ELECTRONIC SUPPLEMENTARY INFORMATION

Characterization of the binding of six actinyls $AnO_2^{2+/+}$ (An = U/Np/Pu) with three expanded porphyrins by density functional theory

Meixiu Yang[†, ‡], Wanjian Ding[†,*], Dongqi Wang[‡,*]

[†]Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China

and

[‡]CAS Key Laboratory of Nuclear Radiation and Nuclear Energy Techniques, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

Content

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1. The optimized structures of H_2L1^{2-}, $L2^{2-}$, and $L3^{3-}$ ligands and their complexes with $AnO_2^{2+/+}$ in vacuum and in methanol.

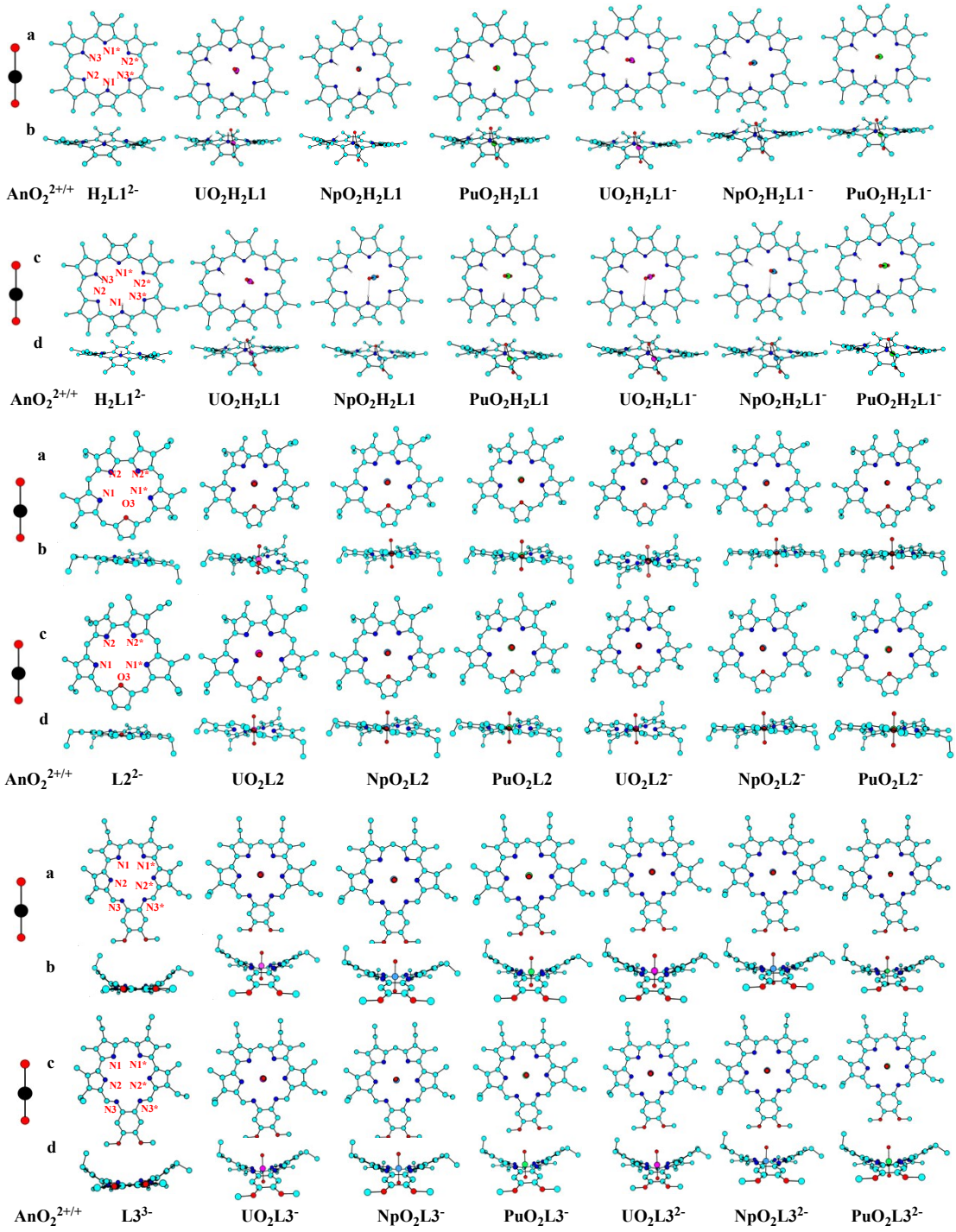

Figure S1. The optimized structures of the ligands H_2L1^{2-}, $L2^{2-}$, and $L3^{3-}$, and their complexes with $AnO_2^{2+/+}$ (hydrogens are omitted for clarity) in vacuum (a,b) and in methanol (c,d). (a,c) top view; (b,d) side view.

2. The calculated energies of different isomers of the three ligands in vacuum and in methanol

Table S1. The relative energies of isomers of the three ligands in vacuum and in methanol.

		ΔG(kcal/mol)		ΔE(kcal/mol)		ΔH(kcal/mol)	
		Gas	MeOH	Gas	MeOH	Gas	MeOH
H_4L1	131*3*	0.0	0.0	0.0	0.0	0.0	0.0
	131*2*	0.2	0.2	0.1	-0.1	0.0	-0.1
	1*233*	13.6	10.5	13.6	10.3	13.6	10.2
	1*2*23	17.8	13.1	18.0	13.2	18.1	13.3
	232*3*	22.9	18.8	23.0	18.5	22.9	18.5
	1231*	33.2	19.7	33.3	19.5	33.3	19.7
H_2L2	12*	0.0	0.0	0.0	0.0	0.0	0.0
	11*	1.7	1.8	2.9	2.5	3.2	2.7
	22*	5.8	4.5	5.3	4.5	5.2	4.4
	12	17.8	13.4	18.4	13.5	18.5	13.5
H_3L3	122*	0.0	0.0	0.0	0.0	0.0	0.0
	132*	3.4	2.8	3.2	2.4	3.0	2.2
	123*	8.2	5.8	8.0	5.8	7.9	5.7
	131*	18.7	15.1	19.4	15.5	19.4	15.4
	121*	19.5	14.7	20.1	15.0	20.2	15.0
	133*	20.7	16.2	21.6	16.6	21.7	16.7
	231*	21.1	15.2	21.2	15.2	21.0	15.0
	232*	23.9	17.3	24.2	17.3	24.1	17.2
	123	30.1	20.2	29.7	20.2	29.4	20.0
	233*	44.6	34.2	46.1	34.2	46.2	34.2

3. The influence of protonation on the complexation

In order to understand the effect of protonation on the complexation of penta-aquo actinyl complexes with the ePor and find an optimal pathway in terms of thermodynamics, H_4L1 was selected to elucidate the complexation and the deprotonation processes. The following stepwise mechanism has been considered and the results are plotted in Figure S2:

Step 1: $AnO_2(H_2O)_5^{2+/+} + Et_3N + H_4L1 \rightarrow [AnO_2H_3L1]^{+/0} + Et_3NH^+ + (H_2O)_5$

Step 2: $[AnO_2H_3L1]^{+/0} + Et_3N \rightarrow [AnO_2H_2L1]^{0/-} + Et_3NH^+$

Step 3: $[AnO_2H_2L1]^{0/-} + Et_3N \rightarrow [AnO_2HL1]^{-/2-} + Et_3NH^+$

Step 4: $[AnO_2HL1]^{-/2-} + Et_3N \rightarrow [AnO_2L1]^{2-/3-} + Et_3NH^+$

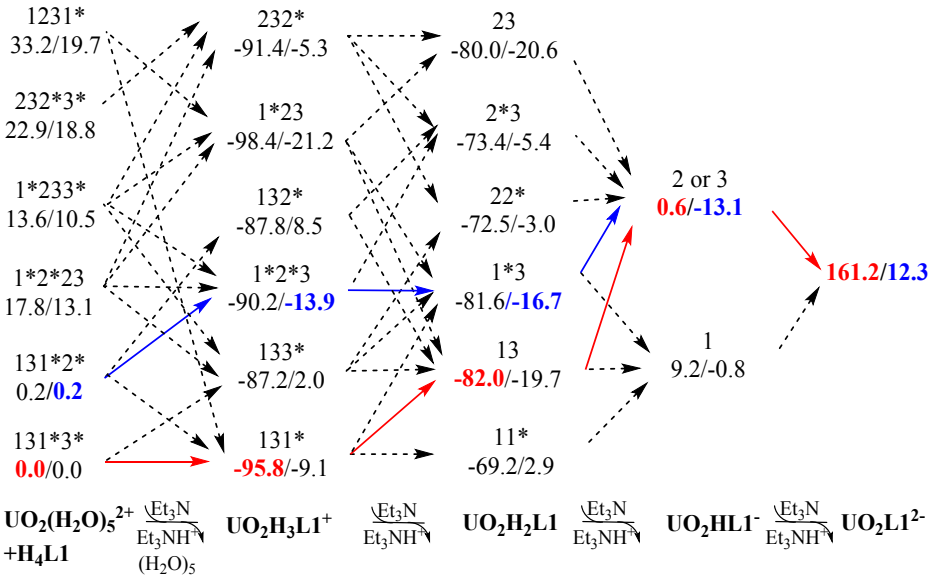

Figure S2. Stepwise mechanism for the complexation of $UO_2(H_2O)_5^{2+}$ with H_4L1 assisted by Et_3N. The Gibbs free energy change (kcal/mol) of the sequential deprotonation reaction is given in the format of $\Delta G_{vacuum}/\Delta G_{MeOH}$ with respect to the total free energy of H_4L1_{131*3*}, $UO_2(H_2O)_5^{2+}$, and 4 Et_3N, and the $\Delta G_{vacuum}/\Delta G_{MeOH}$ of $UO_2(H_2O)_5^{2+}$ + H_4L1 is with respect to the total free energy of $UO_2(H_2O)_5^{2+}$, H_4L1_{131*3*} and 4Et_3N. The solid arrows represent the optimal deprotonation path (red for in vacuum and blue for in MeOH).

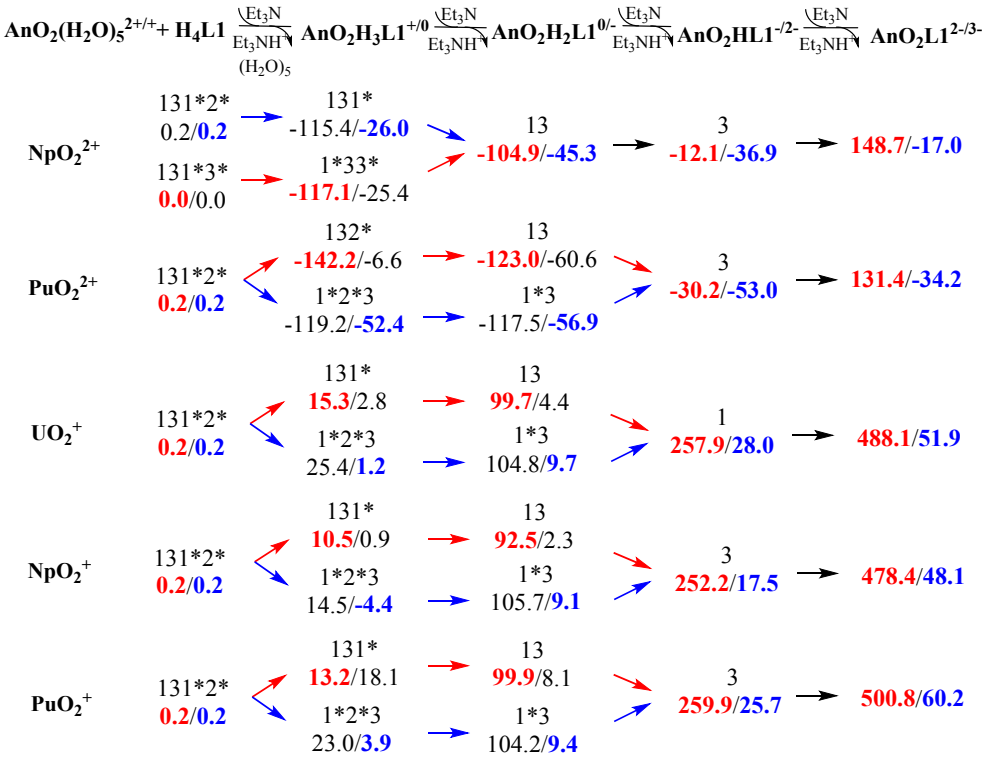

Figure S3. The optimum pathways (red for in vacuum and blue for in MeOH) for the coordination of $AnO_2(H_2O)_5^{2+/+}$ (An = Np/Pu) and $UO_2(H_2O)_5^{+}$ with H_4L1_{131*3*} or H_4L1_{131*2*} assisted by Et_3N. The Gibbs free energy change (kcal/mol) of the sequential deprotonation reaction is given in the format of $\Delta G_{vacuum}/\Delta G_{MeOH}$.

4. Key geometrical parameters of the actinyl and the corresponding complexes

Table S2. Key geometrical parameters (bond length in Å, bond angle in degree) for the $AnO_2^{2+/+}$ and their complexes with H_2L1^{2-}, $L2^{2-}$, $L3^{3-}$ ligand in methanol.

		An-X			An-O^{yl}			^{bare}An-O^{yl}
		N1/ N1*	N2/N2*	N3(O3)[(a)]/N3*	đ [(b)]	O1/O2	∠O-An-O	O1/O2
$AnO_2H_2L1^{0/-}$	U^{VI}	3.02/2.47	3.88/2.38	3.80/2.46	3.00	1.76/1.76	179.7	1.72/1.72
	Np^{VI}	3.24/2.54	3.86/2.46	3.60/2.57	3.04	1.80/1.81	179.2	1.70/1.70
	Pu^{VI}	3.20/2.53	3.81/2.46	3.57/2.57	3.02	1.77/1.79	179.4	1.68/1.68
	U^{V}	3.31/2.53	3.94/2.45	3.66/2.59	2.97	1.80/1.82	171.2	1.79/1.79
	Np^{V}	3.25/2.53	3.91/2.44	3.66/2.54	3.06	1.81/1.82	177.8	1.76/1.76
	Pu^{V}	3.19/2.53	3.86/2.44	3.66/2.53	3.04	1.78/1.79	178.4	1.75/1.75
$AnO_2L2^{0/-}$	U^{VI}	2.56/2.56	2.47/2.47	2.68	2.55	1.76/1.76	176.0	
	Np^{VI}	2.66/2.63	2.55/2.54	2.73	2.62	1.81/1.80	178.3	
	Pu^{VI}	2.65/2.63	2.55/2.54	2.73	2.62	1.78/1.78	178.9	
	U^{V}	2.54/2.54	2.46/2.46	2.68	2.54	1.77/1.77	175.7	
	Np^{V}	2.66/2.67	2.55/2.55	2.75	2.64	1.81/1.81	177.4	
	Pu^{V}	2.66/2.66	2.55/2.55	2.75	2.63	1.79/1.79	178.3	
$AnO_2L3^{-/2-}$	U^{VI}	2.67/2.67	2.52/2.52	2.79/2.79	2.66	1.76/1.77	179.1	
	Np^{VI}	2.73/2.74	2.57/2.58	2.87/2.87	2.72	1.81/1.82	179.5	
	Pu^{VI}	2.69/2.68	2.50/2.50	2.79/2.79	2.66	1.73/1.73	179.5	
	U^{V}	2.59/2.59	2.54/2.54	2.91/2.91	2.68	1.78/1.78	178.0	
	Np^{V}	2.74/2.73	2.58/2.59	2.90/2.90	2.74	1.82/1.82	179.2	
	Pu^{V}	2.76/2.75	2.58/2.58	2.88/2.88	2.74	1.80/1.80	179.2	

[(a)] For the complexes of $AnO_2H_2L1^{0/-}$ and $AnO_2L3^{-/2-}$, X = N3/N3*, and for the complex $AnO_2L2^{0/-}$, X = O3;

[(b)] Arithmetic mean of the bond lengths in the equatorial plane of actinides;

Table S3. Key geometrical parameters (bond length in Å, bond angle in degree) of UO_2^{2+} and its complexes with H_4L1 ligand in vacuum.

