Supporting Information

Theoretical insights into selective extraction of uranium from seawater with tetradentate N,O-mixed donor ligands

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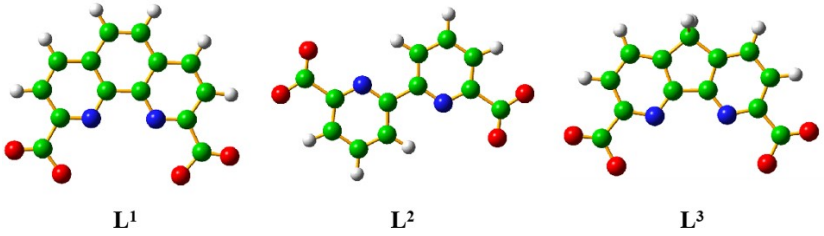

Figure S1. The optimized structures of the L^1, L^2 and L^3 ligands in the gas phase by the B3LYP method. White, green, red and blue represent H, C, O and N, respectively.

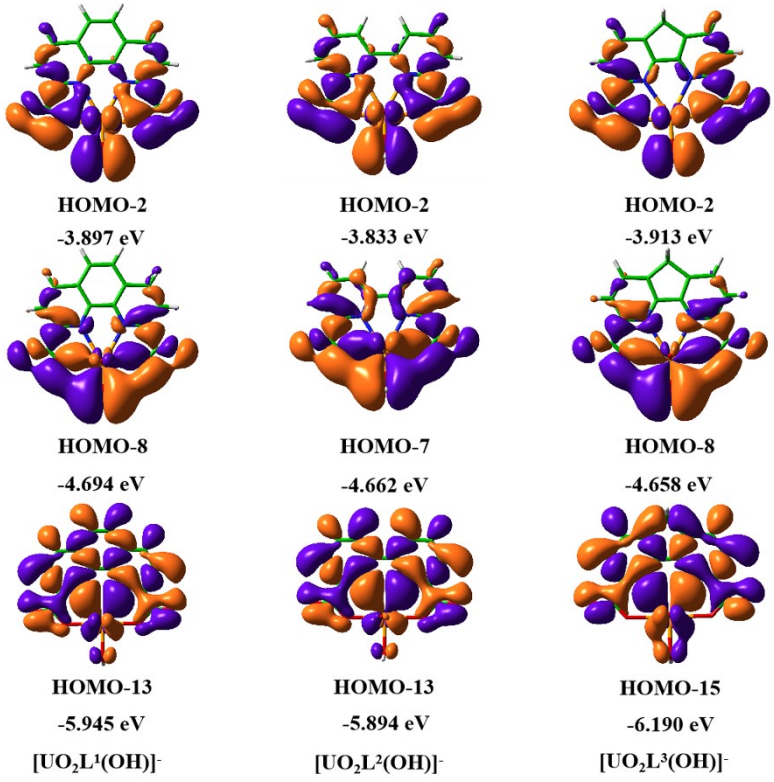

Figure S2. Main molecular orbitals (MOs) of the $[UO_2L(OH)]^-$ complexes supporting to the metal-ligand bonding by the B3LYP method (the isosurface value is set as 0.01 a.u.).

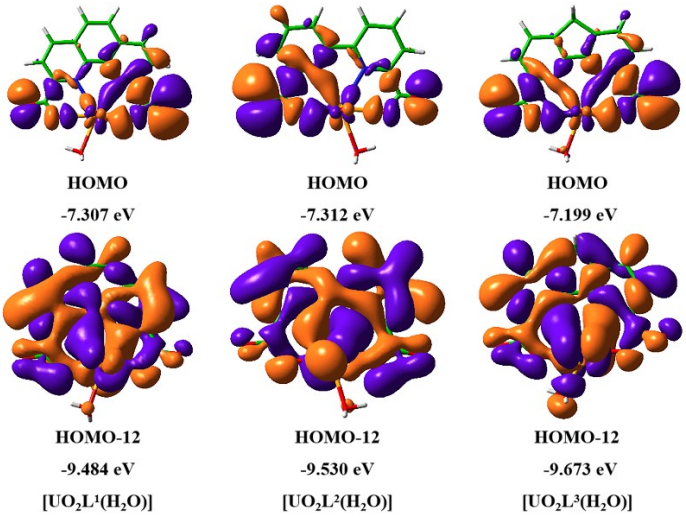

Figure S3. Main molecular orbitals (MOs) of the $[UO_2L(H_2O)]$ complexes supporting to the metal-ligand bonding by the B3LYP method (the isosurface value is set as 0.01 a.u.).

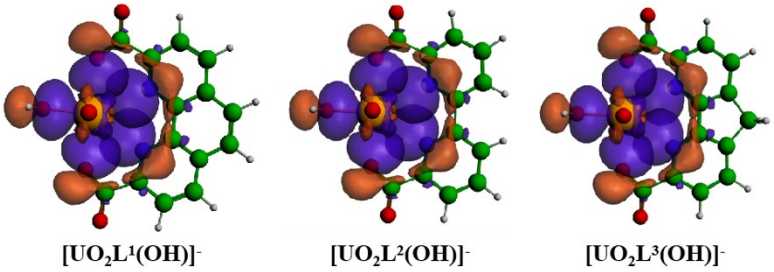

Figure S4. NBO orbitals of the U-N bonds and U-O bonds of the $[UO_2L(OH)]^-$ complexes by the PBE/TZP/ZORA method (the isosurface value is set as 0.02 a.u.).

