SUPPORTING INFORMATION

A Study of Hg_2^{2+} and Complexes of NpO_2^+ and UO_2^{2+} in Solution. Examples
of Cation-Cation Interactions

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Table S1. Cartesian Coordinates of Species Optimized at the BPW91/TZ2P Level in the Gas-Phase and in Solution using COSMO and at the B3LYP/LANL2DZ Level

Geometries Optimized at BPW91/TZ2P Level:

	X	Y	Z
Hg ₂ (2+)			
Hg	0.000000	0.000000	-0.019935
Hg	0.000000	0.000000	-2.721065
Hg ₂ (2+) COSMO			
Hg	0.000000	0.000000	-0.081113
Hg	0.000000	0.000000	-2.659887
NpO ₂ (+)			
Np	0.000000	0.000000	0.000000
O	1.754804	0.000000	0.000000
O	-1.754804	0.000000	0.000000
NpO ₂ (+) COSMO			
Np	0.000000	0.000000	0.000000
O	1.789856	0.000000	0.000000
O	-1.789856	0.000000	0.000000
UO ₂ (2+)			
U	0.000000	0.000000	0.000000
O	1.719126	0.000000	0.000000
O	-1.719126	0.000000	0.000000
UO ₂ (2+) COSMO			
U	0.000000	0.000000	0.000000
O	1.735553	0.000000	0.000000
O	-1.735553	0.000000	0.000000
(ONpO-ONpO)(2+)			
Np	0.000000	0.000000	-0.121491
O	0.000000	0.000000	-1.865281
O	0.000000	0.000000	1.706022
Np	0.000000	0.000000	4.326812
O	-1.754634	0.000000	4.326812
O	1.754634	0.000000	4.326812
(ONpO-ONpO)(2+) COSMO			
Np	0.000000	0.000000	-0.007546
O	0.000000	0.000000	-1.789560
O	0.000000	0.000000	1.830189
Np	0.000000	0.000000	4.214533
O	-1.795205	0.000000	4.214533
O	1.795205	0.000000	4.214533
(ONpO-OUO)(3+)			
Np	0.000000	0.000000	-0.078999
O	0.000000	0.000000	-1.806442
O	0.000000	0.000000	1.813884
U	0.000000	0.000000	4.279192
O	-1.729763	0.000000	4.279192
O	1.729763	0.000000	4.279192
(ONpO-OUO)(3+) COSMO			
Np	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.773400

O	0.000000	0.000000	1.885100
U	0.000000	0.000000	4.118300
O	-1.748100	0.000000	4.118300
O	1.748100	0.000000	4.118300

(OUO-ONpO) (3+)

U	0.000000	0.000000	-0.076347
O	0.000000	0.000000	-1.805334
O	0.000000	0.000000	1.821912
Np	0.000000	0.000000	4.276880
O	-1.727595	0.000000	4.276880
O	1.727595	0.000000	4.276880

(OUO-ONpO) (3+) COSMO

U	0.000000	0.000000	0.042430
O	0.000000	0.000000	-1.730904
O	0.000000	0.000000	1.927932
Np	0.000000	0.000000	4.161035
O	-1.748487	0.000000	4.161035
O	1.748487	0.000000	4.161035

(OUO-OUO) (4+) COSMO

U	0.000000	0.000000	-0.027604
O	0.000000	0.000000	-1.749866
O	0.000000	0.000000	1.743566
U	0.000000	0.000000	4.235007
O	-1.739962	0.000000	4.235007
O	1.739962	0.000000	4.235007

Geometries Optimized at B3LYP/LANL2DZ Level unless otherwise noted:

Hg2(2+) (Optimized at B3LYP/SDD level)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	80	0	0.000000	0.000000	1.369167
2	80	0	0.000000	0.000000	-1.369167

ONpO(+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	1.788962
2	93	0	0.000000	0.000000	0.000000
3	8	0	0.000000	0.000000	-1.788962