U^{VI}	U-N_i						U-O^{yl}			T_A[(b)]
	N1	N2	N3	N1*	N2*	N3*	$\overline{d}$ [(a)]	O1	O2	∠O-U-O	
UO_2^{2+}								1.68	1.68	180.0	
UO_2L1^{2-}	2.62	2.91	2.91	2.62	2.91	2.91	2.81	1.74	1.74	180.0	360.2
$UO_2L1H^{-}_{(1)}$	3.29	3.06	2.68	2.43	2.68	3.06	2.86	1.74	1.75	174.0	360.9
$UO_2L1H^{-}_{(2)}$	2.61	3.76	3.44	2.51	2.48	2.48	2.88	1.75	1.75	174.5	360.3
$UO_2L1H_{2(23)}$	2.59	3.73	3.71	2.53	2.42	2.41	2.90	1.75	1.75	170.6	360.3
$UO_2L1H_{2(11*)}$	2.83	2.79	2.77	2.76	2.77	2.79	2.79	1.74	1.74	178.5	363.4
$UO_2L1H_{2(13)}$	2.81	3.64	3.68	2.49	2.41	2.48	2.92	1.74	1.75	171.8	359.1
$UO_2L1H_{2(12)}$	2.94	3.86	3.32	2.41	2.42	2.49	2.91	1.75	1.75	170.8	360.3

$UO_2L1H_{2(2*3)}$	2.42	2.67	2.92	2.64	3.37	2.96	2.83	1.74	1.75	176.7	360.3
$UO_2L1H_{2(22*)}$	2.50	2.99	3.37	2.54	2.67	2.93	2.83	1.74	1.74	179.1	360.5
$UO_2L1H_3^+{}_{(1*23)}$	2.80	3.84	3.64	2.49	2.36	2.43	2.93	1.75	1.75	168.5	359.7
$UO_2L1H_3^+{}_{(1*2*3)}$	2.32	2.66	3.26	3.17	3.25	2.66	2.89	1.74	1.74	169.7	360.5
$UO_2L1H_3^+{}_{(133*)}$	2.82	3.18	3.27	2.43	2.55	2.90	2.86	1.74	1.74	173.3	360.5
$UO_2L1H_3^+{}_{(232*)}$	2.58	3.67	3.60	2.45	2.44	2.62	2.89	1.75	1.74	174.8	360.2
$UO_2L1H_3^+{}_{(131*)}$	2.66	2.42	2.42	2.78	3.82	3.52	2.94	1.74	1.74	171.9	360.5
$UO_2L1H_3^+{}_{(132*)}$	2.68	2.87	3.01	2.51	2.99	2.85	2.82	1.73	1.74	177.2	360.0

(a) Arithmetic mean of the bond lengths in the equatorial plane of actinides;

(b) The sum of the bond angles in the equatorial plane of actinide atoms.

Table S4. Key geometrical parameters (bond length in Å, bond angle in degree) of UO_2^{2+} and its complexes with H_4L1 ligand in MeOH.

U^{VI}	U-N_i							U-O^{yl}			T_A(b)
	N1	N2	N3	N1*	N2*	N3*	$\bar{d}$ (a)	O1	O2	∠O-U-O	
UO_2^{2+}								1.72	1.72	180.0	
UO_2L1^{2-}	2.59	2.86	2.87	2.59	2.89	2.89	2.78	1.76	1.76	179.4	361.1
$UO_2L1H^-{}_{(1)}$	3.45	3.33	2.72	2.39	2.56	2.88	2.89	1.75	1.76	177.2	360.6
$UO_2L1H^-{}_{(2)}$	2.59	3.78	3.52	2.52	2.46	2.46	2.89	1.76	1.76	176.9	360.1
$UO_2L1H_{2(23)}$	2.56	3.86	3.85	2.53	2.41	2.40	2.93	1.76	1.77	179.6	360.7
$UO_2L1H_{2(11*)}$	2.84	2.77	2.75	2.74	2.75	2.77	2.77	1.75	1.75	176.4	364.3
$UO_2L1H_{2(13)}$	3.02	3.88	3.80	2.47	2.38	2.46	3.00	1.76	1.76	179.7	354.9
$UO_2L1H_{2(12)}$	3.18	4.11	3.55	2.42	2.37	2.45	3.01	1.76	1.76	178.3	356.2
$UO_2L1H_{2(2*3)}$	2.46	2.50	2.67	2.59	3.72	3.41	2.89	1.75	1.75	176.6	359.3
$UO_2L1H_{2(22*)}$	2.49	3.31	3.66	2.54	2.53	2.76	2.88	1.75	1.75	176.0	361.1
$UO_2L1H_3^+{}_{(1*23)}$	3.54	4.28	3.75	2.44	2.36	2.46	3.14	1.76	1.77	179.1	343.3
$UO_2L1H_3^+{}_{(1*2*3)}$	2.31	2.55	3.75	4.09	3.75	2.55	3.16	1.75	1.76	178.2	344.1
$UO_2L1H_3^+{}_{(133*)}$	3.21	3.90	3.75	2.40	2.39	2.66	3.05	1.75	1.75	175.5	354.3
$UO_2L1H_3^+{}_{(232*)}$	2.54	3.83	3.80	2.48	2.43	2.57	2.94	1.76	1.75	175.0	360.8
$UO_2L1H_3^+{}_{(131*)}$	2.92	2.41	2.40	2.80	3.88	3.86	3.05	1.75	1.75	176.6	352.7
$UO_2L1H_3^+{}_{(132*)}$	2.64	2.86	3.06	2.53	3.06	2.86	2.84	1.74	1.74	175.4	359.2

(a) Arithmetic mean of the bond lengths in the equatorial plane of actinides;

(b) The sum of the bond angles in the equatorial plane of actinide atoms.

Table S5. Key geometrical parameters (bond length in Å, bond angle in degree) of NpO_2^{2+} and its complexes with H_4L1 ligand in vacuum.

Np^{VI}	Np-N_i							Np-O^{yl}			T_A(b)
	N1	N2	N3	N1*	N2*	N3*	$\bar{d}$ (a)	O1	O2	∠O-Np-O	
NpO_2^{2+}								1.66	1.66	180.0	
NpO_2L1^{2-}	2.70	2.92	2.93	2.71	2.93	2.92	2.85	1.79	1.79	179.8	360.3

$NpO_2L1H^-_{(1)}$	3.18	3.03	2.78	2.55	2.78	3.03	2.89	1.78	1.79	174.8	360.0
$NpO_2L1H^-_{(2)}$	2.70	3.49	3.24	2.59	2.62	2.62	2.88	1.80	1.78	173.8	360.2
$NpO_2L1H_{2(23)}$	2.61	3.48	3.49	2.63	2.55	2.55	2.88	1.79	1.79	168.6	360.4
$NpO_2L1H_{2(11*)}$	2.91	2.81	2.81	2.91	2.96	2.96	2.89	1.77	1.77	179.1	360.6
$NpO_2L1H_{2(13)}$	2.94	3.51	3.50	2.58	2.52	2.60	2.94	1.77	1.79	174.6	356.2
$NpO_2L1H_{2(12)}$	3.08	3.75	3.28	2.49	2.49	2.59	2.95	1.76	1.79	174.7	356.6
$NpO_2L1H_{2(2*3)}$	2.47	2.79	3.21	2.88	3.20	2.79	2.89	1.77	1.79	175.5	358.3
$NpO_2L1H_{2(22*)}$	2.61	2.84	3.13	2.61	2.84	3.13	2.86	1.78	1.78	179.8	360.8
$NpO_2L1H_3^+{}_{(1*23)}$	3.37	4.04	3.63	2.53	2.42	2.56	3.09	1.76	1.83	171.8	343.8
$NpO_2L1H_3^+{}_{(1*2*3)}$	2.45	2.76	3.18	3.06	3.18	2.76	2.90	1.76	1.77	174.4	360.1
$NpO_2L1H_3^+{}_{(133*)}$	2.82	3.00	3.15	2.56	2.73	3.02	2.88	1.77	1.78	176.2	360.5
$NpO_2L1H_3^+{}_{(232*)}$	2.65	3.39	3.34	2.55	2.58	2.79	2.88	1.78	1.77	174.5	360.1
$NpO_2L1H_3^+{}_{(131*)}$	2.76	2.56	2.58	2.83	3.54	3.31	2.93	1.77	1.78	175.7	360.1
$NpO_2L1H_3^+{}_{(132*)}$	2.71	2.82	2.98	2.68	3.19	2.97	2.89	1.75	1.77	179.6	356.9

[a] Arithmetic mean of the bond lengths in the equatorial plane of actinides;

[b] The sum of the bond angles in the equatorial plane of actinide atoms.

Table S6. Key geometrical parameters (bond length in Å, bond angle in degree) of NpO_2^{2+} and its complexes with H_4L1 ligand in MeOH.

Np^{VI}	Np-N_i						Np-O^{yl}			T_A[b]
	N1	N2	N3	N1*	N2*	N3*	$\overline{d}$ [a]	O1	O2	∠O-Np-O	
NpO_2^{2+}								1.70	1.70	180.0	
NpO_2L1^{2-}	2.66	2.91	2.92	2.66	2.91	2.90	2.83	1.81	1.81	180.0	360.3
$NpO_2L1H^-_{(1)}$	3.21	2.99	2.72	2.52	2.79	3.10	2.89	1.80	1.80	176.3	359.9
$NpO_2L1H^-_{(2)}$	2.68	3.57	3.30	2.57	2.57	2.57	2.88	1.81	1.81	176.2	360.1
$NpO_2L1H_{2(23)}$	2.60	3.53	3.56	2.61	2.52	2.52	2.89	1.81	1.81	172.9	360.0
$NpO_2L1H_{2(11*)}$	2.89	2.74	2.74	2.88	3.05	3.05	2.89	1.79	1.79	179.5	360.6
$NpO_2L1H_{2(13)}$	3.24	3.86	3.60	2.54	2.46	2.57	3.04	1.80	1.81	179.2	348.4
$NpO_2L1H_{2(12)}$	3.35	3.95	3.47	2.49	2.45	2.58	3.05	1.79	1.80	179.1	348.5
$NpO_2L1H_{2(2*3)}$	2.45	2.77	3.28	3.00	3.27	2.76	2.92	1.79	1.80	178.8	356.3
$NpO_2L1H_{2(22*)}$	2.61	2.85	3.16	2.60	2.82	3.14	2.86	1.80	1.80	179.7	360.9
$NpO_2L1H_3^+{}_{(1*23)}$	3.57	4.16	3.70	2.57	2.45	2.61	3.18	1.79	1.84	178.7	335.6
$NpO_2L1H_3^+{}_{(1*2*3)}$	2.41	2.63	3.78	4.06	3.78	2.63	3.22	1.78	1.82	178.5	332.6
$NpO_2L1H_3^+{}_{(133*)}$	2.81	3.12	3.27	2.56	2.66	2.96	2.90	1.79	1.79	177.7	360.4
$NpO_2L1H_3^+{}_{(232*)}$	2.63	3.55	3.48	2.54	2.53	2.76	2.92	1.80	1.80	175.0	361.0
$NpO_2L1H_3^+{}_{(131*)}$	3.08	2.51	2.49	2.87	3.74	3.80	3.08	1.79	1.80	178.6	348.3
$NpO_2L1H_3^+{}_{(132*)}$	3.27	2.60	2.61	2.56	3.63	3.87	3.09	1.77	1.79	176.0	342.1

[a] Arithmetic mean of the bond lengths in the equatorial plane of actinides;

[b] The sum of the bond angles in the equatorial plane of actinide atoms.

Table S7. Key geometrical parameters (bond length in Å, bond angle in degree) of PuO_2^{2+} and its complexes with H_4L1 ligand in vacuum.

Pu^{VI}	Pu-N_i							Pu-O^{yl}			T_A[b]
	N1	N2	N3	N1*	N2*	N3*	$\overline{d}$ [a]	O1	O2	∠O-Pu-O	
PuO_2^{2+}								1.64	1.64	180.0	
PuO_2L1^{2-}	2.70	2.93	2.92	2.68	2.92	2.93	2.85	1.77	1.77	179.9	360.3
$PuO_2L1H^-_{(1)}$	3.19	3.04	2.77	2.53	2.77	3.04	2.89	1.76	1.77	176.4	359.9
$PuO_2L1H^-_{(2)}$	2.69	3.51	3.25	2.58	2.60	2.61	2.88	1.77	1.76	176.1	360.1
$PuO_2L1H_{2(23)}$	2.62	3.51	3.51	2.62	2.53	2.53	2.89	1.77	1.77	174.0	360.3
$PuO_2L1H_{2(11*)}$	2.91	2.97	2.97	2.91	2.80	2.80	2.89	1.75	1.75	179.3	360.5
$PuO_2L1H_{2(13)}$	2.94	3.50	3.49	2.57	2.51	2.60	2.93	1.75	1.77	176.3	356.8
$PuO_2L1H_{2(12)}$	3.02	3.74	3.30	2.48	2.49	2.58	2.93	1.75	1.77	175.7	357.6
$PuO_2L1H_{2(2*3)}$	2.47	2.80	3.18	2.81	3.18	2.80	2.87	1.75	1.77	177.1	358.8
$PuO_2L1H_{2(22*)}$	2.59	2.84	3.13	2.60	2.84	3.13	2.86	1.76	1.76	179.9	360.7
$PuO_2L1H_3^+{}_{(1*23)}$	3.33	4.01	3.61	2.53	2.41	2.54	3.07	1.74	1.80	174.5	346.3
$PuO_2L1H_3^+{}_{(1*2*3)}$	2.42	2.74	3.23	3.13	3.23	2.74	2.91	1.76	1.78	174.2	359.6
$PuO_2L1H_3^+{}_{(133*)}$	2.80	3.04	3.19	2.55	2.70	3.00	2.88	1.75	1.76	177.3	360.4
$PuO_2L1H_3^+{}_{(232*)}$	2.64	3.39	3.34	2.54	2.57	2.79	2.88	1.76	1.75	176.8	360.1
$PuO_2L1H_3^+{}_{(131*)}$	2.74	2.57	2.59	2.82	3.51	3.27	2.92	1.75	1.76	177.0	360.2
$PuO_2L1H_3^+{}_{(132*)}$	2.71	2.89	3.09	2.67	3.09	2.89	2.89	1.74	1.76	179.8	357.0

[a] Arithmetic mean of the bond lengths in the equatorial plane of actinides;

[b] The sum of the bond angles in the equatorial plane of actinide atoms.