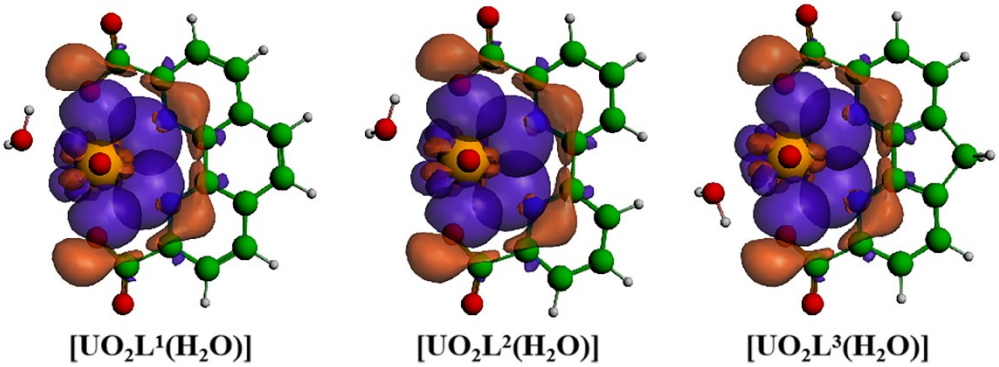

Figure S5. NBO orbitals of the U-N bonds and U-O bonds of the $[UO_2L(H_2O)]$ complexes by the PBE/TZP/ZORA method (the isosurface value is set as 0.02 a.u.).

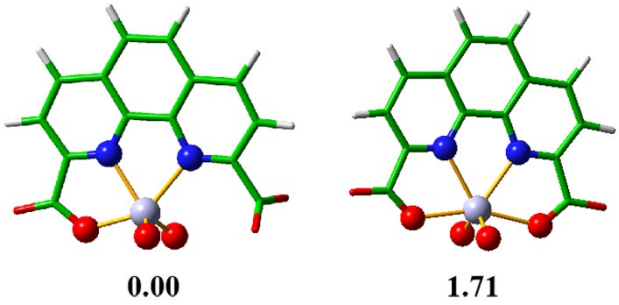

Figure S6. The isomers of $[VO_2L^1]^-$ and relative energies (kcal/mol) by the B3LYP method.

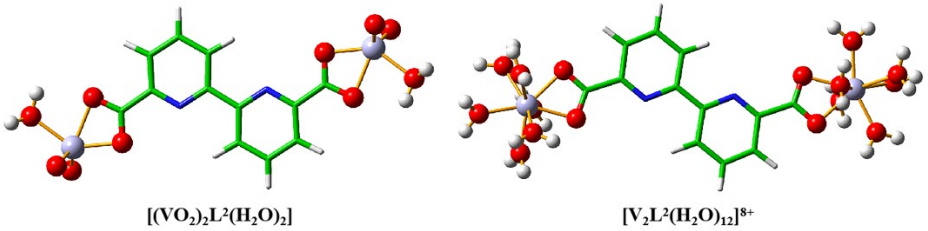

Figure S7. The optimized structures of the $[(VO_2)_2L^2(H_2O)_2]$ and $[V_2L^2(H_2O)_{12}]^{8+}$ complexes by the B3LYP method.

Table S1. Compositions of σ-Bonds about Metal-ligand Bonding on $[UO_2L(CO_3)]^{2-}$ by the B3LYP Method.

Species	MO	U			N(L)	O(L)	$O(CO_3^{2-})$
		5f	6d	7s	2p	2p	2p
$[UO_2L^1(CO_3)]^{2-}$	HOMO-4	1.22	—	—	1.58	5.02	1.49
	HOMO-10	1.99	—	1.50	—	35.16	1.22
$[UO_2L^2(CO_3)]^{2-}$	HOMO-4	1.09	—	—	2.05	4.33	1.86
	HOMO-10	2.15	—	1.58	—	33.82	2.09
$[UO_2L^3(CO_3)]^{2-}$	HOMO-4	2.38	—	—	—	6.37	4.94
	HOMO-8	1.32	1.54	—	—	37.16	—

Table S2. Compositions of σ-Bonds about Metal-ligand Bonding on $[UO_2L(OH)]^-$ by the B3LYP Method.

Species	MO	U			N(L)		O(L)	$O(OH^-)$
		5f	6d	7p	2s	2p	2p	2p
$[UO_2L^1(OH)]^-$	HOMO-2	1.08	—	1.91	—	—	34.88	42.81
	HOMO-8	5.56	7.33	1.16	—	—	31.47	42.31
	HOMO-13	1.57	3.01	—	6.81	54.46	—	—
$[UO_2L^2(OH)]^-$	HOMO-2	1.35	—	1.71	—	—	28.68	43.53
	HOMO-7	5.37	7.30	1.17	—	—	32.42	38.95
	HOMO-13	1.39	2.82	—	7.24	57.00	—	—
$[UO_2L^3(OH)]^-$	HOMO-2	—	—	1.69	—	—	51.32	26.35
	HOMO-8	6.22	6.89	1.24	—	—	18.80	58.76
	HOMO-15	1.71	3.80	—	7.32	52.1	—	—

Table S3. Compositions of σ-Bonds about Metal-ligand Bonding on $[UO_2L(H_2O)]$ by the B3LYP Method.

Species	MO	U			N(L)		O(L)
		5f	6d	7p	2s	2p	2p
$[UO_2L^1(H_2O)]$	HOMO	1.27	—	—	—	—	7.57
	HOMO-12	3.84	2.55	1.36	3.59	37.23	3.92
$[UO_2L^2(H_2O)]$	HOMO	1.18	—	—	—	—	7.46
	HOMO-12	3.88	2.76	1.32	4.04	43.73	3.54
$[UO_2L^3(H_2O)]$	HOMO	1.73	—	—	—	—	8.78
	HOMO-12	5.07	2.78	2.00	5.34	40.78	7.57

Table S4. Compositions of the U-O and U-N σ-Bonds in $[UO_2L(CO_3)]^{2-}$ Complexes by the PBE/TZP/ZORA Method.