OUO(2+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	1.731935

2	92	0	0.000000	0.000000	0.000000
3	8	0	0.000000	0.000000	-1.731935

(ONpO(H₂O)₅)(+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	93	0	0.000000	0.000000	0.000000
2	8	0	0.000000	2.582331	0.000000
3	8	0	-1.517856	-2.089150	0.000000
4	8	0	-2.455943	0.797984	0.000000
5	8	0	2.455943	0.797984	0.000000
6	8	0	1.517856	-2.089150	0.000000
7	8	0	0.000000	0.000000	1.849200
8	8	0	0.000000	0.000000	-1.849200
9	1	0	-1.617384	-2.690365	0.760688
10	1	0	-2.058890	-2.369592	-0.760688
11	1	0	2.058890	-2.369592	0.760688
12	1	0	1.617384	-2.690365	-0.760688
13	1	0	2.889848	1.225876	0.760688
14	1	0	3.058488	0.706855	-0.760688
15	1	0	-0.272865	3.127225	0.760688
16	1	0	0.272865	3.127225	-0.760688
17	1	0	-3.058488	0.706855	0.760688
18	1	0	-2.889848	1.225876	-0.760688

(OUO(H₂O)₅)(2+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	92	0	0.000000	0.000000	0.000000
2	8	0	0.000000	2.488935	-0.000000
3	8	0	-1.462959	-2.013590	-0.000000
4	8	0	-2.367118	0.769123	-0.000000
5	8	0	2.367118	0.769123	-0.000000
6	8	0	1.462959	-2.013590	-0.000000
7	8	0	0.000000	0.000000	1.779633
8	8	0	0.000000	0.000000	-1.779633
9	1	0	-1.503808	-2.674650	0.722313
10	1	0	-2.079042	-2.256719	-0.722313
11	1	0	2.079042	-2.256719	0.722313
12	1	0	1.503808	-2.674650	-0.722313
13	1	0	2.788726	1.279922	0.722313
14	1	0	3.008446	0.603694	-0.722313
15	1	0	-0.355514	3.047754	0.722313
16	1	0	0.355514	3.047754	-0.722313
17	1	0	-3.008446	0.603694	0.722313
18	1	0	-2.788726	1.279922	-0.722313

(ONpO-ONpO)(2+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	8	0	-0.000000	1.793577	2.234847
2	93	0	0.000000	-0.000000	2.275797
3	8	0	-0.000000	0.000000	-0.425003
4	8	0	-0.000000	-1.793577	2.234847
5	93	0	-0.000000	0.000000	-2.275438
6	8	0	-0.000000	0.000000	-4.048867

(ONpO-OUO) (3+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.000000	1.741065	-2.209074
2	92	0	0.000000	-0.000000	-2.189669
3	8	0	0.000000	0.000000	0.240664
4	8	0	-0.000000	-1.741065	-2.209074
5	93	0	0.000000	0.000000	2.185051
6	8	0	0.000000	0.000000	3.957464

(OUO-ONpO) (3+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.000000	1.757408	2.165359
2	93	0	0.000000	0.000000	2.166026
3	8	0	0.000000	-0.000000	-0.258786
4	8	0	-0.000000	-1.757408	2.165359
5	92	0	0.000000	-0.000000	-2.199644
6	8	0	0.000000	-0.000000	-3.956078

(ONpO(H2O)5-ONpO(H2O)4) (2+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	93	0	2.100891	-0.221800	-0.000000
2	8	0	1.689497	0.293462	2.484093
3	8	0	1.689497	0.293462	-2.484093
4	8	0	3.882344	-1.282500	1.562482
5	8	0	3.882344	-1.282500	-1.562482
6	8	0	1.284738	-1.929529	-0.000000
7	8	0	2.985486	1.395902	-0.000000
8	1	0	2.189523	-0.229202	-3.140444
9	1	0	1.584478	1.220315	-2.773411
10	1	0	3.932713	-2.248509	-1.700514
11	1	0	4.724065	-0.847612	-1.802803
12	1	0	3.932713	-2.248509	1.700514
13	1	0	4.724065	-0.847612	1.802803
14	1	0	2.189523	-0.229202	3.140444
15	1	0	1.584478	1.220315	2.773411
16	93	0	-2.114558	0.274817	0.000000
17	8	0	-2.501776	-0.491234	2.410305
18	8	0	-2.501776	-0.491234	-2.410305

