002141000	4.396511000	23.595381000
8	3.220429000	5.673934000	20.964711000
8	7.759194000	4.624324000	24.516364000
6	6.431611000	3.000734000	23.329382000
1	6.906352000	2.619642000	22.413091000
1	6.696323000	2.341968000	24.156125000
1	2.850715000	4.845853000	21.341991000
1	2.995121000	5.686328000	20.018567000
8	5.464777000	7.369813000	21.745017000
1	6.123340000	7.403305000	22.470020000
1	4.710516000	7.935541000	21.977418000

[VO(8a)(H₂O)₂]

6	-3.529305000	-3.585761000	-2.159010000
6	-3.493177000	-5.119228000	0.663681000
8	-1.553900000	-6.886000000	-2.074874000
8	-2.287301000	-4.078128000	-2.189420000
8	0.244167000	-5.579184000	0.021310000
8	-2.243037000	-5.310878000	0.244715000
8	-3.780150000	-2.498506000	-2.647121000
8	-3.741510000	-4.983205000	1.849375000
23	-1.330404000	-5.485146000	-1.396045000
1	-0.240339000	-5.434310000	0.861409000
1	1.006928000	-4.978952000	-0.012239000
8	0.154359000	-4.567482000	-2.673335000
1	-0.433626000	-3.909078000	-3.103476000

1	0.492948000	-5.153069000	-3.372190000
6	-4.606975000	-5.143589000	-0.358384000
6	-4.625602000	-4.459591000	-1.595841000
6	-5.753326000	-5.850646000	0.043410000
6	-5.790561000	-4.505446000	-2.381403000
6	-6.879211000	-5.933291000	-0.771985000
6	-6.898664000	-5.254184000	-1.993048000
1	-5.744184000	-6.330365000	1.016786000
1	-5.810810000	-3.935338000	-3.304741000
1	-7.742110000	-6.508447000	-0.447047000
1	-7.777022000	-5.292626000	-2.631818000

[VO(9a)(H₂O)]

6	1.034003000	2.070596000	1.152384000
7	-0.210410000	1.644470000	0.921231000
6	-1.303065000	2.403006000	1.040730000
6	0.099467000	4.147865000	1.888601000
6	1.232381000	3.349322000	1.667538000
6	-1.185055000	3.693028000	1.552166000
1	-2.065292000	4.318733000	1.654546000
1	2.238417000	3.706756000	1.859679000
23	-0.448891000	-0.250076000	0.276500000
6	-2.520500000	1.709864000	0.432024000
8	-2.189259000	0.560042000	-0.130990000
6	2.061991000	1.058381000	0.650613000
8	1.478230000	0.038856000	0.043338000
8	-3.620835000	2.228434000	0.443104000
8	3.257081000	1.250481000	0.771376000
1	0.222881000	5.150412000	2.289176000
8	-0.650187000	-1.270566000	1.454650000
8	-0.501257000	-1.265875000	-1.537362000
1	-1.342212000	-1.674646000	-1.805084000
1	0.226485000	-1.881989000	-1.729496000

[VO(10a)(H₂O)₂]⁺

23	0.198699000	-0.506762000	0.024401000
8	0.461416000	-1.716692000	-0.926106000
8	1.502548000	0.944732000	-0.797734000
8	1.478444000	-0.348324000	1.648738000
6	-2.350485000	0.703478000	0.046578000
8	-1.098853000	0.757375000	-0.442593000
8	-3.227875000	1.491835000	-0.196068000
1	2.297887000	0.176121000	1.585366000
1	1.468837000	-0.803910000	2.508357000
1	2.065116000	0.659522000	-1.542041000
1	0.956485000	1.688665000	-1.124970000
6	-2.530574000	-0.478208000	0.965476000
7	-1.422415000	-1.223722000	1.169963000
6	-3.741996000	-0.827984000	1.566806000
6	-1.523739000	-2.320597000	1.938541000
7	-3.848228000	-1.907392000	2.348690000
6	-2.750514000	-2.649204000	2.525657000
1	-4.628332000	-0.221834000	1.401905000
1	-0.641287000	-2.940122000	2.066652000
1	-2.842708000	-3.534870000	3.148467000