Complexes	Element	Composition (%)	Contributions of each atomic orbital (%)
$[UO_2L^1(CO_3)]^{2-}$	U	5.67	7s(10.87) 6d(54.88) 5f(33.89)
	O(L)	94.33	2s(18.71) 2p(81.22)
	U	12.67	7s(25.63) 6d(31.87) 5f(42.40)
	$O(CO_3^{2-})$	87.34	2s(20.82) 2p(79.05)
$[UO_2L^2(CO_3)]^{2-}$	U	6.29	7s(10.29) 6d(55.71) 5f (33.91)
	O(L)	93.72	2s(18.74) 2p(81.21)
	U	12.86	7s(24.47) 6d(33.28) 5f(42.19)
	$O(CO_3^{2-})$	87.14	2s(20.49) 2p(79.38)
$[UO_2L^3(CO_3)]^{2-}$	U	4.91	7s(6.47) 6p(2.02) 6d(45.83) 5f(45.68)
	N(L)	95.09	2s(27.01) 2p(72.90)
	U	11.47	7s(20.35) 6p(l.25) 6d(36.62) 5f (41.78)
	$O(CO_3^{2-})$	88.53	2s(20.60) 2p(79.26)

Table S5. Compositions of the U-O and U-N σ-Bonds in $[UO_2L(OH)]^-$ Complexes by the PBE/TZP/ZORA Method.

Complexes	Element	Composition (%)	Contributions of each atomic orbital (%)
$[UO_2L^1(OH)]^-$	U	7.52	7s(14.90)6p(1.90)6d(34.38)5f(48.83)
	O(L)	92.48	2s(21.97)2p(77.98)
	U	7.39	7s(22.89)6d(42.48)5f(34.23)
	N(L)	92.61	2s(28.34)2p(71.61)
	U	13.79	7s(6.23)6d(31.29)5f(62.43)
	$O(OH^-)$	86.21	2s(36.25)2p(63.70)
$[UO_2L^2(OH)]^-$	U	7.69	7s(15.32)6p(1.67)6d(34.29)5f(48.73)
	O(L)	92.31	2s(22.77)2p(77.17)
	U	7.24	7s(22.15)6d(42.64)5f(34.78)
	N(L)	92.76	2s(27.99)2p(71.95)
	U	13.84	7s(6.87)6d(30.79)5f(62.28)
	$O(OH^-)$	86.16	2s(36.41)2p(63.54)
$[UO_2L^3(OH)]^-$	U	6.95	7s(12.97)6p(2.91)6d(34.55)5f(49.57)
	O(L)	93.05	2s(19.15)2p(80.78)
	U	7.58	7s(25.73)6d(41.84)5f(32.01)
	N(L)	92.42	2s(28.94)2p(71.00)
	U	13.54	7s(4.16)6d(33.08)5f(62.72)
	$O(OH^-)$	86.46	2s(35.94)2p(64.02)

Table S6. Compositions of the U-O and U-N σ-Bonds in $[UO_2L(H_2O)]$ Complexes by the PBE/TZP/ZORA Method.

Complexes	Element	Composition (%)	Contributions of each atomic orbital (%)
$[UO_2L^1(H_2O)]$	U	11.30	7s(12.59)6d(43.86)5f(43.53)
	O(L)	88.70	2s(21.93)2p(78.03)
	U	10.24	7s(28.52)6d(59.12)5f(12.30)
	N(L)	89.77	2s(29.58)2p(70.40)
$[UO_2L^2(H_2O)]$	U	11.40	7s(13.04)6d(43.30)5f(43.64)
	O(L)	88.60	2s(22.31)2p(77.64)
	U	10.09	7s(28.44)6d(59.80)5f(11.68)
	N(L)	89.92	2s(29.46)2p(70.51)
$[UO_2L^3(H_2O)]$	U	11.03	7s(10.70)6d(45.13)5f(44.13)
	O(L)	88.98	2s(20.66)2p(79.30)
	U	10.44	7s(28.02)6d(57.41)5f(14.50)
	N(L)	89.56	2s(30.05)2p(69.93)

Table S7. V=O, V-O(L) and V-N(L) Average Bond Lengths (Å) of the $[VO_2L]^-$ (L=L^1, L^2, L^3) and $[VL_2]^+$ Complexes by the B3LYP Method.

Species	V=O	V−O(L)	V−N(L)
$[VO_2L^1]^-$	1.592	2.017, —	2.156, 2.251
$[VO_2L^2]^-$	1.592	2.215	2.406
$[VO_2L^3]^-$	1.588	2.025, —	2.150, 2.580
$[V(L^1)_2]^+$	—	1.926	2.184
$[V(L^2)_2]^+$	—	1.908	2.205
$[V(L^3)^2]^+$	—	1.952	2.173

Table S8. Mayer Bond Orders (MBOs) of V=O, V-O(L) and V-N(L) Bonds by the PBE Method.

Species	V=O	V−O(L)	V−N(L)
$[VO_2L^1]^-$	1.907	0.438, —	0.284, 0.342
$[VO_2L^2]^-$	1.952	0.353	0.229
$[VO_2L^3]^-$	1.930	0.443, —	0.278, 0.263
$[V(L^1)_2]^+$	—	0.693	0.477
$[V(L^2)_2]^+$	—	0.696	0.474
$[V(L^3)^2]^+$	—	0.687	0.476

Table S9. Changes of Gibbs Free Energy (kcal/mol) for the Substitution Reactions of HVO_4^{2-} and Ligands in Aqueous Solution by the B3LYP Method.

Reactions	ΔG_{sol}		
	L^1	L^2	L^3
$HVO_4^{2-} + H_2L^x \rightarrow [VO_2L^x]^- + H_2O + OH^-$	45.0	44.9	58.2
$[VO_2L^x]^- + H_2L^x \rightarrow [V(L^x)_2]^+ + 2OH^-$	140.2	132.2	179.6

Table S10. Changes of Gibbs Free Energy (kcal/mol) for the Substitution Reactions of $H_2VO_4^-$ and L^2 in Aqueous Solution by the B3LYP Method.