Table S8. Key geometrical parameters (bond length in Å, bond angle in degree) of PuO_2^{2+} and its complexes with H_4L1 ligand in MeOH.

Pu^{VI}	Pu-N_i							Pu-O^{yl}			T_A[b]
	N1	N2	N3	N1*	N2*	N3*	$\overline{d}$ [a]	O1	O2	∠O-Pu-O	
PuO_2^{2+}								1.68	1.68	180.0	
PuO_2L1^{2-}	2.66	2.91	2.91	2.66	2.91	2.91	2.83	1.79	1.79	180.0	360.3
$PuO_2L1H^-_{(1)}$	3.20	3.05	2.75	2.51	2.75	3.05	2.89	1.78	1.78	177.3	359.9
$PuO_2L1H^-_{(2)}$	2.67	3.58	3.32	2.57	2.56	2.57	2.88	1.79	1.79	177.6	360.0
$PuO_2L1H_{2(23)}$	2.62	3.70	3.61	2.60	2.48	2.48	2.91	1.79	1.79	178.4	360.2
$PuO_2L1H_{2(11*)}$	2.86	2.99	2.99	2.86	2.78	2.78	2.88	1.76	1.76	179.4	360.4
$PuO_2L1H_{2(13)}$	3.20	3.81	3.57	2.53	2.46	2.57	3.02	1.77	1.79	179.4	350.6
$PuO_2L1H_{2(12)}$	3.31	3.94	3.45	2.48	2.45	2.58	3.04	1.78	1.79	179.4	349.4
$PuO_2L1H_{2(2*3)}$	2.46	2.90	3.33	2.82	3.06	2.71	2.88	1.76	1.77	178.6	358.5
$PuO_2L1H_{2(22*)}$	2.58	2.81	3.13	2.59	2.87	3.16	2.86	1.77	1.77	179.8	360.8
$PuO_2L1H_3^+{}_{(1*23)}$	3.52	4.12	3.68	2.56	2.44	2.59	3.15	1.76	1.81	179.2	338.9
$PuO_2L1H_3^+{}_{(1*2*3)}$	2.40	2.63	3.77	4.07	3.77	2.63	3.21	1.77	1.80	178.6	333.3
$PuO_2L1H_3^+{}_{(133*)}$	2.84	3.14	3.27	2.52	2.63	2.99	2.90	1.78	1.78	179.0	360.5

$PuO_2L1H_3^{+}{}_{(232*)}$	2.64	3.67	3.55	2.53	2.48	2.67	2.92	1.78	1.77	179.2	360.8
$PuO_2L1H_3^{+}{}_{(131*)}$	2.85	2.52	2.51	2.81	3.65	3.56	2.98	1.76	1.77	178.4	355.6
$PuO_2L1H_3^{+}{}_{(132*)}$	3.19	2.58	2.60	2.55	3.61	3.83	3.06	1.74	1.76	177.3	345.0

(a) Arithmetic mean of the bond lengths in the equatorial plane of actinides;

(b) The sum of the bond angles in the equatorial plane of actinide atoms.

Table S9. Key geometrical parameters (bond length in Å, bond angle in degree) of NpO_2^+ and its complexes with H_4L1 ligand in vacuum.

Np^V	Np-N_i							Np-O^{yl}			T_A(b)
	N1	N2	N3	N1*	N2*	N3*	$\bar{d}$ (a)	O1	O2	∠O-Np-O	
NpO_2^+								1.71	1.71	180.0	
NpO_2L1^{3-}	2.72	2.95	2.95	2.72	2.95	2.95	2.87	1.79	1.79	180.0	360.6
$NpO_2L1H^{2-}{}_{(1)}$	3.26	3.08	2.78	2.53	2.78	3.08	2.92	1.78	1.79	174.2	360.3
$NpO_2L1H^{2-}{}_{(2)}$	2.71	3.58	3.33	2.61	2.60	2.60	2.91	1.80	1.79	173.4	360.5
$NpO_2L1H_2^{-}{}_{(23)}$	2.62	3.58	3.59	2.67	2.52	2.51	2.92	1.80	1.80	169.1	360.6
$NpO_2L1H_2^{-}{}_{(11*)}$	2.98	2.90	2.90	2.98	2.90	2.90	2.93	1.78	1.78	180.0	360.9
$NpO_2L1H_2^{-}{}_{(13)}$	3.02	3.64	3.58	2.57	2.49	2.57	2.98	1.78	1.80	173.4	355.8
$NpO_2L1H_2^{-}{}_{(12)}$	3.10	3.83	3.37	2.49	2.47	2.57	2.97	1.77	1.79	174.0	357.2
$NpO_2L1H_2^{-}{}_{(2*3)}$	2.50	2.83	3.23	2.82	3.23	2.83	2.91	1.78	1.79	176.8	358.9
$NpO_2L1H_2^{-}{}_{(22*)}$	2.60	2.86	3.19	2.60	2.86	3.19	2.88	1.79	1.79	180.0	361.3
$NpO_2L1H_{3(1*23)}$	3.43	4.08	3.65	2.55	2.41	2.53	3.11	1.77	1.83	170.0	345.0
$NpO_2L1H_{3(1*2*3)}$	2.42	2.75	3.28	3.19	3.25	2.73	2.94	1.77	1.79	171.7	360.4
$NpO_2L1H_{3(133*)}$	2.89	3.14	3.25	2.51	2.65	3.02	2.91	1.78	1.78	174.6	360.8
$NpO_2L1H_{3(232*)}$	2.67	3.52	3.43	2.53	2.55	2.77	2.91	1.79	1.78	174.5	360.4
$NpO_2L1H_{3(131*)}$	2.79	2.50	2.51	2.83	3.69	3.48	2.97	1.78	1.79	172.6	360.4
$NpO_2L1H_{3(132*)}$	2.76	2.63	2.75	2.65	3.45	3.30	2.92	1.75	1.78	178.2	356.0

(a) Arithmetic mean of the bond lengths in the equatorial plane of actinides;

(b) The sum of the bond angles in the equatorial plane of actinide atoms.

Table S10. Key geometrical parameters (bond length in Å, bond angle in degree) of NpO_2^+ and its complexes with H_4L1 ligand in MeOH.

Np^V	Np-N_i							Np-O^{yl}			T_A(b)
	N1	N2	N3	N1*	N2*	N3*	$\bar{d}$ (a)	O1	O2	∠O-Np-O	
NpO_2^+								1.76	1.76	180.0	
NpO_2L1^{3-}	2.68	3.04	3.04	2.68	2.85	2.85	2.85	1.81	1.81	179.5	360.7
$NpO_2L1H^{2-}{}_{(1)}$	3.25	3.08	2.76	2.51	2.76	3.07	2.90	1.80	1.81	175.7	360.4
$NpO_2L1H^{2-}{}_{(2)}$	2.67	3.68	3.42	2.58	2.54	2.54	2.91	1.82	1.82	175.8	360.6
$NpO_2L1H_2^{-}{}_{(23)}$	2.61	3.76	3.70	2.63	2.47	2.47	2.94	1.82	1.82	176.4	360.5
$NpO_2L1H_2^{-}{}_{(11*)}$	2.89	2.90	2.90	2.89	2.90	2.90	2.90	1.79	1.79	180.0	360.7
$NpO_2L1H_2^{-}{}_{(13)}$	3.25	3.91	3.66	2.53	2.44	2.54	3.06	1.81	1.82	177.8	351.6

$NpO_2L1H_2^{-}{}_{(12)}$	3.35	3.97	3.47	2.49	2.45	2.57	3.05	1.80	1.81	178.1	351.4
$NpO_2L1H_2^{-}{}_{(2*3)}$	2.49	2.97	3.37	2.75	3.03	2.73	2.89	1.80	1.81	178.0	359.4
$NpO_2L1H_2^{-}{}_{(22*)}$	2.60	2.86	3.18	2.60	2.86	3.18	2.88	1.80	1.80	180.0	361.3
$NpO_2L1H_{3(1*23)}$	3.59	4.17	3.69	2.55	2.45	2.58	3.17	1.79	1.84	177.1	339.1
$NpO_2L1H_{3(1*2*3)}$	2.40	2.63	3.72	4.06	3.71	2.61	3.19	1.79	1.82	178.2	342.1
$NpO_2L1H_{3(133*)}$	2.88	3.35	3.39	2.50	2.57	2.90	2.93	1.78	1.79	177.9	360.7
$NpO_2L1H_{3(232*)}$	2.64	3.71	3.61	2.54	2.50	2.68	2.94	1.81	1.80	179.3	361.2
$NpO_2L1H_{3(131*)}$	2.93	2.49	2.47	2.79	3.73	3.69	3.02	1.80	1.80	175.7	357.1
$NpO_2L1H_{3(132*)}$	3.28	2.63	2.62	2.51	3.62	3.88	3.09	1.78	1.79	177.6	345.0

[(a)] Arithmetic mean of the bond lengths in the equatorial plane of actinides;

[(b)] The sum of the bond angles in the equatorial plane of actinide atoms.

5. The population analysis of the complexes in methanol.

Table S11. The Mulliken atomic charges (q) and the Mulliken atomic spin densities (s) of key atoms and groups, and the Mayer atomic bond orders of the complexes $AnO_2L1^{2-/3-}$, $AnO_2L2^{0/-}$, and $AnO_2L3^{-/2-}$ in methanol.

	$q^{(a)}$				$s^{(a)}$		MBO[(b)]	
	Actinyl		N_i		Actinyl		An-O^{yl}	An-N_i
	An/O^{yl}1/O^{yl}2	Q_A^{tot}	N1/N2/N3*(O3)	Q_N^{tot}	An/ O^{yl}1/O^{yl}2	s^{tot}	O^{yl}1/O^{yl}2	
$L1^{4-}$				**-3.66**				
U^{VI}	2.55/-0.73/-0.76	**1.05**	-0.78/-0.64/-0.64	**-4.07**	-	**-**	1.21/1.19	0.22/0.25/0.26
Np^{VI}	2.43/-0.95/-0.95	**0.53**	-0.69/-0.60/-0.61	**-3.81**	2.21/-0.09/-0.09	**2.03**	0.97/0.97	0.18/0.21/0.20
Pu^{VI}	2.34/-0.90/-0.90	**0.55**	-0.69/-0.60/-0.60	**-3.77**	3.37/-0.16/-0.16	**3.04**	0.94/0.94	0.20/0.21/0.21
U^{V}	2.55/-1.06/-1.06	**0.43**	-0.76/-0.65/-0.63	**-4.06**	1.12/-0.05/-0.05	**1.02**	0.99/0.99	0.15/0.17/0.16
Np^{V}	2.38/-0.97/-0.96	**0.45**	-0.74/-0.62/-0.61	**-4.00**	2.22/-0.10/-0.10	**2.03**	0.99/0.99	0.20/0.18/0.21
Pu^{V}	2.29/-0.90/-0.90	**0.50**	-0.73/-0.59/-0.69	**-4.03**	3.35/-0.17/-0.17	**3.02**	1.03/1.03	0.21/0.14/0.21
$L2^{2-}$			[(c)]	**-2.65**				[(c)]
U^{VI}	2.57/-0.62/-0.62	**1.33**	-0.74/-0.79/-0.52	**-3.57**	-	**-**	1.45/1.45	0.19/0.23/0.15
Np^{VI}	2.37/-0.85/-0.85	**0.67**	-0.65/-0.68/-0.45	**-3.08**	2.21/-0.09/-0.09	**2.03**	1.27/1.27	0.13/0.13/0.08
Pu^{VI}	2.21/-0.78/-0.79	**0.64**	-0.64/-0.66/-0.44	**-3.00**	3.37/-0.16/-0.16	**3.04**	1.32/1.32	0.15/0.16/0.09
U^{V}	2.56/-0.66/-0.66	**1.24**	-0.80/-0.83/-0.53	**-3.80**	-0.01/0.00/0.00	**-0.01**	1.40/1.40	0.21/0.27/0.14
Np^{V}	2.38/-0.88/-0.89	**0.62**	-0.68/-0.73/-0.50	**-3.31**	2.21/-0.09/-0.09	**2.03**	1.22/1.22	0.15/0.16/0.09
Pu^{V}	2.23/-0.81/-0.82	**0.60**	-0.66/-0.71/-0.49	**-3.23**	3.37/-0.16/-0.16	**3.04**	1.27/1.27	0.17/0.18/0.09
$L3^{3-}$				**-3.30**				
U^{VI}	2.70/-0.75/-0.78	**1.17**	-0.68/-0.75/-0.61	**-4.09**	-	**-**	1.17/1.16	0.28/0.23/0.18

Np^{VI}	2.58/-0.97/-0.97	**0.65**	-0.62/-0.69/-0.56	**-3.74**	2.22/-0.09/-0.10	**2.03**	1.26/1.24	0.18/0.12/0.15
Pu^{VI}	2.26/-0.55/-0.60	**1.11**	-0.64/-0.71/-0.59	**-3.88**	2.35/-0.13/-0.12	**2.10**	0.95/0.94	0.20/0.14/0.15
U^{V}	2.71/-0.80/-0.85	**1.07**	-0.80/-0.77/-0.61	**-4.36**	0.16/-0.01/0.00	**0.15**	1.12/1.10	0.30/0.23/0.17
Np^{V}	2.56/-1.00/-1.01	**0.55**	-0.66/-0.72/-0.59	**-3.95**	2.22/-0.09/-0.10	**2.03**	0.91/0.88	0.22/0.17/0.16
Pu^{V}	2.46/-0.93/-0.97	**0.55**	0.65/-0.71/-0.59	**-3.89**	3.37/-0.16/-0.16	**3.05**	0.90/0.81	0.24/0.19/0.17

(a) The atomic charge q and spin density s are given in the format of An/O^{yl}1/O^{yl}2 for actinyl, and N1/N2/N3*(O3) for the coordinating atoms in the first coordination shell. The values at the equivalent positions of N1*/N2*/N3 are not shown for simplicity. The group charge and group spin density were calculated as: for actinyl, $Q_A^{tot} = q_{An}+q_{O1}+q_{O2}$; for ligands $L1^{4-}$ and $L3^{3-}$, $Q_N^{tot} = \sum_{i=1}^{6}(qN)_i$; for ligand $L2^{2-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N1*}+q_{N2*}+q_{O3}$; for $AnO_2L1^{2-/3-}$ and $AnO_2L3^{-/2-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N3}+q_{N1*}+q_{N2*}+q_{N3*}$; for $AnO_2L2^{0/-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N1*}+q_{N2*}+q_{O3}$.

(b) MBO is give in the format of An-O^{yl}1/An-O^{yl}2, and An-N1/An-N2/An-N3* for the bonds between actinides and ligands. The values for the equivalent bonds of An-$N1^{*}$/$N2^{*}$/N3 are not shown for simplicity.

(c) For the complexes with $L2^{2-}$ ligand, the values are given in the format of N1/N2/O3.