[VO(11)(H₂O)₂]⁺

23	0.016179000	0.038182000	-0.950518000
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8	-1.601777000	0.773977000	-0.381029000
7	-0.807979000	-1.778103000	-0.571369000
8	0.085768000	-2.889899000	-0.552316000
6	-2.023999000	-2.077949000	-0.204598000
6	-3.068267000	-1.117810000	-0.051111000
6	-2.827518000	0.286013000	-0.161142000
6	-3.899733000	1.174721000	0.005501000
6	-5.176042000	0.689408000	0.273884000
6	-5.424703000	-0.691373000	0.392007000
6	-4.378885000	-1.581882000	0.235621000
1	-2.235000000	-3.130208000	-0.013069000
1	-4.550963000	-2.651699000	0.323281000
1	-6.425946000	-1.051039000	0.604681000
1	-5.994404000	1.393516000	0.396428000
1	-3.711415000	2.240160000	-0.079425000
1	0.239837000	-3.112051000	-1.492789000
8	0.273450000	-0.021221000	-2.496482000
8	0.772580000	1.966563000	-0.462733000
1	0.024586000	2.523207000	-0.171359000
1	1.227845000	2.453704000	-1.173170000
8	1.575425000	-0.728702000	0.160701000
1	1.601334000	-1.709676000	0.178787000
1	2.458350000	-0.358987000	0.329558000

[VO(12)(H₂O)₂]⁺

23	-0.280817000	0.276150000	-0.643607000
8	-0.690385000	0.404405000	-2.151263000
8	-1.725005000	-1.165301000	-0.024123000
1	-1.663101000	-1.728670000	0.766506000
1	-2.153367000	-1.683797000	-0.728458000
8	-1.405029000	1.603923000	0.523035000
1	-0.938473000	2.442249000	0.700938000
1	-2.336251000	1.808277000	0.326849000
8	1.098626000	1.494042000	-0.136936000
7	2.352983000	0.949652000	-0.160458000
6	2.448089000	-0.356576000	-0.331877000
7	1.272596000	-0.974921000	-0.463070000
1	3.118388000	1.603379000	-0.046303000
1	1.330795000	-1.973803000	-0.637668000
6	3.790210000	-1.022722000	-0.369620000
1	3.953469000	-1.478957000	-1.352310000
1	3.838709000	-1.812948000	0.387199000
1	4.600725000	-0.313955000	-0.180048000

[VO(13)(H₂O)₂]⁺

8	2.035017000	-1.825014000	0.700433000
8	0.572029000	0.117017000	2.181825000
1	2.159756000	-2.510974000	0.022239000
1	2.227140000	-2.223246000	1.567934000
8	2.006585000	0.808198000	-0.377208000
1	1.627818000	1.589564000	-0.822405000
1	2.849876000	1.069319000	0.032655000
23	0.552960000	-0.288581000	0.666293000
7	-1.821345000	0.275465000	-0.634133000
6	-2.025693000	-0.978394000	-0.244823000
8	-0.578662000	0.806320000	-0.403932000
7	-0.957685000	-1.550704000	0.317953000
1	-1.077431000	-2.530403000	0.556447000
1	-2.544797000	0.944346000	-0.869732000

6	-3.335595000	-1.618389000	-0.460358000
6	-4.060586000	-1.381631000	-1.642232000
6	-3.864693000	-2.467933000	0.527455000
6	-5.302196000	-1.989310000	-1.828713000
6	-5.107794000	-3.069408000	0.333631000
6	-5.826591000	-2.831283000	-0.842641000
1	-3.641280000	-0.757209000	-2.426766000
1	-3.325641000	-2.627906000	1.457613000
1	-5.854922000	-1.813969000	-2.746869000
1	-5.519598000	-3.715126000	1.103491000
1	-6.793943000	-3.302348000	-0.991074000

[VO₂(1b)(H₂O)]

23	0.188762000	-0.337803000	0.299484000
8	0.423531000	0.674590000	1.495294000
8	0.947481000	0.170042000	-1.004826000
8	-1.716357000	0.296794000	-0.336831000
6	0.056061000	-2.721358000	0.763913000
8	1.128315000	-2.046651000	0.853459000
8	-1.008276000	-2.124569000	0.409986000
1	-2.261584000	-0.489245000	-0.523531000
1	-1.662102000	0.828144000	-1.149796000
1	0.057469000	-3.794643000	0.989549000

[VO₂(2b)(H₂O)]

23	0.112242000	-0.358834000	0.186277000
8	0.233259000	0.499623000	1.515107000
8	0.889249000	0.352709000	-1.011075000
8	-1.795833000	0.279578000	-0.461527000
6	0.084300000	-2.786988000	0.339503000
8	1.114718000	-2.064409000	0.559703000
8	-0.985263000	-2.164540000	0.009838000
1	-2.281298000	-0.502944000	-0.780437000
1	-1.711579000	0.904348000	-1.202271000
6	0.123236000	-4.276410000	0.485592000
1	-0.337897000	-4.546546000	1.443619000
1	1.154162000	-4.635278000	0.475512000
1	-0.460193000	-4.747009000	-0.310643000