Reactions	ΔG_{sol}
$2H_2VO_4^- + H_2L^2 \rightarrow [(VO_2)_2L^2H_2O)_2] + 2OH^-$	141.9
$[(VO_2)_2L^2H_2O)_2] + 14H_2O \rightarrow [V_2L^2H_2O)_{12}]^{8+} + 8OH^-$	799.1

Cartesian coordinates of the optimized uranyl complexes:

$[UO_2L^1(CO_3)]^{2-}$

C	2.56118500	3.45134100	-0.00014200
C	3.78824700	2.83466400	-0.00164300
C	3.85562600	1.42212000	-0.00169100
C	2.62257400	0.72194600	-0.00018700
C	1.38790300	2.66048300	0.00124200
C	5.08169500	0.68202300	-0.00321400
C	2.62273100	-0.72152400	-0.00018100
C	3.85591400	-1.42144500	-0.00176600
C	5.08183500	-0.68110200	-0.00326000
C	3.78883500	-2.83401200	-0.00181600
H	4.71036200	-3.41147100	-0.00301700
C	2.56191000	-3.45094300	-0.00032400
C	1.38846400	-2.66031000	0.00126600
H	6.01855700	1.23254500	-0.00434400
H	2.42857700	4.52550600	0.00005800
H	4.70963900	3.41233700	-0.00275600
H	6.01881000	-1.23143200	-0.00443100
H	2.42946400	-4.52512800	-0.00026200
N	1.42663300	-1.34078500	0.00135900
N	1.42635600	1.34095700	0.00122000
C	-0.00233800	-3.31703400	0.00303900
C	-0.00305600	3.31693300	0.00296600
O	-0.01660100	-4.55653900	0.00297800
O	-0.01760200	4.55640100	0.00347500
O	-0.95607100	-2.49560800	0.00444300
O	-0.95660700	2.49527900	0.00365700
O	-1.16736000	-0.00130000	-1.78671600
O	-1.17362200	0.00087500	1.78829600
O	-3.35656300	-1.08547100	-0.00142200
C	-4.12206600	0.00014000	-0.00512500
O	-5.34887200	0.00010300	-0.00723200
O	-3.35650200	1.08542800	-0.00606000
U	-1.32939900	-0.00018000	0.00054800

$[UO_2L^2(CO_3)]^{2-}$

C	-2.81468700	3.48027600	0.10190300
C	-4.06403500	2.88663600	0.19404500
C	-4.15752900	1.49755000	0.15830100
C	-2.98378600	0.74454600	0.02908900
C	-1.68952700	2.65552400	-0.00864500
C	-2.98365200	-0.74466100	-0.03062600
C	-4.15713700	-1.49768200	-0.16205600
C	-4.06356200	-2.88676600	-0.19757000
H	-4.96120900	-3.49038200	-0.30167700
C	-2.81436700	-3.48035800	-0.10296400
C	-1.68941200	-2.65557300	0.00965500
H	-2.65306200	4.55012200	0.11597100
H	-4.96192100	3.49020000	0.29638900
H	-2.65272500	-4.55019600	-0.11661000
N	-1.77960900	-1.32753800	0.04144800
N	-1.77964100	1.32748900	-0.04071300
C	-0.28139700	-3.27002800	0.10476700
C	-0.28124000	3.26988800	-0.10117800
O	-0.22740200	-4.50662500	0.12757700
O	-0.22708800	4.50651800	-0.12295000
O	0.65178400	-2.42381300	0.15126900
O	0.65181700	2.42359300	-0.14675600
O	0.98281900	0.11794500	1.78461400
O	0.98057000	-0.11736800	-1.78355800
O	3.16135900	-1.08406700	0.07346800
C	3.92604000	-0.00010000	-0.00291400
O	5.15300700	-0.00025100	-0.00481600
O	3.16137900	1.08400300	-0.07698600
U	1.13487500	0.00006200	0.00044200
H	-5.12281600	1.01433900	0.24392700
H	-5.12222600	-1.01441800	-0.24958100

$[UO_2L^3(CO_3)]^{2-}$

C	1.48023300	2.73280900	-0.00006400
C	2.74366400	3.35122500	0.00002700
C	3.92159800	2.59037800	0.00022700
C	3.79736700	1.20163300	0.00029900

C	2.49196800	0.71616600	0.00022300
H	2.75760800	4.43423400	-0.00009700
H	4.89105900	3.08320100	0.00027400
C	3.79719600	-1.20212700	0.00041200
C	3.92121600	-2.59089500	0.00022100
C	2.74316100	-3.35156100	-0.00001200
C	1.47982700	-2.73296100	-0.00012300
C	2.49186400	-0.71647100	0.00028000
H	4.89059500	-3.08388000	0.00026700
H	2.75695100	-4.43457300	-0.00014600
N	1.36690400	-1.40536800	0.00002200
N	1.36711200	1.40523700	0.00005100
C	0.13108300	-3.47852900	-0.00044700
C	0.13169800	3.47860900	-0.00042300
O	0.19045800	-4.71861600	-0.00056800
O	0.19130400	4.71869300	-0.00083100
O	-0.85815600	-2.69997100	-0.00054700
O	-0.85777500	2.70029100	-0.00027200
O	-0.99390300	-0.00023500	1.78502900
O	-0.99451000	0.00030800	-1.78521900
O	-3.17127800	1.08515500	0.00092800
C	-3.93875700	0.00017600	0.00061800
O	-5.16418900	0.00030100	0.00102200
O	-3.17145900	-1.08488600	-0.00021100
U	-1.15523100	0.00005900	-0.00007300
C	4.75290700	-0.00030900	0.00046400
H	5.40648800	-0.00039100	-0.88037800
H	5.40632200	-0.00032300	0.88142700