Table S12. The natural charges (*q'*) and the spin densities (*s'*) of key atoms and groups, and the Wiberg bond index (WBI) of the complexes $AnO_2L1^{2-/3-}$, $AnO_2L2^{0/-}$, and $AnO_2L3^{-/2-}$ in methanol.

	q'[(a)]				*s'*[(a)]		WBI[(b)]	
	Actinyl		N_i		Actinyl		An-O^{yl}	An-N_i
	An/O^{yl}1/O^{yl}2	Q_A^{tot}	N1/N2/N3*(O3)	Q_N^{tot}	An/O^{yl}1/O^{yl}2	s^{tot}	O^{yl}1/O^{yl}2	
$L1^{4-}$				**-3.58**				
U^{VI}	1.62/-0.58/-0.59	**0.45**	-0.56/-0.54/-0.54	**-3.26**	-	**-**	2.13/2.13	0.47/0.35/0.34
Np^{VI}	1.33/-0.71/-0.71	**-0.09**	-0.54/-0.54/-0.54	**-3.23**	2.18/-0.09/-0.09	**2.00**	1.95/1.95	0.36/0.29/0.29
Pu^{VI}	1.27/-0.65/-0.65	**-0.03**	-0.55/-0.54/-0.53	**-3.23**	3.32/-0.16/-0.16	**3.00**	1.96/1.96	0.34/0.27/0.27
U^{V}	1.45/-0.82/-0.82	**-0.18**	-0.56/-0.54/-0.54	**-3.28**	1.05/-0.04/-0.04	**0.97**	1.88/1.88	0.39/0.28/0.32
Np^{V}	1.36/-0.73/-0.73	**-0.09**	-0.57/-0.54/-0.55	**-3.31**	2.17/-0.09/-0.09	**1.99**	1.93/1.93	0.36/0.25/0.31
Pu^{V}	1.37/-0.66/-0.67	**0.04**	-0.58/-0.54/-0.55	**-3.39**	3.27/-0.15/-0.15	**2.97**	1.95/1.95	0.33/0.16/0.32
$L2^{2-}$			*(c)*	**-2.78**				*(c)*
U^{VI}	1.69/-0.55/-0.55	**0.59**	-0.57/-0.56/-0.49	**-2.75**	-	**-**	2.15/2.15	0.48/0.52/0.27
Np^{VI}	1.39/-0.67/-0.67	**0.05**	-0.55/-0.53/-0.47	**-2.63**	2.15/-0.09/-0.09	**1.97**	1.99/1.99	0.35/0.38/0.19
Pu^{VI}	1.29/-0.60/-0.60	**0.08**	-0.54/-0.52/-0.47	**-2.61**	3.29/-0.16/-0.16	**2.97**	2.01/2.01	0.34/0.37/0.19
U^{V}	1.64/-0.57/-0.57	**0.49**	-0.60/-0.57/-0.48	**-2.84**	-0.01/0.00/0.00	**-0.01**	2.13/2.13	0.51/0.54/0.27

Np^{V}	1.40/-0.69/-0.69	**0.01**	-0.56/-0.55/-0.50	**-2.73**	2.14/-0.09/-0.09	**1.96**	1.97/1.97	0.35/0.39/0.20
Pu^{V}	1.31/-0.63/-0.63	**0.05**	-0.56/-0.55/-0.50	**-2.71**	3.29/-0.16/-0.16	**2.97**	1.99/1.99	0.34/0.38/0.19
$L3^{3-}$				**-3.41**				
U^{VI}	1.46/-0.57/-0.57	**0.32**	-0.52/-0.52/-0.50	**-3.08**	-	**-**	2.13/2.13	0.46/0.52/0.37
Np^{VI}	1.21/-0.69/-0.69	**-0.17**	-0.54/-0.51/-0.48	**-3.04**	2.14/-0.08/-0.08	**1.98**	1.98/1.98	0.34/0.39/0.27
Pu^{VI}	1.17/-0.38/-0.39	**0.40**	-0.52/-0.51/-0.50	**-3.06**	2.30/-0.15/-0.15	**2.00**	2.18/2.17	0.42/0.51/0.34
U^{V}	1.44/-0.61/-0.62	**0.20**	-0.56/-0.53/-0.52	**-3.23**	0.17/-0.01/-0.01	**0.15**	2.09/2.09	0.51/0.51/0.31
Np^{V}	1.22/-0.71/-0.71	**-0.20**	-0.52/-0.53/-0.51	**-3.13**	2.14/-0.08/-0.08	**1.98**	1.97/1.96	0.35/0.39/0.26
Pu^{V}	1.14/-0.64/-0.65	**-0.15**	-0.52/-0.53/-0.51	**-3.12**	3.32/-0.16/-0.16	**3.00**	1.98/1.97	0.33/0.38/0.26

(a) The atomic charge q and spin density s are given in the format of An/O^{yl}1/O^{yl}2 for actinyl, and N1/N2/N3*(O3) for the coordinating atoms in the first coordination shell. The values at the equivalent positions of N1*/N2*/N3 are not shown for simplicity. The group charge and group spin density were calculated as: for actinyl, $Q_A^{tot} = q_{An}+q_{O1}+q_{O2}$; for ligands $L1^{4-}$ and $L3^{3-}$, $Q_N^{tot} = \sum_{i=1}^{6}(qN)_i$; for ligand $L2^{2-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N1*}+q_{N2*}+q_{O3}$; for $AnO_2L1^{2-/3-}$ and $AnO_2L3^{-/2-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N3}+q_{N1*}+q_{N2*}+q_{N3*}$; for $AnO_2L2^{0/-}$, $Q_N^{tot} = q_{N1}+q_{N2}+q_{N1*}+q_{N2*}+q_{O3}$.

(b) WBI is give in the format of An-O^{yl}1/An-O^{yl}2, and An-N1/An-N2/An-N3* for the bonds between actinides and ligands. The values for the equivalent bonds of An-$N1^{*}$/$N2^{*}$/N3 are not shown for simplicity.

(c) For the complexes with $L2^{2-}$ ligand, the values are given in the format of N1/N2/O3.

Table S13. The atomic natural charges (*q'*) and the spin densities (*s*) of key atoms and groups, and the Wiberg bond index (WBI) of the complexes $AnO_2H_2L1^{2-/3-}$ in methanol.

	q'[(a)]				*s*[(a)]		WBI[(b)]	
	Actinyl		N_i		Actinyl		An-O^{yl}	An-N_i
	An/O^{yl}1/O^{yl}2	Q_A^{tot}	N1/N2/N3/ N1*/N2*/N3*	Q_N^{tot}	An/O^{yl}1/O^{yl}2	s^{tot}	O^{yl}1/O^{yl}2	N1/N2/N3/ N1*/N2*/N3*
H_2L1^{2-}				**-3.40**				
U^{VI}	2.07/-0.59/-0.60	**0.89**	-0.57/-0.55/-0.52/ -0.60/-0.60/-0.60	**-3.44**	-	-	2.10/2.08	0.13/0.06/0.02/ 0.51/0.53/0.50
Np^{VI}	1.77/-0.70/-0.74	**0.33**	-0.53/-0.55/-0.53/ -0.59/-0.60/-0.59	**-3.38**	2.15/-0.09/-0.09	**1.97**	1.95/1.86	0.04/0.05/0.02/ 0.35/0.38/0.34
Pu^{VI}	1.64/-0.63/-0.67	**0.34**	-0.54/-0.54/-0.52/ -0.58/-0.58/-0.58	**-3.36**	3.29/-0.15/-0.14	**3.00**	1.97/1.88	0.05/0.05/0.02/ 0.34/0.38/0.33
U^{V}	1.91/-0.81/-0.84	**0.25**	-0.54/-0.55/-0.53/ -0.60/-0.60/-0.59	**-3.41**	1.07/-0.04/-0.04	**0.99**	1.87/1.78	0.04/0.05/0.02/ 0.40/0.41/0.38
$Np^{V)}$	1.73/-0.71/-0.74	**0.28**	-0.54/-0.55/-0.53/	**-3.43**	2.14/-0.09/-0.08	**1.97**	1.94/1.86	0.04/0.05/0.02/

			-0.61/-0.61/-0.59					0.37/0.38/0.37
Pu^{V}	1.61/-0.64/-0.67	**0.30**	-0.54/-0.55/-0.53/ -0.60/-0.60/-0.59	**-3.42**	3.28/-0.15/-0.15	**2.98**	1.96/1.89	0.05/0.05/0.02/ 0.36/0.36/0.36

6. The four quantities in the framework of AIM technique in the complexes

Table S14. The three quantities in the framework of AIM technique in the complexes of $AnO_2H_2L1^{0/-}$, $AnO_2L2^{0/-}$, $AnO_2L3^{-/2-}$ and $AnO_2L1^{2-/3-}$ in vacuum. The data are given in the format of U(VI)/Np(VI)/Pu(VI)/U(V)/Np(V)/Pu(V).

	ρ_b	$\nabla^2\rho_b$	$H_b(r)$
$AnO_2H_2L1_{13}^{0/-}$			
An-N1	0.031/0.020/0.020/0.018/0.018/-	0.088/0.078/0.076/0.069/0.070/-	-0.001/0.001/0.001/0.001/0.001/-
An-N2[(b)]	0.006/0.008/0.007/-/-/-	0.019/0.024/0.024/-/-/-	0.001/0.001/0.001/-/-/-
An-N3[(b)]	-/-/-/-/-/-	-/-/-/-/-/-	-/-/-/-/-/-
An-N1*	0.065/0.048/0.048/0.052/0.050/0.050	0.157/0.152/0.154/0.149/0.153/0.157	-0.011/-0.004/-0.004/-0.005/-0.005/-0.005
An-N2*	0.077/0.055/0.053/0.059/0.059/0.061	0.180/0.170/0.175/0.169/0.179/0.185	-0.016/-0.006/-0.005/-0.007/-0.007/-0.008
An-N3*	0.067/0.047/0.045/0.049/0.050/0.050	0.158/0.147/0.147/0.144/0.151/0.156	-0.012/-0.004/-0.003/-0.005/-0.004/-0.005
An-O^{yl}1	**0.331/0.302/0.312/0.283/0.295/0.307**	**0.152/0.171/0.189/0.178/0.184/0.201**	**-0.336/-0.276/-0.284/-0.253/-0.264/-0.274**
An-O^{yl}2	**0.323/0.285/0.295/0.261/0.280/0.291**	**0.169/0.206/0.221/0.226/0.215/0.228**	**-0.322/-0.248/-0.256/-0.217/-0.239/-0.248**
$AnO_2L2^{0/-(a)}$			
An-O3	0.031/0.028/0.027/0.0290.025/0.024	0.120/0.115/0.114/0.112/0.103/0.101	0.001/0.001/0.002/0.001/0.001/0.002
An-N1	0.053/0.042/0.040/0.054/0.039/0.038	0.138/0.136/0.134/0.138/0.124/0.121	-0.006/-0.002/-0.002/-0.006/-0.002/-0.001
An-N2	0.065/0.048/0.047/0.066/0.047/0.047	0.165/0.167/0.166/0.163/0.161/0.161	-0.011/-0.003/-0.003/-0.011/-0.003/-0.003
An-O^{yl}1	**0.327/0.291/0.303/0.323/0.287/0.298**	**0.168/0.202/0.210/0.173/0.210/0.217**	**-0.329/-0.257/-0.268/-0.320/-0.249-0.260**
$AnO_2L3^{-/2-(a)}$			
An-N1	0.043/0.032/0.040/0.052/0.033/0.031	0.113/0.109/0.116/0.129/0.110/0.108	-0.003/0.000/-0.002/-0.006/0.000/0.000
An-N2	0.057/0.046/0.056/0.055/0.044/0.043	0.148/0.150/0.157/0.143/0.143/0.148	-0.007/-0.003/-0.007/-0.006/-0.002/-0.002
An-N3	0.030/0.024/0.028/0.022/0.021/0.020	0.086/0.084/0.086/0.064/0.072/0.073	-0.001/0.001/0.000/0.000/0.001/0.001
An-O^{yl}1	**0.323/0.286/0.341/0.319/0.281/0.292**	**0.170/0.204/0.217/0.174/0.212/0.227**	**-0.321/-0.248/-0.331/-0.313/-0.240/-0.249**
$AnO_2L1^{2-/3-(a)}$			
An-N1	0.049/0.036/0.036/0.037/0.035/0.036	0.121/0.117/0.123/0.106/0.112/0.117	-0.005/-0.001/-0.001/-0.002/-0.001/-0.001
An-N2	0.026/0.022/0.021/0.022/0.021/0.021	0.069/0.073/0.074/0.066/0.068/0.066	0.000/0.001/0.001/0.000/0.001/0.001
An-N3	0.026/0.023/0.021/0.022/0.021/0.021	0.069/0.075/0.072/0.065/0.068/0.066	0.000/0.001/0.001/0.000/0.001/0.001
An-O^{yl}1	**0.330/0.288/0.298/0.270/0.286/0.286**	**0.163/0.199/0.216/0.216/0.204/0.269**	**-0.333/-0.253/-0.260/-0.231/-0.248/-0.237**

[(a)] The values for the equivalent bonds of An-N1*/N2*/N3* are not shown for simplicity.

[(b)] The "-" means that the BCP of An-N does not exist.

Table S15. The three quantities in the framework of AIM technique in the complexes of $AnO_2L1^{2-/3-}$, $AnO_2H_2L1^{0/-}$, $AnO_2L2^{0/-}$, and $AnO_2L3^{-/2-}$ in methanol. The data are

given in the format of U(VI)/Np(VI)/Pu(VI)/U(V)/Np(V)/Pu(V).