19	8	0	-1.300651	-2.076894	0.000000
20	8	0	-2.501776	2.287194	1.520579
21	8	0	-2.501776	2.287194	-1.520579
22	8	0	-0.232273	0.664140	-0.000000
23	8	0	-3.924375	-0.084912	0.000000
24	1	0	-1.859532	-0.650192	-3.127082
25	1	0	-3.365050	-0.905833	-2.604987
26	1	0	-2.051064	3.151376	-1.553165
27	1	0	-3.276107	2.273125	-2.115689
28	1	0	-2.051064	3.151376	1.553165
29	1	0	-3.276107	2.273125	2.115689
30	1	0	-1.859532	-0.650192	3.127082
31	1	0	-3.365050	-0.905833	2.604987
32	1	0	-0.293318	-2.199047	0.000000
33	1	0	-1.789790	-2.918943	0.000000

(ONpO(H₂O)₅-OUO(H₂O)₄)(3+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	92	0	-0.029099	-2.118341	-0.000000
2	8	0	0.433800	-1.614810	2.421382
3	8	0	0.433800	-1.614810	-2.421382
4	8	0	-0.736878	-4.019644	1.508274
5	8	0	-0.736878	-4.019644	-1.508274
6	8	0	-1.768773	-1.631032	-0.000000
7	8	0	1.646649	-2.724331	-0.000000
8	1	0	-0.034475	-2.070950	-3.150133
9	1	0	1.277709	-1.232716	-2.735807
10	1	0	-1.663978	-4.286816	-1.681833
11	1	0	-0.121305	-4.713545	-1.826977
12	1	0	-1.663978	-4.286816	1.681833
13	1	0	-0.121305	-4.713545	1.826977
14	1	0	-0.034475	-2.070950	3.150133
15	1	0	1.277709	-1.232716	2.735807
16	93	0	0.072207	2.100409	0.000000
17	8	0	-0.736878	2.605460	2.361541
18	8	0	-0.736878	2.605460	-2.361541
19	8	0	-2.292918	1.279009	0.000000
20	8	0	2.010463	2.542501	1.558812
21	8	0	2.010463	2.542501	-1.558812
22	8	0	0.432957	0.138166	0.000000
23	8	0	-0.315702	3.890934	0.000000
24	1	0	-0.959351	2.039103	-3.126157
25	1	0	-1.092567	3.509277	-2.496492
26	1	0	2.972391	2.385804	-1.476334
27	1	0	1.836003	3.155539	-2.303288
28	1	0	2.972391	2.385804	1.476334
29	1	0	1.836003	3.155539	2.303288
30	1	0	-0.959351	2.039103	3.126157
31	1	0	-1.092567	3.509277	2.496492
32	1	0	-2.504396	0.319585	-0.000000
33	1	0	-3.108448	1.820310	0.000000

(OUO(H₂O)₅-ONpO(H₂O)₄)(3+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	93	0	-0.078022	-2.082431	0.000000
2	8	0	0.352446	-1.622658	2.418943
3	8	0	0.352446	-1.622658	-2.418943
4	8	0	-0.791125	-3.993675	1.482219
5	8	0	-0.791125	-3.993675	-1.482219
6	8	0	-1.805791	-1.556046	0.000000
7	8	0	1.608219	-2.666037	0.000000
8	1	0	-0.166655	-2.050225	-3.130202
9	1	0	1.210320	-1.299358	-2.759730
10	1	0	-1.719197	-4.268688	-1.636952
11	1	0	-0.176766	-4.685027	-1.809022
12	1	0	-1.719197	-4.268688	1.636952
13	1	0	-0.176766	-4.685027	1.809022
14	1	0	-0.166655	-2.050225	3.130202
15	1	0	1.210320	-1.299358	2.759730
16	92	0	0.128906	2.104854	0.000000
17	8	0	-0.791125	2.562075	2.315006
18	8	0	-0.791125	2.562075	-2.315006
19	8	0	-2.264396	1.319405	0.000000
20	8	0	2.099230	2.521984	1.520744
21	8	0	2.099230	2.521984	-1.520744
22	8	0	0.459529	0.143244	0.000000
23	8	0	-0.152988	3.888910	0.000000
24	1	0	-1.024993	2.003049	-3.081113
25	1	0	-1.051418	3.492582	-2.480849
26	1	0	2.947757	2.049301	-1.631301
27	1	0	2.129939	3.375944	-2.000804
28	1	0	2.947757	2.049301	1.631301
29	1	0	2.129939	3.375944	2.000804
30	1	0	-1.024993	2.003049	3.081113
31	1	0	-1.051418	3.492582	2.480849
32	1	0	-2.513987	0.369074	0.000000
33	1	0	-3.054667	1.895880	0.000000