$[UO_2L^1(OH)]^-$

C	-2.01834300	3.45060000	-0.00795700
C	-3.25002200	2.83821500	-0.00751500
C	-3.32965900	1.42593400	-0.00664600
C	-2.10568100	0.71931800	-0.00552600
C	-0.85150400	2.65656100	-0.00632900
C	-4.55568000	0.68276800	-0.00722600
C	-2.10605500	-0.71840600	-0.00570600
C	-3.33040800	-1.42441700	-0.00681000
C	-4.55604700	-0.68062400	-0.00729000
C	-3.25147600	-2.83671300	-0.00773700
H	-4.16606500	-3.42223200	-0.00832700
C	-2.02007700	-3.44972100	-0.00813500

C	-0.85287900	-2.65626200	-0.00673900
H	-5.49267500	1.23036500	-0.00768200
H	-1.88948000	4.52497500	-0.00963100
H	-4.16432500	3.42417400	-0.00809600
H	-5.49333000	-1.22772200	-0.00775600
H	-1.89181500	-4.52416700	-0.00951800
N	-0.90634100	-1.33478500	-0.00537500
N	-0.90564000	1.33512000	-0.00486000
C	0.54916800	-3.27920600	-0.00838700
C	0.55083400	3.27891300	-0.00844300
O	0.62387300	-4.50445700	-0.01929400
O	0.62590300	4.50417100	-0.01963100
O	1.48583200	-2.41339900	-0.00110400
O	1.48720800	2.41287700	0.00130900
O	1.33594500	-0.00217500	1.80184500
O	1.39358600	0.00152900	-1.77341200
U	1.45633700	-0.00035700	0.01714500
O	3.61090000	-0.00076900	0.00895700
H	4.05957600	0.00114000	-0.84132400

$[UO_2L^2(OH)]^-$

C	3.48646400	2.20570500	-0.01047500
C	2.89511200	3.45955000	-0.00917300
C	1.50667100	3.55557800	-0.00766200
C	0.74307800	2.38456700	-0.00696100
C	2.66185800	1.08015100	-0.00883400
C	-0.74317500	2.38455600	-0.00705400
C	-1.50681100	3.55552100	-0.00848600
C	-2.89525800	3.45943300	-0.00998100
H	-3.50149500	4.35931300	-0.01088600
C	-3.48656400	2.20557600	-0.01065900
C	-2.66191400	1.08005000	-0.00853100
H	4.55650300	2.04699700	-0.01267500
H	3.50132000	4.35944900	-0.00950300
H	-4.55659900	2.04685400	-0.01282400
N	-1.32885400	1.17414000	-0.00655200
N	1.32878800	1.17419500	-0.00691000
C	-3.26418500	-0.33122600	-0.01001500
C	3.26418500	-0.33108000	-0.01047700
O	-4.48784400	-0.42329100	-0.02287800
O	4.48783100	-0.42314600	-0.02304400
O	-2.39084400	-1.25988600	0.00109100

O	2.39083200	-1.25977900	0.00011100
O	0.00034000	-1.08222300	1.80365500
O	-0.00028800	-1.14460400	-1.77376900
U	0.00003200	-1.20756400	0.01804500
H	1.03171700	4.52729300	-0.00696600
H	-1.03192100	4.52726800	-0.00854600
O	0.00012000	-3.36309100	0.01269500
H	0.00007900	-3.81172500	-0.83754200

$[UO_2L^3(OH)]^-$

C	-2.70086500	1.02010000	-0.00312600
C	-3.34199500	2.27141200	-0.01194000
C	-2.60165500	3.46856700	-0.01383700
C	-1.20649900	3.38354200	-0.00673000
C	-0.70849400	2.08958300	0.00338000
H	-4.42481800	2.28090000	-0.01880700
H	-3.12271700	4.42128100	-0.02207300
C	1.21508600	3.38049500	-0.00678500
C	2.61045000	3.46199300	-0.01390900
C	3.34776900	2.26297200	-0.01197800
C	2.70347900	1.01328800	-0.00312800
C	0.71381300	2.08779300	0.00334400
H	3.13392600	4.41338200	-0.02216000
H	4.43061200	2.26974900	-0.01882200
N	1.37550100	0.94915600	0.00523900
N	-1.37306100	0.95261500	0.00526800
C	3.35927700	-0.38006400	-0.00742700
C	-3.36016600	-0.37160800	-0.00745600
O	4.58473000	-0.44196800	-0.01966300
O	-4.58577400	-0.43040400	-0.01974600
O	2.49228300	-1.32128100	-0.00004000
O	-2.49556900	-1.31503000	-0.00003700
O	-0.00165700	-1.25225700	1.79942400
O	-0.00165800	-1.28447800	-1.76963300
U	-0.00172300	-1.35319500	0.01705700
C	0.00550200	4.34087800	-0.01139400
H	0.00629000	4.98826100	-0.89495500
H	0.00636000	4.99699800	0.86572900
O	-0.00451600	-3.50522700	-0.00665300
H	-0.00513600	-3.95756100	-0.85501700

$[VO_2L^1]^-$

V	-0.11314900	-1.69875700	0.10025700
O	0.27848600	-2.23463200	1.54638000
O	3.54248600	-1.85337800	0.85213000
O	4.01455000	-1.06569300	-1.23324600
O	-2.00024500	-2.38377800	-0.09287600
O	-4.22505900	-1.97901300	-0.19435900
N	1.21354700	0.11896800	0.04355300
N	-1.39133100	0.03210600	-0.04365300
C	-2.69497000	-0.16014100	-0.09453700
C	-0.86668400	1.26578100	-0.00067100
C	0.55491100	1.31748600	0.04362300
C	1.17183100	2.57884500	0.07797200
C	2.59203600	2.58195400	0.08719900
H	3.13205800	3.52335000	0.11575100
C	3.25056300	1.38816400	0.02560600
H	4.32986500	1.33985300	-0.03034300
C	2.55244600	0.13916100	0.01171400
C	-3.05607100	-1.63981900	-0.13175400
C	3.44795000	-1.10585900	-0.12012600
C	0.35056100	3.75126500	0.08338400
H	0.84572000	4.71671300	0.11467400
C	-1.01633200	3.68984400	0.04391600
H	-1.60987300	4.59744800	0.04571200
C	-1.67595000	2.42344600	-0.00398500
C	-3.07514100	2.20879100	-0.05883300
H	-3.74205200	3.06545600	-0.06444800
C	-3.58715900	0.92651300	-0.10628400
H	-4.64862700	0.72050300	-0.15027300
O	0.62126700	-2.50125900	-1.06298300