	ρ_b	$\nabla^2\rho_b$	$H_b(r)$
		$AnO_2H_2L1^{0/-}$	
An-N1[a]	0.019/-/-/-/-/-	0.059/-/-/-/-/-	0.000/-/-/-/-/-
An-N1*	0.068/0.053/0.052/0.057/0.056/0.054	0.161/0.165/0.167/0.155/0.160/0.163	-0.012/-0.005/-0.005/-0.007/-0.007/-0.006
An-N2[a]	-/-/-/-/-/-	-/-/-/-/-/-	-/-/-/-/-/-
An-N2*	0.081/0.063/0.061/0.066/0.067/0.065	0.185/0.187/0.194/0.175/0.186/0.193	-0.018/-0.009/-0.008/-0.011/-0.011/-0.010
An-N3[a]	-/-/-/-/-/-	-/-/-/-/-/-	-/-/-/-/-/-
An-N3*	0.070/0.050/0.049/0.054/0.054/0.053	0.163/0.154/0.154/0.149/0.162/0.163	-0.013/-0.004/-0.004/-0.006/-0.006/-0.006
An-O^{yl}1	**0.319/0.282/0.294/0.262/0.275/0.288**	**0.170/0.205/0.221/0.207/0.226/0.232**	**-0.313/-0.242/-0.252/-0.218/-0.229/-0.242**
An-O^{yl}2	**0.317/0.272/0.284/0.252/0.266/0.280**	**0.180/0.229/0.242/0.228/0.245/0.248**	**-0.309/-0.225/-0.236/-0.203/-0.215/-0.230**
		$AnO_2L2^{0/-}$	
An-O3	0.033/0.028/0.027/0.033/0.027/0.026	0.127/0.113/0.113/0.125/0.106/0.105	0.001/0.001/0.002/0.001/0.001/0.002
An-N1	0.056/0.044/0.043/0.058/0.041/0.040	0.142/0.137/0.136/0.146/0.127/0.125	-0.007/-0.003/-0.003/-0.008/-0.002/-0.002
An-N1*	0.056/0.041/0.041/0.058/0.041/0.040	0.142/0.128/0.131/0.147/0.124/0.126	-0.007/-0.002/-0.002/-0.008/-0.002/-0.002
An-N2	0.067/0.051/0.050/0.069/0.051/0.050	0.166/0.170/0.169/0.166/0.164/0.163	-0.011/-0.004/-0.004/-0.012/-0.004/-0.004
An-N2*	0.067/0.050/0.049/0.069/0.051/0.050	0.166/0.162/0.166/0/166/0.160/0.164	-0.011/-0.004/-0.004/-0.012/-0.004/-0.004
An-O^{yl}1	**0.319/0.277/0.289/0.3110.271/0.284**	**0.177/0.228/0.233/0.185/0.237/0.242**	**-0.313/-0.232/-0.244/-0.299/-0.223/-0.236**
An-O^{yl}2	**0.319/0.277/0.289/0.311/0.271/0.284**	**0.177/0.228/0.233/0.185/0.237/0.241**	**-0.313/-0.233/-0.245/-0.299/-0.223/-0.236**
		$AnO_2L3^{-/2-}$	
An-N1	0.043/0.034/0.039/0.052/0.034/0.031	0.112/0.110/0.112/0.131/0.116/0.103	-0.003/0.001/-0.002/-0.006/0.001/0.000
An-N1*	0.043/0.034/0.039/0.052/0.035/0.032	0.112/0.110/0.113/0.132/0.109/0.105	-0.003/0.001/-0.002/-0.006/0.001/0.000
An-N2	0.060/0.049/0.059/0.058/0.048/0.047	0.149/0.154/0.159/0.148/0.148/0.152	-0.008/-0.004/-0.008/-0.007/-0.004/-0.003
An-N2*	0.060/0.048/0.059/0.058/0.047/0.046	0.149/0.152/0.159/0.148/0.146/0.151	-0.008/-0.004/-0.008/-0.007/-0.003/-0.003
An-N3	0.034/0.026/0.031/0.025/0.024/0.024	0.092/0.085/0.093/0.072/0.078/0.080	-0.001/0.000/0.001/0.000/0.000/0.001
An-N3*	0.034/0.026/0.031/0.026/0.024/0.024	0.092/0.085/0.093/0.073/0.079/0.081	-0.001/0.000/0.001/0.000/0.000/0.001
An-O^{yl}1	**0.313/0.270/0.333/0.300/0.267/0.277**	**0.180/0.231/0.226/0.192/0.237/0.251**	**-0.303/-0.222/-0.317/-0.279/-0.216/-0.224**
An-O^{yl}2	**0.311/0.268/0.331/0.297/0.264/0.275**	**0.181/0.234/0.226/0.193/0.241/0.254**	**-0.299/-0.218/-0.313/-0.275/-0.211/-0.220**
		$AnO_2L1^{2-/3-}$	
An-N1	0.052/0.040/0.039/0.042/0.040/0.039	0.125/0.124/0.126/0.115/0.119/0.116	-0.006/-0.002/-0.002/-0.002/-0.002/-0.002
An-N1*	0.052/0.040/0.039/0.042/0.040/0.039	0.125/0.125/0.126/0.115/0.119/0.118	-0.006/-0.002/0.001/-0.002/-0.002/-0.002
An-N2	0.029/0.023/0.023/0.021/0.018/0.011	0.073/0.075/0.074/0.061/0.056/0.033	0.001/0.000/0.001/0.000/0.001/0.001
An-N2*	0.027/0.024/0.022/0.026/0.027/0.041	0.070/0.077/0.073/0.078/0.083/0.123	0.001/0.000/0.001/0.000/0.000/-0.002
An-N3	0.030/0.023/0.022/0.021/0.018/0.011	0.075/0.076/0.073/0.061/0.056/0.033/	0.001/0.000/0.001/0.000/0.001/0.001
An-N3*	0.027/0.023/0.023/0.026/0.027/0.040	0.070/0.076/0.074/0.078/0.083/0.122	0.001/0.000/0.001/0.000/0.000/-0.002
An-O^{yl}1	**0.319/0.271/0.284/0.256/0.270/0.280**	**0.172/0.233/0.237/0.219/0.229/0.245**	**-0.312/-0.223/-0.225/-0.208/-0.221/-0.230**
An-O^{yl}2	**0.318/0.271/0.284/0.256/0.270/0.280**	**0.171/0.234/0.237/0.219/0.229/0.245**	**-0.312/-0.222/-0.236/-0.209/-0.221/-0.230**

[a] The "-" means that the BCP of An-N does not exist.

Table S16. The value of DI in the framework of AIM technique in the complexes of $AnO_2H_2L1^{0/-}$, $AnO_2L2^{0/-}$, $AnO_2L3^{-/2-}$ and $AnO_2L1^{2-/3-}$ in vacuum and in methanol. The data are

given in the format of U(VI)/Np(VI)/Pu(VI)/U(V)/Np(V)/Pu(V).

	Vacuum	MeOH
$AnO_2H_2L1^{0/-}$	DI	DI
An-N1	0.639/0.445/0.444/0.395/0.390/0.368	0.458/0.251/0.276/0.223/0.252/0.282
An-N1*	1.121/0.955/0.958/0.995/0.990/0.993	1.138/1.066/1.000/1.043/1.038/1.030
An-N2	0.341/0.372/0.378/0.324/0.312/0.293	0.231/0.197/0.219/0.181/0.197/0.219
An-N2*	1.173/1.012/0.943/1.035/1.038 /1.044	1.188/1.066/1.059/1.087 /1.086 /1.079
An-N3	0.143/0.171/0.172/0.155/0.146/0.140	0.108/0.135/0.142/0.123/0.123/0.126
An-N3*	1.116/0.949/1.008/0.981/0.984/0.990	1.135/0.988/0.982/1.026/1.032/1.028
An-O^{yl}1	**2.917/2.869/2.875/2.845/2.855/2.861**	**2.879/2.814/2.825/2.776/2.797/2.812**
An-O^{yl}2	**2.887/2.781/2.794/2.726/2.766/2.781**	**2.860/2.721/2.745/2.678/2.717/2.748**
$AnO_2L2^{0/-}$	DI	DI
An-O	0.770/0.708/0.709/0.754/0.696/0.694	0.795/0.722/0.723/0.792/0.724/0.724
An-N1	1.025/0.909/0.907/1.038/0.893/0.890	1.054/0.947/0.945/1.087/0.940/0.937
An-N1*	1.023/0.897/0.899/1.041/0.888/0.890	1.053/0.921/0.922/1.091/0.938/0.938
An-N2	1.081/0.938/0.937/1.097/0.9470.947	1.105/0.984/0.982/1.129/0.994/0.991
An-N2*	1.080/0.937/0.936/1.097/0.949/0.948	1.103/0.972/0.967/1.130/0.999/0.993
An-O^{yl}1	**2.904/2.841/2.851/2.893/2.832/2.843**	**2.882/2.804/2.817/2.864//2.791/2.806**
An-O^{yl}2	**2.904/2.840/2.850/2.894/2.832/2.843**	**2.883/2.805/2.818/2.865/2.792/2.806**
$AnO_2L3^{-/2-}$	DI	DI
An-N1	0.926/0.811/0.913/1.028/0.832/0.821	0.948/0.855/0.925/1.051/0.867/0.851
An-N1*	0.926/0.812/0.913/1.027/0.832/0.822	0.947/0.853/0.924/1.048/0.871/0.855
An-N2	1.007/0.904/1.022/0.996/0.898/0.904	1.043/0.952/1.058/1.039/0.854/0.955
An-N2*	1.008/0.906/1.023/0.996/0.900/0.903	1.041/0.947/1.055/1.040/0.951/0.953
An-N3	0.766/0.688/0.756/0.669/0.653/0.658	0.811/0.727/0.801/0.732/0.716/0.722
An-N3*	0.768/0.691/0.759/0.671/0.654/0.656	0.809/0.724/0.799/0.733/0.713/0.719
An-O^{yl}1	**2.894/2.826/2.902/2.885/2.822/2.830**	**2.867/2.876/2.881/2.841/2.777/2.789**
An-O^{yl}2	**2.895/2.829/2.899/2.886/2.820/2.829**	**2.866/2.784/2.877/2.839/2.773/2.785**
$AnO_2L1^{2-/3-}$	DI	DI
An-N1	0.989/0.838/0.855/0.842/0.850/0.863	1.032/0.909/0.909/0.932/0.919/0.911
An-N1*	0.989/0.850/0.842/0.843/0.850/0.863	1.028/0.915/0.904/0.932/0.920/0.915
An-N2	0.787/0.719/0.720/0.704/0.707/0.695	0.839/0.763/0.761/0.729/0.695/0.543
An-N2*	0.783/0.724/0.714/0.712/0.707/0.693	0.816/0.768/0.760/0.804/0.816/0.929
An-N3	0.787/0.724/0.714/0.700/0.707/0.694	0.847/0.765/0.760/0.726/0.695/0.542
An-N3*	0.783/0.719/0.720/0.711/0.707/0.693	0.826/0.768/0.761/0.800/0.817/0.927
An-O^{yl}1	**2.911/2.838/2.845/2.813/2.833/2.823**	**2.884/2.793/2.808/2.766/2.790/2.801**
An-O^{yl}2	**2.911/2.837/2.846/2.813/2.833/2.823**	**2.883/2.792/2.808/2.767/2.790/2.801**

7. The NICS values of the ligands and their complexation states with $AnO_2^{2+/+}$ (An = U, Np, Pu) in methanol

Table S17. The NICS values of the three ligands in their deprotonated free states (H_2L1^{2-}, $L2^{2-}$, $L3^{3-}$ and $L1^{4-}$,) and their complexation states with $AnO_2^{2+/+}$ (An = U, Np, Pu) in methanol. The definition of the rings please see Scheme 1.

NICS(0)		A Ring	B Ring	C Ring	A* Ring	B* Ring	C* Ring	G Ring
H_2L1^{2-}	**H_2L1^{2-}**	**-8.55**	**-2.67**	**5.16**	**-7.79**	**-2.85**	**-6.55**	**4.61**
	U^{VI}	-13.68	2.18	-11.78	8.43	7.10	7.17	-15.96
	U^{V}	-10.17	0.41	-7.58	-4.66	2.93	-3.62	-2.31
	Np^{V}	-8.78	-1.50	-6.92	-8.89	-2.30	-7.72	2.52
	Pu^{V}	-8.56	-1.78	-6.90	-8.89	-2.81	-7.80	2.84
$L2^{4-}$	**$L2^{2-}$**	**-3.10**	**-1.67**	**-10.02**	**-3.14**	**-1.28**		**-5.89**
	U^{VI}	-3.89	-16.53	-7.79	-4.17	-15.89		-1.28
	Np^{V}	-5.88	-4.12	-14.64	-5.95	-3.98		-11.97
	Pu^{V}	-5.57	-4.02	-14.05	-5.68	-3.80		-11.02
$L3^{3-}$	**$L3^{3-}$**	**-4.12**	**-7.17**	**-10.66**	**-4.09**	**-7.25**	**-**	**1.23**
	U^{VI}	5.99	-7.24	-0.58	6.01	-7.25	-	2.80
	Pu^{VI}	5.87	-7.44	-1.15	5.87	-7.44	-	2.29
	Np^{V}	1.20	-8.03	-0.97	1.24	-8.35	-	5.84
	Pu^{V}	-4.65	-7.41	-10.82	-4.72	-7.51		-0.41
$L1^{4-}$	**$L1^{4-}$**	**-8.63**	**-4.19**	**-4.20**	**-8.63**	**-4.19**	**-4.20**	**2.93**
	U^{VI}	-8.12	-3.87	-3.76	-8.04	-3.81	-3.94	2.29
	U^{V}	-8.43	-4.18	-4.24	-8.42	-4.18	-4.50	2.84
	Np^{V}	-8.32	-4.04	-4.30	-8.32	-4.13	-4.17	3.18
	Pu^{V}	-8.43	-4.18	-4.47	-8.42	-4.31	-4.49	3.08
NICS(1)		A Ring	B Ring	C Ring	A* Ring	B* Ring	C* Ring	G Ring
H_2L1^{2-}	**H_2L1^{2-}**	**-10.46**	**-5.34**	**4.19**	**-12.03**	**-6.45**	**-7.65**	**3.97**
	U^{VI}	-21.55	-2.99	-17.63	-0.55	2.15	0.83	-7.27
	U^{V}	-14.95	-2.85	-9.34	-9.76	1.29	-4.32	0.82
	Np^{V}	-13.20	-4.30	-8.36	-11.43	-3.68	-7.08	3.66
	Pu^{V}	-13.22	-4.44	-8.66	-11.02	-4.46	-7.16	3.72
$L2^{2-}$	**$L2^{2-}$**	**-5.10**	**-7.08**	**-9.07**	**-5.20**	**-6.85**		**-5.70**
	U^{VI}	-19.11	-11.99	-11.04	-17.01	-11.64		0.61
	Np^{V}	-8.05	-9.01	-13.30	-8.13	-8.99		-10.14
	Pu^{V}	-7.84	-8.88	-12.90	-8.03	-8.80		-9.45
$L3^{3-}$	**$L3^{3-}$**	**-6.84**	**-15.18**	**-9.58**	**-7.17**	**-15.31**	**-**	**1.34**
	U^{VI}	-3.38	-11.72	1.30	-3.30	-13.24	-	8.23
	Pu^{VI}	-3.52	-12.01	0.62	-3.43	-13.50	-	7.33
	Np^{V}	-4.58	-11.09	1.44	-4.27	-12.74	-	9.92
	Pu^{V}	-7.57	-11.61	-10.84	-7.50	-13.02		0.25
$L1^{4-}$	**$L1^{4-}$**	**-12.60**	**-6.44**	**-6.44**	**-12.59**	**-6.44**	**-6.44**	**2.37**
	U^{VI}	-8.08	-5.21	-5.03	-10.95	-6.37	-6.91	3.20

U^V	-9.77	-5.58	-5.65	-10.23	-5.72	-6.02	3.03
Np^V	-10.04	-5.65	-5.82	-9.95	-5.69	-5.72	3.21
Pu^V	-10.17	-6.41	-6.62	-10.20	-5.50	-5.64	3.06

8. The population analysis of the bare $AnO_2^{2+/+}$ and $AnO_2(H_2O)_5^{2+/+}$ in vacuum and in methanol.

Table S18. The natural charges (*q'*) and the spin densities (*s*) of key atoms in bare $AnO_2^{2+/+}$, and the Mayer atomic bond orders (MBO) and the Wiberg bond index (WBI) of the bare $AnO_2^{2+/+}$ in vacuum and in MeOH.