[VO₂(3b)]⁻

6	-0.228264000	5.446531000	7.009074000
1	-0.646247000	4.522022000	6.593254000
1	-1.064401000	6.149866000	7.146919000
6	0.354187000	5.078281000	8.385937000
6	1.153620000	7.344658000	6.269668000
1	1.036114000	7.618991000	7.325578000
1	0.520224000	8.021061000	5.674749000
6	2.634448000	7.561452000	5.900083000
8	-0.391338000	4.971928000	9.353218000
8	3.010776000	8.627088000	5.423810000
7	0.800510000	5.936739000	6.098292000
8	4.265980000	4.482729000	7.755022000
8	2.631490000	3.680719000	5.894551000
8	1.648378000	4.877515000	8.416179000
8	3.411433000	6.545316000	6.176889000
23	2.919828000	4.845320000	6.967598000
6	0.551161000	5.606482000	4.693810000
1	1.398539000	5.937896000	4.086279000

1	0.471511000	4.522523000	4.587279000
1	-0.366250000	6.093083000	4.313709000

[VO₂(4b)(H₂O)]

23	0.117943000	-0.496021000	0.092049000
8	0.284023000	0.762652000	1.050590000
8	0.811246000	-0.231998000	-1.314067000
8	-1.821788000	0.040545000	-0.526154000
7	0.210785000	-2.803602000	1.038866000
8	1.209381000	-1.974664000	0.955472000
8	-0.879226000	-2.282579000	0.568672000
1	-1.866863000	0.122373000	-1.495305000
1	-2.035668000	0.916158000	-0.157334000
8	0.295268000	-3.907765000	1.495311000

[VO₂(5b)(H₂O)]⁻

23	-0.418700000	-0.271709000	0.418030000
8	-0.903399000	-0.579022000	1.910907000
8	-1.463489000	-0.872020000	-0.656634000
8	-1.452559000	1.655134000	0.181811000
1	-2.005765000	1.417134000	-0.582414000
1	-0.684737000	2.152605000	-0.164611000
8	0.987018000	1.121840000	-0.028757000
8	1.278025000	-1.185399000	0.148235000
16	2.173935000	0.078381000	-0.203684000
8	2.624587000	0.035352000	-1.601912000
8	3.213583000	0.289505000	0.811230000

[VO₂(6b)(H₂O)]⁻

6	-3.354110000	-4.954506000	-1.762923000
6	-3.166722000	-5.714163000	-0.405365000
8	0.342969000	-5.697888000	-2.293536000
8	0.040710000	-3.421307000	-0.935192000
8	-2.202535000	-4.532767000	-2.239938000
8	0.524043000	-5.582393000	0.548556000
8	-1.891664000	-5.756090000	-0.063942000
8	-4.444384000	-4.791549000	-2.279734000
8	-4.088119000	-6.186243000	0.233636000
23	-0.581679000	-4.875139000	-1.276028000
1	-0.277742000	-5.839571000	1.047357000
1	0.790933000	-4.702784000	0.866910000

[VO₂(7b)(H₂O)]⁻

8	4.262276000	1.980978000	23.579866000
6	4.804849000	2.995230000	23.154262000
8	5.546338000	5.543584000	20.366282000
23	4.847274000	5.662386000	21.819889000
8	6.260530000	5.564120000	23.084365000
8	4.139081000	3.993503000	22.609234000
8	4.228494000	7.116602000	22.073250000
6	6.870914000	4.517088000	23.594298000
8	2.906155000	5.060701000	20.681160000
8	7.833560000	4.601564000	24.348275000
6	6.328821000	3.143380000	23.178756000
1	6.679097000	2.966773000	22.149791000

1	6.758985000	2.374483000	23.821253000
1	2.839345000	4.208555000	21.157042000
1	3.367082000	4.879153000	19.844378000

[VO₂(8b)(H₂O)]

23	-1.056933000	0.592013000	0.553927000
8	-1.702617000	1.068151000	1.923684000
8	-1.282905000	-1.392865000	0.358721000
8	-1.738036000	1.340912000	-0.666571000
8	0.834740000	0.624516000	0.505275000
8	1.127269000	-1.801696000	-0.377119000
15	1.782737000	-0.445898000	-0.158898000
1	2.258437000	0.114834000	-1.359900000
1	2.910397000	-0.519521000	0.679926000
1	-0.370153000	-1.763383000	0.029532000
1	-1.565237000	-1.890063000	1.144922000

[VO₂(9b)(H₂O)]⁻

23	-0.668856000	0.237574000	0.412029000
8	-1.253524000	0.588510000	1.878329000
8	-1.731815000	-1.708726000	0.600934000
8	-1.604136000	0.841088000	-0.739952000
8	1.064563000	1.077747000	0.261656000
8	0.677112000	-1.253338000	0.084325000
15	1.905481000	-0.248991000	0.028744000
8	2.383393000	-0.217986000	-1.553712000
8	3.111663000	-0.514931000	0.875362000
1	3.345962000	-0.338255000	-1.555513000
1	-0.895174000	-2.216182000	0.536608000
1	-1.944370000	-1.628811000	1.546788000