$[VO_2L^2]^-$

C	3.46583500	1.48226300	-0.00700600
C	2.91458300	2.75388200	-0.01080800
C	1.52792500	2.89144400	-0.00807500
C	0.73733900	1.74264300	-0.00280600
C	2.60784000	0.38220000	-0.00137500
C	-0.73744800	1.74266000	0.00134900
C	-1.52811900	2.89140200	0.00686100
C	-2.91476700	2.75377200	0.01089300
H	-3.54791600	3.63489800	0.01563100

C	-3.46597400	1.48212800	0.00821500
C	-2.60790700	0.38213800	0.00179900
H	4.52972600	1.28554900	-0.00755100
H	3.54770700	3.63502900	-0.01529100
H	-4.52985200	1.28534500	0.01019300
N	-1.28071400	0.51306900	-0.00033000
N	1.28062300	0.51306100	-0.00069500
C	-3.12205400	-1.05385900	-0.00715500
C	3.12220800	-1.05378700	0.00818900
O	-4.34384300	-1.21650100	-0.00391900
O	4.34406100	-1.21612900	0.00792400
O	-2.18296800	-1.89871200	-0.01958900
O	2.18323500	-1.89871900	0.01693900
H	1.07402100	3.87358600	-0.01025800
H	-1.07426500	3.87357200	0.00840400
V	-0.00007900	-1.52377900	-0.00055700
O	0.01057300	-2.39310400	-1.33395400
O	-0.01027300	-2.38999700	1.33489700

$[VO_2L^3]^-$

C	-2.73208200	0.09324100	-0.00016800
C	-3.39446200	1.34808600	-0.00047300
C	-2.72064800	2.56715400	-0.00012600
C	-1.32612100	2.51303100	0.00026300
C	-0.78628300	1.23417900	0.00025700
H	-4.47482700	1.27762300	-0.00105000
H	-3.26933300	3.50438000	-0.00026900
C	1.07338500	2.65291200	0.00033300
C	2.45460600	2.82176300	0.00016400
C	3.27750200	1.67426100	-0.00012500
C	2.70930000	0.40090200	-0.00023400
C	0.63133200	1.33451200	0.00028500
H	2.91169800	3.80636900	0.00015300
H	4.35696800	1.75413400	-0.00032100
N	1.38169000	0.25639500	0.00003600
N	-1.38783900	0.04253500	0.00010800
C	3.39380200	-0.96262700	-0.00096500
C	-3.60941400	-1.21098700	-0.00011900
O	4.60838100	-1.04460000	-0.00118600
O	-4.83443200	-0.95984100	-0.00287800
O	2.52112000	-1.92191900	-0.00127700
O	-2.97115300	-2.26731400	0.00274400

C	-0.18021000	3.53715500	0.00042800
H	-0.21405600	4.18818900	-0.87998500
H	-0.21405600	4.18793800	0.88103300
V	0.50697900	-1.70841000	0.00015700
O	0.12084500	-2.50063600	-1.32055200
O	0.12297500	-2.49809200	1.32298600

$[V(L^1)_2]^+$

C	2.77244700	-2.68592500	2.10312800
C	4.04112900	-2.24649300	1.75901000
C	4.19243200	-1.13741300	0.89058500
C	3.00245900	-0.55434700	0.43410000
C	1.65052900	-2.01808500	1.58019300
C	5.41695700	-0.53919600	0.42211200
C	3.00248500	0.55438600	-0.43402700
C	4.19248500	1.13733800	-0.89059200
C	5.41698400	0.53901300	-0.42218400
C	4.04122900	2.24641500	-1.75902100
H	4.91596400	2.75038400	-2.15374500
C	2.77256300	2.68595000	-2.10307400
C	1.65061900	2.01819000	-1.58009000
H	6.35943600	-0.96025300	0.75176200
H	2.61624600	-3.52931100	2.76355600
H	4.91584100	-2.75053200	2.15369100
H	6.35948500	0.95998100	-0.75188200
H	2.61640400	3.52936100	-2.76347700
N	1.78591700	0.99004100	-0.77503600
N	1.78587400	-0.98993000	0.77515100
C	0.19706400	2.31655400	-1.81359500
C	0.19692700	-2.31628800	1.81381400
O	-0.22394000	3.19943500	-2.50492400
O	-0.22407400	-3.19905100	2.50530500
O	-0.56808200	1.44937200	-1.13452100
O	-0.56821900	-1.44922600	1.13465300
V	-0.00002200	0.00006500	0.00006200
C	-2.77229800	-2.10324600	-2.68598000
C	-4.04100400	-1.75919400	-2.24656500
C	-4.19237700	-0.89071100	-1.13753700
C	-3.00244300	-0.43410700	-0.55450000
C	-1.65041600	-1.58020000	-2.01815900
C	-5.41693200	-0.42230000	-0.53933000
C	-3.00252400	0.43403700	0.55423200