	q'		***s***		**MBO**	**WBI**
	An	**O1/O2**	**An**	**O1/O2**	**An-**	**An-**
Vacuu						
$\mathbf{UO_2^{2+}}$	2.8	-0.40/-	-	-	2.02/2.02	2.23/2.23
$\mathbf{NpO_2^{2}}$	2.6	-0.32/-	1.1	-0.06/-	2.02/2.02	2.26/2.26
$\mathbf{PuO_2^{2}}$	2.4	-0.24/-	2.2	-0.14/-	2.10/2.10	2.27/2.27
$\mathbf{UO_2^{+}}$	2.3	-0.65/-	1.0	-0.04/-	1.92/1.92	2.01/2.01
$\mathbf{NpO_2^{+}}$	2.1	-0.58/-	2.1	-0.09/-	1.95/1.95	2.05/2.05
$\mathbf{PuO_2^{+}}$	2.0	-0.52/-	3.3	-0.14/-	2.04/2.04	2.06/2.06
MeOH						
$\mathbf{UO_2^{2+}}$	3.2	-0.62/-	-	-	1.82/1.82	2.00/2.00
$\mathbf{NpO_2^{2}}$	3.0	-0.51/-	1.1	-0.06/-	1.85/1.85	2.06/2.06
$\mathbf{PuO_2^{2}}$	2.8	-0.43/-	2.2	-0.14/-	1.94/1.94	2.09/2.09
$\mathbf{UO_2^{+}}$	2.7	-0.88/-	1.0	-0.04/-	1.63/1.63	1.74/1.74
$\mathbf{NpO_2^{+}}$	2.5	-0.79/-	2.1	-0.09/-	1.70/1.70	1.81/1.81
$\mathbf{PuO_2^{+}}$	2.4	-0.71/-	3.3	-0.15/-	1.79/1.79	1.85/1.85

Table S19 The bond length (*d*), the Mulliken atomic charges (*q*), the natural charges (*q'*), and the spin densities (*s*) of key atoms in bare $AnO_2^{2+/+}$, and the Wiberg bond index (WBI) of the $AnO_2(H_2O)_5^{2+/+}$ in vacuum and in MeOH.

	d		***q***			***q'***			***s***		**WBI**	
	An-O^{yl}	**An-O^{w}**	**An**	**O^{yl}**	Q_A^{tot}	**An**	**O^{yl}**	Q_A^{tot}	**An**	**O^{yl}**	**An-O^{yl}**	**An-O^{w}**
Vacuum												
$\mathbf{U^{VI}}$	1.79	2.55	1.94	-0.07	1.80	1.88	-0.47	0.93	-	-	2.25	0.39
$\mathbf{Np^{VI}}$	1.71	2.46	1.72	0.04	1.81	1.63	-0.35	0.92	1.09	-0.05	2.30	0.39
$\mathbf{Pu^{VI}}$	1.69	2.44	1.54	0.14	1.82	1.45	-0.26	0.93	2.24	-0.12	2.32	0.39
$\mathbf{U^{V}}$	1.73	2.47	1.94	-0.38	1.17	1.61	-0.70	0.21	1.05	-0.04	2.03	0.30
$\mathbf{Np^{V}}$	1.76	2.54	1.74	-0.29	1.19	1.42	-0.60	0.22	2.15	-0.09	2.09	0.29
$\mathbf{Pu^{V}}$	1.75	2.55	1.79	-0.26	1.26	1.40	-0.54	0.32	3.28	-0.14	2.09	0.25
MeOH												
$\mathbf{U^{VI}}$	1.74	2.44	2.13	-0.15	1.83	1.87	-0.50	0.87	-	-	2.22	0.42
$\mathbf{Np^{VI}}$	1.71	2.43	1.89	-0.03	1.83	1.61	-0.38	0.85	1.09	-0.06	2.28	0.42
$\mathbf{Pu^{VI}}$	1.69	2.41	1.69	0.08	1.85	1.43	-0.28	0.86	2.24	-0.12	2.30	0.41
$\mathbf{U^{V}}$	1.81	2.53	2.22	-0.54	1.13	1.63	-0.75	0.13	1.05	-0.04	1.97	0.33

Np^V	1.78	2.52	2.02	-0.43	1.14	1.45	-0.63	0.16	2.16	-0.08	2.04	0.32
Pu^V	1.77	2.53	1.99	-0.42	1.14	1.42	-0.58	0.26	3.28	-0.15	2.05	0.27

9. The integration accuracy and the convergence criteria in our calculations.

The integration accuracy in our calculations is default FineGrid, which is a pruned (75,302) grid, having 75 radial shells and 302 angular points per shell, resulting in about 7000 points per atom. The optimization convergence criteria is 0.00045 au for maximum force, 0.0003 au for RMS force, 0.0018 au for maximum displacement, and 0.0012 au for RMS displacement.

10. Coordinates and energies of stationary points (in vacuum)

H_4L1

E (CAM-B3LYP) = -1800.96504298 Hartree
Zero-point correction= 0.733461 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1800.231582 Hartree
Sum of electronic and thermal Enthalpies= -1800.186918 Hartree
Sum of electronic and thermal Free Energies= -1800.306173 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-0.263661	-2.577600	-0.433241
2	7	2.597929	-1.673887	-0.029015
3	7	2.801597	1.153092	0.127633
4	7	0.263608	2.577524	0.433131
5	7	-2.597913	1.673969	0.028770
6	7	-2.801547	-1.153177	-0.127710
7	6	-1.446108	-3.146012	-0.031111
8	6	-1.135056	-4.299768	0.673735
9	6	0.281442	-4.424606	0.680803
10	6	0.796234	-3.347296	-0.024099
11	6	2.179422	-2.953021	-0.234257
12	6	3.298823	-3.724584	-0.553724
13	6	4.422827	-2.873653	-0.494639
14	6	3.962769	-1.595110	-0.167974
15	6	4.682663	-0.390981	0.055758
16	1	5.764607	-0.483907	0.073387
17	6	4.162336	0.853548	0.249411
18	6	4.915350	2.069747	0.506119
19	6	4.008492	3.086166	0.511724
20	6	2.715635	2.459620	0.232147
21	6	1.446070	3.145946	0.031021
22	6	1.134998	4.299820	-0.673686
23	6	-0.281497	4.424729	-0.680601
24	6	-0.796264	3.347344	0.024171
25	6	-2.179434	2.953052	0.234353
26	6	-3.298789	3.724506	0.554127
27	6	-4.422800	2.873576	0.494938

28	6	-3.962719	1.595105	0.167876
29	6	-2.715656	-2.459693	-0.232299
30	6	-4.008467	-3.086167	-0.512040
31	6	-4.915292	-2.069768	-0.506448
32	6	-4.162293	-0.853596	-0.249617
33	6	-4.682630	0.390947	-0.055942
34	1	-5.764591	0.483899	-0.073588
35	6	5.835033	-3.281883	-0.768725
36	1	5.950908	-3.648777	-1.795469
37	1	6.535298	-2.452908	-0.639244
38	1	6.153052	-4.092371	-0.103298
39	6	3.315431	-5.166383	-0.958414
40	1	3.740304	-5.816021	-0.183913
41	1	2.305977	-5.524952	-1.172786
42	1	3.918775	-5.309096	-1.861956
43	6	1.059180	-5.462758	1.428584
44	1	1.082895	-6.426983	0.907099
45	1	2.092738	-5.144230	1.582350
46	1	0.618508	-5.644541	2.414671
47	6	-2.072663	-5.185610	1.436011
48	1	-3.022777	-4.685860	1.634759
49	1	-2.290354	-6.121540	0.908264
50	1	-1.640085	-5.459264	2.404007
51	6	-4.251831	-4.526237	-0.848541
52	1	-3.330856	-5.008385	-1.186215
53	1	-4.630062	-5.104875	0.001139
54	1	-4.988492	-4.616886	-1.653285
55	6	-6.390587	-2.146184	-0.736029
56	1	-6.950732	-1.964983	0.189276
57	1	-6.725036	-1.404238	-1.468586
58	1	-6.683256	-3.132990	-1.103583
59	6	-3.315447	5.166232	0.959062
60	1	-2.306011	5.524811	1.173505
61	1	-3.740339	5.815976	0.184659
62	1	-3.918807	5.308777	1.862622
63	6	-1.059258	5.463039	-1.428118
64	1	-2.092924	5.144730	-1.581564
65	1	-1.082583	6.427263	-0.906611
66	1	-0.618879	5.644749	-2.414353
67	6	2.072546	5.185657	-1.436072
68	1	2.290363	6.121569	-0.908332
69	1	3.022627	4.685865	-1.634951
70	1	1.639840	5.459336	-2.403999
71	6	6.390687	2.146388	0.735274
72	1	6.726333	1.400791	1.463515
73	1	6.950496	1.971009	-0.191359
74	1	6.682524	3.131469	1.108135
75	6	4.251877	4.526243	0.848220
76	1	4.629872	5.104951	-0.001525
77	1	3.330959	5.008331	1.186180
78	1	4.988778	4.616844	1.652763
79	6	-5.835021	3.281624	0.769299
80	1	-6.153130	4.092435	0.104301
81	1	-6.535240	2.452660	0.639433

82	1	-5.950842	3.647976	1.796244
83	1	-0.208312	-1.747777	-1.000652
84	1	2.048022	-0.848817	0.184484
85	1	0.208284	1.747680	1.000530
86	1	-2.047964	0.848951	-0.184803

H_2L2

E (CAM-B3LYP) = -1689.25529310 Hartree
Zero-point correction= 0.694317 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1688.560976 Hartree
Sum of electronic and thermal Enthalpies= -1688.520329 Hartree
Sum of electronic and thermal Free Energies= -1688.634331 Hartree

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Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	1.306190	1.829780	-0.160228
2	7	-1.572819	1.485033	-0.170842
3	7	-2.599219	-1.330761	0.003214
4	8	0.298221	-3.036710	-0.175068
5	7	2.785560	-0.733628	-0.387423
6	6	-0.985036	2.663732	-0.298192
7	6	-1.899360	3.691161	-0.801499
8	6	-3.108867	3.074974	-0.913308
9	6	-2.895709	1.696003	-0.504806
10	6	0.412857	2.842600	0.006347
11	6	1.117729	3.957799	0.506523
12	6	2.465554	3.594548	0.579645
13	6	2.566501	2.256224	0.154506
14	6	-1.562590	5.075253	-1.268246
15	1	-1.764587	5.845526	-0.516547
16	1	-0.508596	5.154191	-1.544377
17	1	-2.154426	5.330556	-2.153284
18	6	0.554667	5.248134	1.025666
19	1	0.666222	6.078369	0.319746
20	1	-0.506226	5.152799	1.262937
21	1	1.067632	5.538804	1.947636
22	6	-4.404184	3.670474	-1.374109
23	6	-5.239409	4.246490	-0.222636
24	1	-4.993732	2.919021	-1.910989
25	1	-4.200551	4.466542	-2.099349
26	1	-6.176731	4.674425	-0.592469
27	1	-5.483857	3.472180	0.511235
28	1	-4.688495	5.033453	0.301103
29	6	3.590889	4.436388	1.103800
30	6	3.880533	4.191845	2.590508
31	1	3.354637	5.494335	0.948120
32	1	4.501703	4.245675	0.524197
33	1	4.155683	3.147427	2.765250
34	1	4.700410	4.826598	2.941857
35	1	2.998816	4.405459	3.202698
36	6	-3.879589	0.747362	-0.418951
37	1	-4.893560	1.084398	-0.609171
38	6	-3.770597	-0.620420	-0.113406

39	6	-4.840189	-1.520020	0.079964
40	6	-4.290631	-2.775639	0.315759
41	6	-2.880272	-2.643113	0.243240
42	6	-1.998542	-3.752726	0.298640
43	1	-2.523182	-4.683114	0.484351
44	6	-0.676493	-3.974231	0.075533
45	6	-0.084852	-5.277880	-0.008420
46	6	1.208584	-5.116625	-0.347620
47	1	-0.628589	-6.197955	0.154126
48	1	1.959279	-5.876761	-0.512180
49	6	1.473069	-3.706145	-0.428728
50	6	2.712298	-3.195371	-0.657454
51	1	3.415421	-3.999945	-0.845124
52	6	3.341111	-1.915861	-0.599905
53	6	4.810376	-1.833770	-0.689166
54	6	5.118563	-0.531932	-0.470795
55	6	3.734602	1.482759	0.011754
56	6	3.844198	0.150128	-0.280962
57	1	4.663915	2.027307	0.149674
58	6	6.463146	0.121486	-0.422487
59	1	6.537472	0.945472	-1.140641
60	1	6.672967	0.537500	0.569912
61	1	7.260740	-0.589200	-0.652436
62	6	5.755799	-2.977317	-0.913046
63	6	6.081660	-3.756646	0.368055
64	1	6.687874	-2.593736	-1.341773
65	1	5.349618	-3.663597	-1.665727
66	1	6.766947	-4.585492	0.162316
67	1	6.550952	-3.101681	1.108347
68	1	5.175916	-4.168349	0.823891
69	6	-5.039117	-4.042946	0.609762
70	6	-5.128693	-4.356821	2.108542
71	1	-4.576863	-4.887935	0.086730
72	1	-6.051353	-3.965997	0.199892
73	1	-5.688173	-5.281116	2.285093
74	1	-4.132421	-4.471854	2.546698
75	1	-5.631542	-3.546593	2.645229
76	6	-6.292459	-1.155985	0.056899
77	1	-6.916567	-2.030001	-0.145284
78	1	-6.621306	-0.735771	1.014433
79	1	-6.513516	-0.414554	-0.716585
80	1	-1.688418	-0.890182	-0.058872
81	1	1.099433	0.881031	-0.451610

H_3L3

E (CAM-B3LYP) = -1991.80783871 Hartree
Zero-point correction= 0.796283 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1991.011556 Hartree
Sum of electronic and thermal Enthalpies= -1990.963563 Hartree
Sum of electronic and thermal Free Energies= -1991.092942 Hartree

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Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z

1	7	-2.742360	-1.382942	-0.233552
2	7	-0.044115	-2.532060	-0.072409
3	7	2.460291	-1.470105	-0.366758
4	6	-4.543938	0.130962	-0.911164
5	6	-3.593244	-3.397772	-0.680847
6	6	-2.478557	-2.716280	-0.182098
7	6	-1.185461	-3.198005	0.271308
8	6	-0.822117	-4.255664	1.101554
9	6	0.590381	-4.213048	1.242170
10	6	1.042148	-3.127610	0.502861
11	6	2.347582	-2.538778	0.319988
12	6	3.686223	-0.835426	-0.567974
13	6	4.881474	-1.538932	-0.790214
14	6	6.076379	-0.875389	-1.005480
15	6	-3.706616	-4.874601	-0.906122
16	6	-1.747180	-5.213346	1.789756
17	6	1.424550	-5.118799	2.101511
18	6	1.542854	-4.630258	3.550884
19	1	2.144486	-5.319981	4.151642
20	1	2.013118	-3.642894	3.590242
21	1	0.557932	-4.542776	4.019796
22	8	7.266949	-1.476960	-1.255309
23	6	7.292061	-2.883563	-1.313122
24	1	0.992799	-6.125968	2.092259
25	1	-4.274970	-5.381070	-0.117313
26	1	6.987122	-3.332667	-0.359309
27	1	-2.718398	-5.339701	-0.947955
28	1	-4.213780	-5.086610	-1.853350
29	1	-1.442732	-5.378118	2.828175
30	1	-1.772974	-6.195102	1.301896
31	1	2.428343	-5.219379	1.673438
32	1	3.198514	-3.015537	0.822732
33	1	4.844057	-2.620509	-0.827031
34	1	-2.769142	-4.826792	1.804523
35	1	8.325566	-3.159284	-1.525058
36	1	6.644396	-3.266917	-2.111580
37	1	-5.559697	0.170380	-1.292950
38	7	-2.622753	1.414774	-0.158361
39	7	0.032137	2.419400	0.033764
40	7	2.501301	1.236810	-0.343973
41	6	-3.924949	1.319578	-0.647236
42	6	-4.481549	2.650950	-0.827646
43	6	-3.509381	3.526457	-0.439256
44	6	-2.378019	2.700105	-0.025842
45	6	-1.058143	3.146163	0.404218
46	6	-0.612462	4.184070	1.224656
47	6	0.796477	4.054077	1.333441
48	6	1.165014	2.944859	0.578462
49	6	2.435861	2.294161	0.366432
50	6	3.706711	0.565868	-0.557609
51	6	4.923276	1.234701	-0.771624

