

Supplemental Information

Quantifying the binding strength of U(VI) with phthalimidedioxime in comparison with glutarimidedioxime: Implications in the extraction of U(VI) from seawater with amidoxime-based sorbents

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Computational software used:

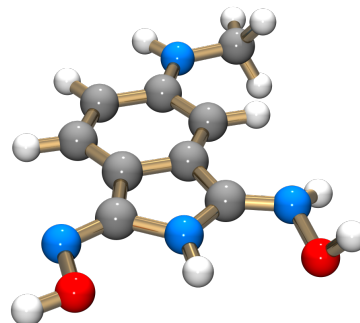
Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

^{III}L protonated (H₃L⁺) at oxime N atom

Energy -718.71936 Hartree

ZPVE 0.20606 Hartree

N	-0.4019	2.0936	0.0367
C	-1.1422	0.9782	0.0305
C	0.9798	1.7594	0.0072
N	1.9483	2.6009	-0.0125
N	-2.4765	0.9936	0.0895
O	-3.0975	2.2170	-0.1468
H	-3.6255	2.4052	0.6543
O	1.4816	3.9032	0.0064
H	2.2877	4.4479	-0.0184
H	-0.7632	3.0393	-0.0136
H	-3.0094	0.1955	-0.2459
C	-0.2749	-0.1900	0.0120
C	1.8395	-1.9507	-0.0252
C	-0.5745	-1.5532	0.0126
C	1.0447	0.3059	-0.0032
C	2.1161	-0.5935	-0.0209
C	0.5069	-2.4663	-0.0082
H	-1.5964	-1.9149	0.0368
H	3.1420	-0.2399	-0.0320
H	2.6658	-2.6572	-0.0407
N	0.3089	-3.8135	-0.0107
H	1.1276	-4.4046	-0.0223
C	-0.9914	-4.4617	0.0066
H	-1.5579	-4.2041	0.9115
H	-0.8401	-5.5424	-0.0019
H	-1.5857	-4.1942	-0.8773

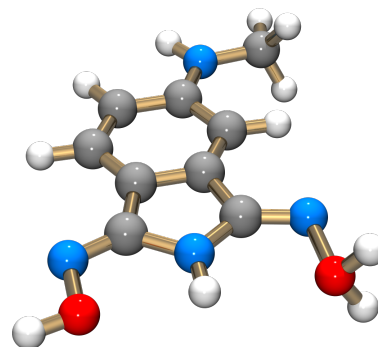


^{III}L protonated (H₃L⁺) at oxime O atom

Energy -718.66291 Hartree

ZPVE 0.020405 Hartree

N	-0.3662	2.0852	-0.0003
C	-1.1439	0.9800	0.0001
C	1.0107	1.7296	0.0000
N	1.9863	2.5612	0.0001
N	-2.4495	0.8357	0.0005
O	-3.0531	2.3453	0.0000
O	1.5130	3.8751	-0.0006
H	2.3220	4.4141	0.0000
H	-0.6815	3.0459	-0.0003
H	-3.6386	2.3485	-0.7894
H	-3.6380	2.3492	0.7899
C	-0.2663	-0.2086	0.0004
C	1.8262	-1.9917	0.0005
C	1.0547	0.2762	0.0005
C	-0.5837	-1.5629	0.0002
C	0.4884	-2.4886	0.0003
C	2.1154	-0.6370	0.0004
H	-1.6134	-1.8989	0.0002
H	3.1446	-0.2923	0.0004
H	2.6450	-2.7069	0.0005
N	0.2699	-3.8342	-0.0002
H	1.0796	-4.4374	0.0003
C	-1.0403	-4.4616	-0.0016
H	-1.6178	-4.1905	0.8921
H	-0.9055	-5.5447	-0.0031
H	-1.6170	-4.1879	-0.8950