C	-4.19255300	0.89053900	1.13717400
C	-5.41701500	0.42203600	0.53885200
C	-4.04134800	1.75898000	2.24624900
H	-4.91610500	2.15365600	2.75021600
C	-2.77270000	2.10308900	2.68580600
C	-1.65072400	1.58012700	2.01808700
H	-6.35939100	-0.75202000	-0.96037800
H	-2.61604100	-2.76369000	-3.52934200
H	-4.91569000	-2.15394900	-2.75059300
H	-6.35953800	0.75168800	0.95981000
H	-2.61658100	2.76349700	3.52922100
N	-1.78597400	0.77508500	0.98992100
N	-1.78582800	-0.77510500	-0.99005600
C	-0.19717400	1.81370300	2.31648500
C	-0.19679000	-1.81368800	-2.31633600
O	0.22381500	2.50503600	3.19935700
O	0.22426100	-2.50509300	-3.19916000
O	0.56809200	1.13457400	1.44936700
O	0.56821000	-1.13453700	-1.44922500

$[V(L^2)_2]^+$

C	-2.67672100	-2.54271800	2.35749500
C	-3.97004300	-2.16633500	2.00859900
C	-4.16339300	-1.15440500	1.07037000
C	-3.05183700	-0.53726600	0.49811100
C	-1.62285100	-1.87920600	1.74215700
C	-3.05196300	0.53705900	-0.49777500
C	-4.16367200	1.15413600	-1.06980900
C	-3.97057000	2.16597300	-2.00819400
H	-4.82479700	2.65422900	-2.46082800
C	-2.67732800	2.54231400	-2.35746000
C	-1.62331700	1.87890700	-1.74225300
H	-2.46365000	-3.32083600	3.07900500
H	-4.82416200	-2.65462700	2.46140000
H	-2.46446100	3.32031400	-3.07915600
N	-1.81590200	0.91767400	-0.85067000
N	-1.81568100	-0.91785000	0.85071700
C	-0.16960800	2.14089600	-1.98571300
C	-0.16905800	-2.14124800	1.98512100
O	0.26279000	2.95955500	-2.74598900
O	0.26346400	-2.96052800	2.74472700
O	0.58482000	1.33164400	-1.23429700

O	0.58515100	-1.33144500	1.23427800
H	-5.16303500	-0.85100200	0.78914800
H	-5.16323000	0.85073700	-0.78828900
V	-0.00000600	0.00013900	-0.00005100
C	2.67689400	2.35783100	2.54237300
C	3.97018900	2.00886400	2.16597600
C	4.16347100	1.07049700	1.15415100
C	3.05188000	0.49823100	0.53710000
C	1.62297900	1.74246600	1.87894300
C	3.05193300	-0.49775500	-0.53712600
C	4.16360100	-1.07001500	-1.15407600
C	3.97042200	-2.00850700	-2.16579200
H	4.82461800	-2.46134400	-2.65391500
C	2.67715800	-2.35763900	-2.54218500
C	1.62318700	-1.74224000	-1.87888900
H	2.46387500	3.07938600	3.32046100
H	4.82434700	2.46169100	2.65417600
H	2.46424300	-3.07936100	-3.32014600
N	1.81585300	-0.85060000	-0.91770100
N	1.81573800	0.85098100	0.91762800
C	0.16945800	-1.98538600	-2.14098200
C	0.16921400	1.98550000	2.14106300
O	-0.26306600	-2.74535400	-2.95988300
O	-0.26325200	2.74536300	2.96012000
O	-0.58484300	-1.23409600	-1.33151900
O	-0.58507400	1.23434400	1.33158500
H	5.16309400	0.78922000	0.85073600
H	5.16318600	-0.78861700	-0.85065000

$[V(L^2)_2]^+$

C	-2.01643300	-1.85590200	-1.68980300
C	-3.29589500	-2.10496200	-2.20877400
C	-4.44510300	-1.52001900	-1.62236200
C	-4.28618700	-0.71572200	-0.48530000
C	-2.98072300	-0.63994100	-0.04818500
H	-3.38842000	-2.70935800	-3.10241500
H	-5.40779000	-1.67444000	-2.09587400
C	-3.97248500	1.00841500	1.22238500
C	-3.77658400	2.15096600	2.01172300
C	-2.45469700	2.51454700	2.36473700
C	-1.35404900	1.77434200	1.90346200
C	-2.80191800	0.34347300	0.92654300

H	-4.59460400	2.78993400	2.32367700
H	-2.27384200	3.40577600	2.95257200
N	-1.56548100	0.68620800	1.18743300
N	-1.89420700	-1.12078100	-0.59954100
C	0.13679000	2.01728400	1.95256300
C	-0.62712900	-2.17243600	-2.19075500
O	0.68370100	2.88591700	2.56989700
O	-0.35514000	-2.87074300	-3.12168000
O	0.77342900	1.11472100	1.18199400
O	0.28743300	-1.52830100	-1.42870900
C	-5.08288600	0.30382700	0.38481900
H	-5.61882700	1.02158200	-0.24178600
H	-5.82510800	-0.18986200	1.01906400
V	0.00002000	-0.26531000	-0.00016600
C	1.35396700	1.77885000	-1.89925900
C	2.45461400	2.52007700	-2.35894100
C	3.77649800	2.15574800	-2.00674300
C	3.97243800	1.01143700	-1.21994100
C	2.80188400	0.34587700	-0.92551700
H	2.27374700	3.41253800	-2.94490200
H	4.59451200	2.79537100	-2.31737200
C	4.28621900	-0.71673400	0.48368500
C	4.44518400	-1.52383600	1.61873800
C	3.29599300	-2.11023500	2.20375400
C	2.01652400	-1.86000300	1.68537200
C	2.98072700	-0.63987100	0.04683500
H	5.40788500	-1.67941500	2.09184400
H	3.38857600	-2.71684800	3.09588400
N	1.89422800	-1.12214900	0.59694900
N	1.56543900	0.68917400	-1.18561800
C	0.62727700	-2.17781400	2.18562200
C	-0.13693500	2.02163100	-1.94795400
O	0.35527800	-2.87847100	3.11474900
O	-0.68390100	2.89141700	-2.56364600
O	-0.28739300	-1.53165300	1.42523000
O	-0.77343200	1.11743200	-1.17932400
C	5.08288200	0.30487100	-0.38408000
H	5.82512800	-0.18729400	-1.01947000
H	5.61878800	1.02117700	0.24421700