52	6	6.097454	0.537754	-0.996304
53	6	-5.857573	2.964677	-1.329580
54	1	-6.162626	2.220442	-2.074093
55	1	-5.844207	3.927051	-1.853357
56	6	-6.903126	3.018952	-0.207572
57	1	-7.896016	3.248602	-0.607153
58	1	-6.645050	3.787446	0.527150
59	1	-6.960414	2.062513	0.321123
60	6	-3.543606	5.020916	-0.525855
61	6	-1.448751	5.180125	1.970390
62	6	1.711997	4.948917	2.115742
63	6	1.987782	6.287933	1.421651
64	1	2.651157	6.915758	2.025386
65	1	2.459359	6.130066	0.446767
66	1	1.059401	6.842232	1.253265
67	8	7.305521	1.106262	-1.238594
68	6	7.373752	2.512200	-1.276703
69	1	1.277222	5.141318	3.104479
70	1	-2.546545	5.425037	-0.721918
71	1	6.738275	2.926383	-2.069498
72	1	-3.909335	5.490759	0.393843
73	1	-4.201140	5.347642	-1.337409
74	1	-1.024990	5.371306	2.961746
75	1	-2.466996	4.813138	2.118427
76	1	2.662178	4.437016	2.303252
77	1	3.311943	2.719394	0.872065
78	1	4.919394	2.317247	-0.794383
79	1	-1.516575	6.147169	1.458781
80	1	8.415276	2.758945	-1.485038
81	1	7.082543	2.956896	-0.316598
82	6	-4.000110	-1.169211	-0.741312
83	6	-4.553922	-2.424040	-1.027080
84	6	-5.914682	-2.690900	-1.596373
85	1	-5.837719	-3.460572	-2.374198
86	1	-6.293034	-1.794939	-2.099877
87	6	-6.928874	-3.146271	-0.539872
88	1	-7.905577	-3.344259	-0.992822
89	1	-6.594610	-4.062242	-0.043431
90	1	-7.057974	-2.380315	0.230930
91	1	-2.173226	-0.601581	0.083119
92	1	0.045498	-1.731334	-0.680010
93	1	0.019573	1.583066	-0.529308

UO_2L1^{2-}

E (CAM-B3LYP) = -2426.14872368 Hartree
Zero-point correction= 0.688535 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2425.460189Hartree
Sum of electronic and thermal Enthalpies= -2425.412810 Hartree
Sum of electronic and thermal Free Energies= -2425.539703 Hartree

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Center Atomic Coordinates(Angstroms)

Number	Number	X	Y	Z
1	6	-3.392124	1.085297	0.072137
2	6	-4.649270	0.707232	0.559236
3	7	-2.611204	0.000521	-0.179963
4	6	-4.649491	-0.704130	0.560867
5	6	-3.392470	-1.083560	0.074500
6	6	-2.805540	-2.379912	-0.126692
7	6	-3.446126	-3.620820	-0.456821
8	7	-1.483455	-2.501116	-0.015621
9	6	-2.436863	-4.558474	-0.469554
10	6	-1.227437	-3.851976	-0.186678
11	6	0.000104	-4.454703	-0.000134
12	1	0.000132	-5.542044	-0.000161
13	6	1.227596	-3.851947	0.186466
14	6	2.437040	-4.558433	0.469348
15	7	1.483581	-2.501055	0.015567
16	6	3.446280	-3.620770	0.456699
17	6	2.805645	-2.379816	0.126732
18	6	3.392552	-1.083432	-0.074274
19	6	4.649656	-0.703926	-0.560361
20	7	2.611183	0.000608	0.180114
21	6	4.649349	0.707433	-0.558718
22	6	3.392097	1.085425	-0.071815
23	6	2.804871	2.381580	0.130633
24	6	3.445122	3.621999	0.463479
25	7	1.483253	2.503138	0.016764
26	6	2.436055	4.559889	0.474833
27	6	1.227096	3.853809	0.188578
28	6	-2.804990	2.381454	-0.130523
29	6	-3.445359	3.621831	-0.463395
30	7	-1.483359	2.503040	-0.017025
31	6	-2.436288	4.559695	-0.475298
32	6	-1.227249	3.853681	-0.189179
33	6	-0.000100	4.456596	-0.000428
34	1	-0.000152	5.543972	-0.000609
35	6	-2.579019	-6.022268	-0.754003
36	1	-3.318200	-6.200352	-1.545257
37	1	-1.636923	-6.469053	-1.085475
38	1	-2.919041	-6.588802	0.124798
39	6	-4.868742	-3.836551	-0.876354
40	1	-5.518236	-4.218719	-0.077086
41	1	-5.311637	-2.901176	-1.229177
42	1	-4.922696	-4.562242	-1.699168
43	6	-5.717204	-1.571024	1.159000
44	1	-6.560937	-1.776552	0.483841
45	1	-5.311526	-2.536884	1.472052
46	1	-6.144392	-1.095568	2.052047
47	6	-5.716777	1.575959	1.155041
48	1	-5.310747	2.542404	1.465830
49	1	-6.560213	1.780236	0.479129

50	1	-6.144446	1.102852	2.049110
51	6	-4.867349	3.836626	-0.885562
52	1	-5.309671	2.900494	-1.237119
53	1	-5.518081	4.220364	-0.088037
54	1	-4.920162	4.560634	-1.709944
55	6	-2.578132	6.023150	-0.761730
56	1	-2.919636	6.590739	0.115830
57	1	-1.635509	6.469602	-1.092175
58	1	-3.316028	6.200245	-1.554416
59	6	4.866938	3.836952	0.886140
60	1	5.309276	2.900873	1.237813
61	1	5.517886	4.220828	0.088855
62	1	4.919358	4.560942	1.710567
63	6	5.716898	1.576233	-1.154331
64	1	5.310848	2.542643	-1.465200
65	1	6.560193	1.780587	-0.478266
66	1	6.144773	1.103154	-2.048315
67	6	5.717545	-1.570767	-1.158255
68	1	6.561134	-1.776257	-0.482904
69	1	5.311986	-2.536648	-1.471402
70	1	6.144910	-1.095289	-2.051203
71	6	2.579162	-6.022277	0.753563
72	1	1.637398	-6.468786	1.086357
73	1	2.917744	-6.588897	-0.125740
74	1	3.319419	-6.200588	1.543748
75	6	4.868936	-3.836444	0.876136
76	1	5.518441	-4.218389	0.076771
77	1	5.311741	-2.901078	1.229102
78	1	4.923003	-4.562268	1.698821
79	6	2.577932	6.023359	0.761140
80	1	2.922071	6.590455	-0.115705
81	1	1.634697	6.470435	1.088970
82	1	3.313835	6.200353	1.555716
83	8	0.123700	-0.002908	-1.739268
84	8	-0.123769	-0.002749	1.739203
85	92	-0.000023	-0.002769	-0.000031

NpO_2L1^{2-}

E (CAM-B3LYP) = -2463.60689570 Hartree
Zero-point correction= 0.684807 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2462.922089 Hartree
Sum of electronic and thermal Enthalpies= -2462.874360 Hartree
Sum of electronic and thermal Free Energies= -2463.001762 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.689715	-0.000193	0.219495
2	7	-1.531261	2.490399	0.015294
3	7	1.527454	2.487474	-0.024512
4	7	2.694429	0.000153	-0.215469

5	7	1.527805	-2.487299	-0.024543
6	7	-1.530916	-2.490645	0.015271
7	6	-3.457822	-1.084520	-0.003927
8	6	-4.765187	-0.692878	-0.453922
9	6	-4.765307	0.692243	-0.453815
10	6	-3.457972	1.084027	-0.003926
11	6	-2.861317	2.377488	0.137034
12	6	-3.481021	3.657434	0.414232
13	6	-2.455692	4.569908	0.391529
14	6	-1.253173	3.819044	0.132196
15	6	0.001100	4.409747	-0.032432
16	1	-0.002080	5.498274	-0.053834
17	6	1.242988	3.822660	-0.172174
18	6	2.455803	4.568863	-0.432008
19	6	3.475382	3.658398	-0.424268
20	6	2.848942	2.376453	-0.127469
21	6	3.457950	1.084344	0.029714
22	6	4.744473	0.697573	0.506755
23	6	4.744577	-0.696946	0.506774
24	6	3.458109	-1.083921	0.029752
25	6	2.849284	-2.376112	-0.127424
26	6	3.475913	-3.657990	-0.424135
27	6	2.456454	-4.568585	-0.431907
28	6	1.243526	-3.822528	-0.172157
29	6	-2.860989	-2.377906	0.137069
30	6	-3.480472	-3.657921	0.414474
31	6	-2.455028	-4.570261	0.391662
32	6	-1.252637	-3.819245	0.132212
33	6	0.001718	-4.409781	-0.032410
34	1	-0.001309	-5.498309	-0.053757
35	6	-2.540757	6.046709	0.629928
36	1	-3.510529	6.323585	1.057696
37	1	-1.764744	6.395692	1.320830
38	1	-2.424671	6.625124	-0.297512
39	6	-4.898706	3.925873	0.826063
40	1	-5.546215	4.254064	0.002515
41	1	-5.354733	3.030685	1.256639
42	1	-4.935975	4.711930	1.590603
43	6	-5.841749	1.563398	-1.028240
44	1	-6.622551	1.837460	-0.305579
45	1	-5.424713	2.492915	-1.423528
46	1	-6.348349	1.054940	-1.857899
47	6	-5.841461	-1.564085	-1.028579
48	1	-5.424268	-2.493467	-1.424011
49	1	-6.622280	-1.838381	-0.306027
50	1	-6.348071	-1.055548	-1.858184
51	6	-4.898025	-3.926558	0.826632
52	1	-5.354108	-3.031416	1.257238
53	1	-5.545655	-4.254937	0.003258
54	1	-4.934990	-4.712557	1.591247
55	6	-2.539862	-6.047058	0.630167

56	1	-2.423724	-6.625521	-0.297235
57	1	-1.763772	-6.395876	1.321065
58	1	-3.509578	-6.324048	1.057992
59	6	4.902288	-3.906642	-0.815624
60	1	5.350813	-3.000121	-1.230291
61	1	5.539458	-4.228977	0.017684
62	1	4.962900	-4.687320	-1.583922
63	6	5.815619	-1.564256	1.098954
64	1	5.400847	-2.503254	1.474746
65	1	6.620521	-1.822195	0.395900
66	1	6.294707	-1.061359	1.948610
67	6	5.815379	1.565062	1.098915
68	1	6.620253	1.823090	0.395861
69	1	5.400463	2.504016	1.474661
70	1	6.294530	1.062273	1.948600
71	6	2.541154	6.039877	-0.700368
72	1	1.811639	6.360984	-1.452887
73	1	2.349390	6.635297	0.202785
74	1	3.535991	6.319199	-1.063102
75	6	4.901700	3.907219	-0.815857
76	1	5.538873	4.229699	0.017393
77	1	5.350326	3.000730	-1.230487
78	1	4.962162	4.687852	-1.584212
79	6	2.542013	-6.039600	-0.700196
80	1	2.350379	-6.635004	0.202995
81	1	1.812511	-6.360853	-1.452666
82	1	3.536874	-6.318793	-1.062961
83	93	0.007112	-0.000001	-0.004086
84	8	0.195030	-0.000309	1.774029
85	8	-0.186235	0.000305	-1.782117

PuO_2L1^{2-}

E (CAM-B3LYP) = -2503.04264384 Hartree
Zero-point correction= 0.684888 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2502.357756 Hartree
Sum of electronic and thermal Enthalpies= -2502.310060 Hartree
Sum of electronic and thermal Free Energies= -2502.437914 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	3.4500910	-1.0823340	0.0418250
2	6	4.7370680	-0.6953870	0.5167170
3	7	2.6844180	0.0010870	-0.2011240
4	6	4.7364950	0.6992330	0.5167230
5	6	3.4492390	1.0851440	0.0417170
6	6	2.8427870	2.3778570	-0.1203090
7	6	3.4721870	3.6570570	-0.4254080
8	7	1.5224040	2.4917740	-0.0166990
9	6	2.4545880	4.5694380	-0.4375270
10	6	1.2403580	3.8266880	-0.1727060

11	6	-0.0008750	4.4152480	-0.0375470
12	1	-0.0045110	5.5037870	-0.0621290
13	6	-1.2547290	3.8226320	0.1266490
14	6	-2.4581340	4.5699940	0.3912060
15	7	-1.5292300	2.4938840	0.0065410
16	6	-3.4810470	3.6545530	0.4151550
17	6	-2.8583440	2.3771880	0.1324280
18	6	-3.4513410	1.0825340	-0.0102510
19	6	-4.7603790	0.6904910	-0.4558790
20	7	-2.6808460	-0.0010270	0.2095190
21	6	-4.7598210	-0.6942750	-0.4558150
22	6	-3.4504800	-1.0852210	-0.0101070
23	6	-2.8564520	-2.3793950	0.1327380
24	6	-3.4781240	-3.6572080	0.4156790
25	7	-1.5272500	-2.4950500	0.0068290
26	6	-2.4544820	-4.5718460	0.3918150
27	6	-1.2516830	-3.8235680	0.1271100
28	6	2.8446710	-2.3755430	-0.1200510
29	6	3.4751190	-3.6542750	-0.4248710
30	7	1.5243780	-2.4904950	-0.0164520
31	6	2.4582390	-4.5674650	-0.4369820
32	6	1.2434040	-3.8256570	-0.1722910
33	6	0.0026460	-4.4151930	-0.0370330
34	1	-0.0001050	-5.5037360	-0.0614520
35	6	2.5421040	6.0386160	-0.7151500
36	1	3.5379630	6.3146750	-1.0776160
37	1	1.8143730	6.3556780	-1.4711370
38	1	2.3490050	6.6400350	0.1837580
39	6	4.8987210	3.9002770	-0.8197030
40	1	5.5378960	4.2242570	0.0114460
41	1	5.3442120	2.9906750	-1.2309640
42	1	4.9606330	4.6775830	-1.5913390
43	6	5.8079660	1.5669770	1.1075620
44	1	6.6145220	1.8213980	0.4050460
45	1	5.3942000	2.5079310	1.4796280
46	1	6.2851070	1.0661650	1.9596730
47	6	5.8092560	-1.5622980	1.1074800
48	1	5.3962550	-2.5036140	1.4794900
49	1	6.6160020	-1.8160290	0.4049300
50	1	6.2860100	-1.0611590	1.9596160
51	6	4.9019270	-3.8963970	-0.8188570
52	1	5.3467650	-2.9864830	-1.2301410
53	1	5.5412000	-4.2197490	0.0124630
54	1	4.9646270	-4.6737460	-1.5903850
55	6	2.5469500	-6.0366140	-0.7143750
56	1	2.3541460	-6.6380510	0.1845860
57	1	1.8196080	-6.3543570	-1.4704530
58	1	3.5430930	-6.3119510	-1.0766060
59	6	-4.8946200	-3.9218520	0.8341960
60	1	-5.3475770	-3.0242420	1.2630060
61	1	-5.5461190	-4.2524150	0.0146880