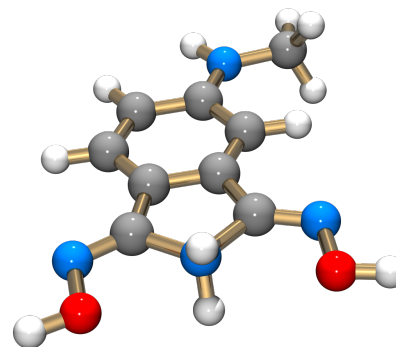


^{III}L protonated (H₃L⁺) at imide N atom

Energy -718.69228 Hartree

ZPVE 0.20667 Hartree

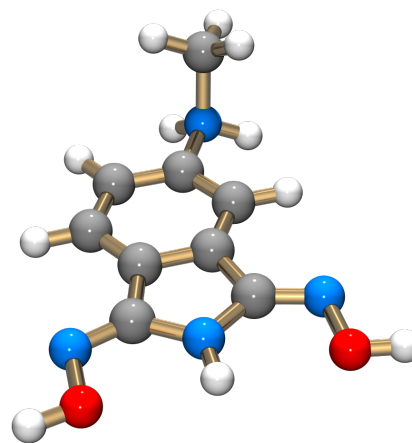
N	0.4473	2.1647	-0.0001
C	-0.9989	1.7267	0.0000
C	1.2494	0.8951	-0.0001
N	2.5231	0.9136	0.0000
N	-1.9409	2.5893	0.0002
O	-1.4242	3.8860	0.0004
H	-2.2119	4.4580	0.0008
O	3.0065	2.2138	0.0002
H	3.9755	2.1146	0.0005
H	0.6632	2.7562	0.8166
H	0.6631	2.7563	-0.8167
C	-1.0056	0.2884	-0.0003
C	-0.4941	-2.4834	0.0000
C	-2.0886	-0.6084	-0.0004
C	0.3133	-0.2161	-0.0002
C	0.5945	-1.5754	-0.0001
C	-1.8281	-1.9636	-0.0004
H	-3.1104	-0.2430	-0.0006
H	1.6200	-1.9241	-0.0002
H	-2.6593	-2.6642	-0.0006
N	-0.3015	-3.8261	0.0006
H	-1.1227	-4.4148	-0.0002
C	0.9977	-4.4829	0.0009
H	1.5771	-4.2220	-0.8934
H	0.8383	-5.5623	0.0027
H	1.5778	-4.2192	0.8940



^{III}L protonated (H₃L⁺) at amine N atom

Energy -718.70515 Hartree
ZPVE 0.20795 Hartree

H	2.9719	0.4131	0.1469
C	1.9238	0.6928	0.1653
C	-0.8397	1.4098	0.2298
C	0.9212	-0.2739	0.0884
C	1.5421	2.0316	0.2733
C	0.1798	2.3548	0.3026
C	-0.4415	0.0797	0.1216
H	2.3021	2.8072	0.3377
H	-1.8942	1.6742	0.2583
C	0.9931	-1.7355	-0.0248
C	-1.2304	-1.1541	0.0314
N	2.0867	-2.4114	-0.0810
N	-2.5171	-1.1976	0.0367
O	-2.9456	-2.5249	-0.0634
H	-3.9149	-2.4612	-0.0471
O	1.7977	-3.7733	-0.1857
H	2.6718	-4.1966	-0.2192
N	-0.3189	-2.1975	-0.0563
H	-0.5762	-3.1729	-0.1267
N	-0.1992	3.7929	0.3861
C	-0.3447	4.4951	-0.9505
H	0.6104	4.4286	-1.4714
H	-0.6193	5.5365	-0.7696
H	-1.1200	3.9805	-1.5182
H	-1.0821	3.8764	0.9042
H	0.4978	4.2925	0.9513



Calculated energies of U(VI) complexes with $^{\text{I}}\text{L}$ and $^{\text{II}}\text{L}$ (B3LYP/6-31+G* and IEFPCM)

Reaction (L = $^{\text{I}}\text{L}$ or $^{\text{II}}\text{L}$)	$\Delta G_{(\text{aq})}$ [kcal/mol]	
	$^{\text{I}}\text{L}$	$^{\text{II}}\text{L}$
$\text{HL}^- + \text{UO}_2^{2+} = \text{UO}_2(\text{HL})^+$	-30.81	-15.31
$\text{HL}^- + \text{UO}_2^{2+} + 2\text{H}_2\text{O} = \text{UO}_2(\text{HL})(\text{H}_2\text{O})_2^+$	-28.43	-13.23
$\text{HL}^- + \text{UO}_2(\text{H}_2\text{O})_5^{2+} = \text{UO}_2(\text{HL})(\text{H}_2\text{O})_2^+ + 3\text{H}_2\text{O}$	-41.96	-26.76
$\text{H}_2\text{L} + \text{UO}_2(\text{H}_2\text{O})_2^{2+} = \text{UO}_2(\text{HL})(\text{H}_2\text{O})_2^+ + \text{H}^+$	-3.41	10.39
$\text{H}_2\text{L}(\text{H}_2\text{O})_2 + \text{UO}_2(\text{H}_2\text{O})_5^{2+} = \text{UO}_2(\text{HL})(\text{H}_2\text{O})_2^+ + 5\text{H}_2\text{O} + \text{H}^+$	-13.28	0.26