[VO₂(10b)]⁻

6	1.021843000	2.002518000	0.893160000
7	-0.209125000	1.551981000	0.648160000
6	-1.298836000	2.300854000	0.821475000
6	0.092574000	4.113076000	1.541350000
6	1.220341000	3.304661000	1.350856000
6	-1.189125000	3.614447000	1.276044000
1	-2.086761000	4.208737000	1.411073000
1	2.229122000	3.653619000	1.545097000
23	-0.447624000	-0.473678000	-0.057713000
8	-0.455372000	-0.894299000	-1.603879000
6	-2.565201000	1.534549000	0.467151000
8	-2.303997000	0.328540000	0.078579000
6	2.072665000	0.938600000	0.609768000
8	1.539719000	-0.164237000	0.193610000
8	-3.666231000	2.076668000	0.568347000
8	3.266557000	1.185245000	0.783861000
1	0.212717000	5.133898000	1.897569000
8	-0.639168000	-1.744579000	0.899192000

[VO₂(11)(H₂O)]

23	0.117536000	0.028898000	-0.948240000
8	-1.604770000	0.626198000	-0.509737000
7	-0.882408000	-1.936404000	-0.503204000
8	-0.086761000	-3.114284000	-0.701526000

6	-2.101744000	-2.210284000	-0.179224000
6	-3.103494000	-1.193812000	0.005218000
6	-2.813921000	0.186602000	-0.220942000
6	-3.867164000	1.119789000	-0.097277000
6	-5.145515000	0.704329000	0.248767000
6	-5.432121000	-0.654607000	0.482903000
6	-4.416119000	-1.587088000	0.356665000
1	-2.386397000	-3.259705000	-0.082953000
1	-4.618614000	-2.643172000	0.523142000
1	-6.436178000	-0.966877000	0.753126000
1	-5.937218000	1.443837000	0.340947000
1	-3.639079000	2.166181000	-0.274157000
1	0.161367000	-3.041483000	-1.645447000
8	0.338706000	-0.403057000	-2.475624000
8	1.041306000	1.298070000	-0.630043000
8	1.496166000	-1.104024000	0.174876000
1	1.441437000	-2.068895000	0.013831000
1	2.405915000	-0.784425000	0.059415000

[VO₂(₁₂)(H₂O)]

23	-0.249349000	0.564376000	-0.602389000
8	-1.019130000	0.254534000	-1.978457000
8	-1.917636000	-0.118120000	0.570717000
7	1.767861000	-1.163738000	0.481136000
6	2.429467000	-0.496639000	-0.458587000
7	1.700968000	0.357961000	-1.144606000
1	2.163807000	0.859570000	-1.893911000
8	-0.325792000	2.122419000	-0.261048000
1	2.190278000	-1.744086000	1.193261000
8	0.451158000	-0.850103000	0.663946000
1	-2.597933000	-0.393660000	-0.067008000
1	-1.583942000	-0.922367000	1.012009000
6	3.892172000	-0.768617000	-0.673714000
1	4.266898000	-1.532664000	0.014269000
1	4.064970000	-1.117039000	-1.697819000
1	4.472640000	0.147892000	-0.522189000

[VO₂(₁₃)(H₂O)]

8	1.528039000	-0.790401000	1.082051000
8	1.911064000	-1.830620000	-1.308122000
8	2.110588000	1.009693000	-0.883524000
1	1.418168000	1.642579000	-1.153215000
1	2.483829000	1.319516000	-0.040919000
23	1.041347000	-0.801911000	-0.449399000
7	-1.552340000	-0.018772000	-1.411446000
6	-1.783755000	-1.220832000	-0.865104000
8	-0.287255000	0.484089000	-1.247082000
7	-0.729879000	-1.802580000	-0.336730000
1	-0.838608000	-2.770072000	-0.053592000
1	-2.277949000	0.683348000	-1.495875000
6	-3.151084000	-1.786605000	-0.920617000
6	-3.949230000	-1.621873000	-2.065000000
6	-3.658480000	-2.493818000	0.181946000
6	-5.239533000	-2.154102000	-2.100902000
6	-4.948121000	-3.024976000	0.139393000
6	-5.741091000	-2.855549000	-1.000365000
1	-3.546905000	-1.107511000	-2.933350000
1	-3.051925000	-2.605647000	1.076670000
1	-5.847366000	-2.031841000	-2.993219000

1	-5.335981000	-3.565383000	0.998500000
1	-6.744305000	-3.271957000	-1.031665000