$[(VO_2)_2L^2(H_2O)_2]$

C	-2.56581500	2.35719900	-0.03474000
C	-1.24928000	2.81105400	-0.04380300

C	-0.21619800	1.88530400	-0.04195900
C	-0.53585200	0.51766700	-0.03227600
C	-2.77971600	0.97856900	-0.02462200
C	0.53587100	-0.51760600	-0.03227300
C	0.21622100	-1.88524200	-0.04184400
C	1.24930700	-2.81098900	-0.04374700
H	1.03357700	-3.87288100	-0.05293000
C	2.56584200	-2.35713200	-0.03486800
C	2.77974100	-0.97850000	-0.02486700
H	-3.40870700	3.03480800	-0.03744000
H	-1.03354800	3.87294500	-0.05307800
H	3.40873400	-3.03474000	-0.03763300
N	1.79507000	-0.07838600	-0.02421300
N	-1.79504900	0.07845000	-0.02402900
C	4.16975000	-0.44524700	-0.01504000
C	-4.16973300	0.44534600	-0.01459500
O	5.17661600	-1.23037200	0.00609300
O	-5.17658200	1.23043700	0.00655900
O	4.41111200	0.80046600	-0.02959100
O	-4.41107200	-0.80041000	-0.02900600
H	0.82395700	2.18197300	-0.04856400
H	-0.82393200	-2.18191800	-0.04832500
V	6.40537900	0.51437900	-0.01002400
O	6.93806600	1.25126700	1.29512500
O	6.95156800	1.23602000	-1.30878600
O	7.78763800	-1.07801500	0.11037100
H	7.31641800	-1.88840200	0.34756000
H	8.48399700	-0.92326500	0.76016900
V	-6.40527200	-0.51442400	-0.01000200
O	-6.95083500	-1.23552600	-1.30931200
O	-6.93896100	-1.25162300	1.29459200
O	-7.78790600	1.07768300	0.11002800
H	-8.48404200	0.92202600	0.75986600
H	-7.31704000	1.88807200	0.34790700

$[V_2L^2(H_2O)_{12}]^{8+}$

C	2.62315700	-2.30714000	-0.02134900
C	1.32229200	-2.80853200	-0.01501200
C	0.27668500	-1.89889900	-0.00890500
C	0.56244200	-0.46484600	-0.01003600
C	2.85410300	-0.85427500	-0.01545200
C	-0.51736400	0.47617200	-0.01540600

C	-0.23546100	1.90809900	-0.02414300
C	-1.28482400	2.81417300	-0.03727400
H	-1.10727200	3.88757700	-0.04772000
C	-2.58444000	2.30974300	-0.03943000
C	-2.81152400	0.85866100	-0.02312900
H	3.46845500	-2.99153600	-0.02729300
H	1.14159900	-3.88148400	-0.01601600
H	-3.43030400	2.99323400	-0.05629800
N	-1.83603700	-0.00652100	-0.01434000
N	1.87994700	0.01444900	-0.00947500
C	-4.30437500	0.40185100	-0.01578200
C	4.34510500	-0.41959900	-0.01162400
O	-5.23347500	1.27340700	0.07021300
O	5.26014000	-1.29718400	-0.06312900
O	-4.73237800	-0.77902600	-0.10492900
O	4.80689100	0.76378100	0.04137400
H	-0.75659300	-2.22851000	-0.00592700
H	0.79649000	2.24179000	-0.02131300
V	-6.85787700	-0.13571200	-0.00383000
V	6.83479200	0.13976400	0.00204600
O	6.71549600	1.50894900	1.58327200
O	7.14912400	2.03831400	-0.85923600
O	6.50429400	0.02052800	-2.07409700
O	8.87988900	0.47812700	0.28515100
O	7.15114800	-0.94492900	1.75964800
O	7.73481100	-1.63133800	-0.64977300
H	7.01283000	-0.61152500	2.66663000
H	7.47718000	1.92267800	2.03874300
H	5.89253700	1.93224100	1.89169700
H	7.52091200	2.22229900	-1.74451800
H	7.05376600	2.88962800	-0.39128600
H	9.44773200	0.05355700	0.96137900
H	9.43906900	1.12305500	-0.19520800
H	8.69345100	-1.74339100	-0.81810100
H	7.28456400	-2.48532600	-0.80184500
H	6.92854100	-0.64042300	-2.65446900
H	5.99198600	0.63969600	-2.62612100
H	7.42882500	-1.88001800	1.81339900
O	-6.18772000	-0.05372000	1.98636700
O	-6.85539700	-2.16343000	-0.00142600
O	-8.63198300	-0.52420900	1.29542700
O	-8.59562500	-0.53023400	-1.13642200
O	-7.71689700	1.70949800	0.01354100
O	-6.33813800	0.07517400	-1.99819000

H	-6.09497300	-2.72993400	0.23829300
H	-8.87879600	-1.38451700	1.69124100
H	-9.07059000	0.16362300	1.83565900
H	-7.28989200	2.54831500	0.28226600
H	-8.60861500	1.92775600	-0.33182600
H	-6.36036900	-0.78927900	2.60569000
H	-6.23922600	0.76664400	2.51391100
H	-6.03647000	-0.64584600	-2.58361400
H	-6.51496500	0.86897500	-2.54019900
H	-8.69683400	-0.55451900	-2.10900000
H	-9.47362400	-0.67259600	-0.72707700
H	-7.55204300	-2.73298000	-0.39041300