62	1	-4.9300900	-4.7047750	1.6020920
63	6	-5.8372470	-1.5660970	-1.0274040
64	1	-5.4211650	-2.4969790	-1.4205080
65	1	-6.6178960	-1.8377770	-0.3036610
66	1	-6.3440770	-1.0592290	-1.8580000
67	6	-5.8385080	1.5613900	-1.0275460
68	1	-6.6193710	1.8325170	-0.3038280
69	1	-5.4231750	2.4925650	-1.4207490
70	1	-6.3449380	1.0540320	-1.8580880
71	6	-2.5459340	6.0458800	0.6344110
72	1	-1.7701320	6.3942100	1.3259340
73	1	-2.4314480	6.6276510	-0.2911810
74	1	-3.5159880	6.3196100	1.0636340
75	6	-4.8977760	3.9181210	0.8335640
76	1	-5.5495090	4.2479980	0.0139670
77	1	-5.3500170	3.0202180	1.2625160
78	1	-4.9339230	4.7011500	1.6013190
79	6	-2.5411390	-6.0477710	0.6351900
80	1	-2.4271260	-6.6295410	-0.2904640
81	1	-1.7645080	-6.3955610	1.3260460
82	1	-3.5106390	-6.3220830	1.0653010
83	8	-0.1386350	-0.0001300	-1.7655440
84	8	0.1488830	0.0000970	1.7583460
85	94	0.0069880	-0.0000140	-0.0035010

UO_2L1^{3-}

E (CAM-B3LYP) = -2426.001667 Hartree
Zero-point correction= 0.683057 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2425.318611 Hartree
Sum of electronic and thermal Enthalpies= -2425.270647 Hartree
Sum of electronic and thermal Free Energies= -2425.3989 Hartree

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Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-3.4832960	-1.0507050	-0.0141420
2	6	-4.7340670	-0.6539510	-0.5276250
3	7	-2.7194550	0.0285040	0.2764120
4	6	-4.7186050	0.7592810	-0.5233450
5	6	-3.4593790	1.1254840	-0.0082210
6	6	-2.8289370	2.4283920	0.1453020
7	6	-3.4352370	3.6990960	0.4610750
8	7	-1.5136930	2.5399350	-0.0083380
9	6	-2.4091580	4.6193190	0.4318420
10	6	-1.2132380	3.8783760	0.1445070
11	6	0.0447260	4.4455460	-0.0138490
12	1	0.0531080	5.5359170	-0.0132420
13	6	1.2941610	3.8555160	-0.1620510
14	6	2.5059810	4.5688250	-0.4529700
15	7	1.5661470	2.5127570	0.0039590
16	6	3.5142500	3.6274590	-0.4615630

17	6	2.8794820	2.3720290	-0.1409220
18	6	3.4805990	1.0555260	0.0152090
19	6	4.7302680	0.6620760	0.5335040
20	7	2.7184730	-0.0252780	-0.2729690
21	6	4.7159640	-0.7511200	0.5359030
22	6	3.4586020	-1.1207340	0.0184220
23	6	2.8303270	-2.4246040	-0.1342350
24	6	3.4399300	-3.6951930	-0.4438890
25	7	1.5133550	-2.5370500	0.0048590
26	6	2.4125150	-4.6153900	-0.4322050
27	6	1.2142420	-3.8752750	-0.1516490
28	6	-2.8815180	-2.3674480	0.1353590
29	6	-3.5162900	-3.6261720	0.4430420
30	7	-1.5671960	-2.5060870	-0.0052260
31	6	-2.5075760	-4.5668290	0.4283960
32	6	-1.2949880	-3.8503070	0.1482570
33	6	-0.0462010	-4.4407790	-0.0023990
34	1	-0.0573520	-5.5306500	-0.0034690
35	6	-2.5107210	6.0832080	0.7391540
36	1	-2.3075280	6.3123390	1.7966180
37	1	-1.8003180	6.6762740	0.1502030
38	1	-3.5151100	6.4662700	0.5181980
39	6	-4.8499540	3.9467740	0.8956240
40	1	-5.5003120	4.3494200	0.1039230
41	1	-5.3076310	3.0128070	1.2349030
42	1	-4.8900290	4.6612760	1.7303050
43	6	-5.7604530	1.6438820	-1.1425470
44	1	-6.6151460	1.8762050	-0.4849960
45	1	-5.3274810	2.6011620	-1.4497680
46	1	-6.1867120	1.1790750	-2.0439440
47	6	-5.7952930	-1.5103280	-1.1535730
48	1	-5.3823120	-2.4712820	-1.4764290
49	1	-6.6511950	-1.7357580	-0.4952610
50	1	-6.2165190	-1.0246410	-2.0462070
51	6	-4.9387670	-3.8466980	0.8615050
52	1	-5.3759500	-2.9108430	1.2222860
53	1	-5.5939530	-4.2148470	0.0576040
54	1	-5.0006310	-4.5831500	1.6767120
55	6	-2.6523890	-6.0346840	0.6945920
56	1	-2.9837540	-6.5996400	-0.1910890
57	1	-1.7106100	-6.4832050	1.0279300
58	1	-3.3973880	-6.2260110	1.4795180
59	6	4.8580670	-3.9438440	-0.8612220
60	1	5.3148700	-3.0163490	-1.2192860
61	1	5.5045390	-4.3272220	-0.0573550
62	1	4.9056700	-4.6796090	-1.6780080
63	6	5.7572040	-1.6308840	1.1629420
64	1	5.3233640	-2.5839920	1.4816580
65	1	6.6103980	-1.8720570	0.5067030
66	1	6.1854890	-1.1565720	2.0583350
67	6	5.7891250	1.5236030	1.1563050

68	1	6.6471980	1.7436910	0.4990030
69	1	5.3746020	2.4871510	1.4693580
70	1	6.2074590	1.0457860	2.0545650
71	6	2.6504210	6.0339220	-0.7339800
72	1	1.7028150	6.4828580	-1.0496490
73	1	3.0034910	6.6045220	0.1396170
74	1	3.3782400	6.2168620	-1.5369850
75	6	4.9360790	3.8437780	-0.8842370
76	1	5.5924710	4.2188380	-0.0844320
77	1	5.3726070	2.9046170	-1.2372570
78	1	4.9970170	4.5730980	-1.7059390
79	6	2.5285160	-6.0851780	-0.7017860
80	1	2.8593230	-6.6570250	0.1796540
81	1	1.5755090	-6.5164750	-1.0256930
82	1	3.2616180	-6.2887840	-1.4948720
83	8	0.1732430	-0.0063200	1.8113030
84	8	-0.1741690	-0.0062110	-1.8134070
85	92	-0.0005680	-0.0059900	-0.0010270

NpO_2L1^{3-}

E (CAM-B3LYP) = -2463.48378189 Hartree
Zero-point correction= 0.683622 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2462.800160 Hartree
Sum of electronic and thermal Enthalpies= -2462.752485 Hartree
Sum of electronic and thermal Free Energies= -2462.879764 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.705013	-0.000766	0.267987
2	7	-1.533312	2.522990	0.004126
3	7	1.531987	2.523765	-0.004070
4	7	2.705091	0.000621	-0.267922
5	7	1.533336	-2.523210	-0.004190
6	7	-1.531923	-2.524028	0.004030
7	6	-3.459310	-1.088039	-0.014868
8	6	-4.715755	-0.707926	-0.526717
9	6	-4.716153	0.705093	-0.526876
10	6	-3.459951	1.086025	-0.015042
11	6	-2.848422	2.396127	0.140737
12	6	-3.474946	3.658765	0.450978
13	6	-2.459133	4.591396	0.438776
14	6	-1.252529	3.865437	0.157929
15	6	-0.001166	4.446597	-0.000131
16	1	-0.001406	5.536524	-0.000302
17	6	1.250482	3.866044	-0.158055
18	6	2.456673	4.592622	-0.439020
19	6	3.473008	3.660562	-0.451061
20	6	2.847155	2.397596	-0.140663
21	6	3.459399	1.087831	0.015178
22	6	4.715743	0.707590	0.527188

23	6	4.716118	-0.705429	0.527040
24	6	3.459954	-1.086235	0.015019
25	6	2.848404	-2.396313	-0.140971
26	6	3.474907	-3.658883	-0.451631
27	6	2.459099	-4.591515	-0.439516
28	6	1.252538	-3.865621	-0.158304
29	6	-2.847046	-2.397800	0.140992
30	6	-3.472864	-3.660696	0.451631
31	6	-2.456597	-4.592834	0.439249
32	6	-1.250430	-3.866307	0.158007
33	6	0.001212	-4.446834	-0.000201
34	1	0.001517	-5.536763	-0.000289
35	6	-2.592316	6.060001	0.706641
36	1	-3.327002	6.255779	1.500279
37	1	-1.644118	6.502896	1.029108
38	1	-2.930828	6.627143	-0.174961
39	6	-4.894865	3.889747	0.872556
40	1	-5.548767	4.266075	0.071361
41	1	-5.339355	2.956575	1.231333
42	1	-4.948714	4.624178	1.690224
43	6	-5.768630	1.574706	-1.149248
44	1	-6.622823	1.805779	-0.490639
45	1	-5.346043	2.532847	-1.467855
46	1	-6.194173	1.097092	-2.044238
47	6	-5.767757	-1.578291	-1.148839
48	1	-5.344628	-2.536269	-1.467221
49	1	-6.621788	-1.809696	-0.490135
50	1	-6.193615	-1.101141	-2.043927
51	6	-4.892574	-3.892265	0.873596
52	1	-5.337407	-2.959223	1.232289
53	1	-5.546486	-4.269043	0.072621
54	1	-4.945903	-4.626557	1.691422
55	6	-2.588937	-6.061485	0.707290
56	1	-2.926453	-6.629034	-0.174435
57	1	-1.640642	-6.503659	1.030469
58	1	-3.324020	-6.257615	1.500467
59	6	4.894811	-3.889655	-0.873385
60	1	5.339156	-2.956362	-1.232031
61	1	5.548826	-4.266038	-0.072313
62	1	4.948685	-4.623924	-1.691194
63	6	5.768498	-1.575221	1.149321
64	1	5.345830	-2.533411	1.467677
65	1	6.622736	-1.806194	0.490735
66	1	6.193988	-1.097828	2.044455
67	6	5.767668	1.577766	1.149703
68	1	6.621735	1.809451	0.491146
69	1	5.344491	2.535611	1.468426
70	1	6.193477	1.100289	2.044638
71	6	2.588858	6.061330	-0.706843
72	1	1.641376	6.502754	-1.033454
73	1	2.922764	6.629297	0.175988

74	1	3.326620	6.257822	-1.497411
75	6	4.892851	3.892102	-0.872607
76	1	5.546632	4.268542	-0.071375
77	1	5.337635	2.959103	-1.231473
78	1	4.946479	4.626615	-1.690209
79	6	2.592139	-6.060091	-0.707632
80	1	2.928402	-6.627751	0.174501
81	1	1.644420	-6.502397	-1.032336
82	1	3.328474	-6.255899	-1.499715
83	93	-0.000010	0.000305	-0.000024
84	8	0.201938	0.000006	1.780151
85	8	-0.201957	0.000633	-1.780204

PuO_2L1^{3-}

E (CAM-B3LYP) = -2502.89467314 Hartree
Zero-point correction= 0.683144 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2502.211530 Hartree
Sum of electronic and thermal Enthalpies= -2502.163686 Hartree
Sum of electronic and thermal Free Energies= -2502.292021 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-3.45383	-0.97225	-0.03946
2	6	-4.69205	-0.55349	-0.54956
3	7	-2.64763	0.09656	0.23164
4	6	-4.64680	0.85925	-0.55850
5	6	-3.37990	1.20473	-0.05742
6	6	-2.75787	2.50560	0.11837
7	6	-3.35641	3.75878	0.47830
8	7	-1.43560	2.61052	-0.06160
9	6	-2.33233	4.68368	0.45491
10	6	-1.14209	3.95497	0.12787
11	6	0.11606	4.51560	-0.03285
12	1	0.14529	5.60685	-0.04471
13	6	1.34842	3.89203	-0.17415
14	6	2.57840	4.55589	-0.48927
15	7	1.57179	2.53771	0.03812
16	6	3.55662	3.58263	-0.47768
17	6	2.88444	2.36519	-0.11104
18	6	3.44094	1.03538	0.07853
19	6	4.67330	0.62622	0.61004
20	7	2.65445	-0.03402	-0.22187
21	6	4.64655	-0.78710	0.60085
22	6	3.39482	-1.14224	0.06916
23	6	2.77146	-2.43275	-0.12040
24	6	3.37127	-3.69198	-0.45891
25	7	1.44268	-2.52857	0.00996
26	6	2.33574	-4.60466	-0.47949
27	6	1.14596	-3.86974	-0.18340
28	6	-2.88953	-2.29418	0.12695

29	6	-3.55139	-3.52443	0.45909
30	7	-1.57399	-2.45710	-0.02517
31	6	-2.56624	-4.49129	0.44084
32	6	-1.34016	-3.81497	0.13696
33	6	-0.11218	-4.43895	-0.03271
34	1	-0.13833	-5.52111	-0.04420
35	6	-2.44786	6.13800	0.79096
36	1	-2.64545	6.29336	1.86103
37	1	-1.53786	6.69695	0.55217
38	1	-3.27644	6.61008	0.24544
39	6	-4.76388	4.01813	0.93300
40	1	-5.40233	4.45841	0.15698
41	1	-5.24798	3.09505	1.25990
42	1	-4.77044	4.71293	1.78378
43	6	-5.69755	1.76001	-1.13887
44	1	-6.52910	1.96555	-0.45597
45	1	-5.27674	2.73147	-1.42905
46	1	-6.13684	1.31982	-2.04029
47	6	-5.79640	-1.38986	-1.13010
48	1	-5.43470	-2.37205	-1.42981
49	1	-6.63727	-1.55290	-0.43798
50	1	-6.22145	-0.90897	-2.02215
51	6	-4.97090	-3.73014	0.89482
52	1	-5.41676	-2.79263	1.24034
53	1	-5.62108	-4.11877	0.10003
54	1	-5.02308	-4.45136	1.71774
55	6	-2.75602	-5.94698	0.74482
56	1	-3.53239	-6.39273	0.11436
57	1	-1.83730	-6.52449	0.60097
58	1	-3.07028	-6.09816	1.78660
59	6	4.79059	-3.95860	-0.85984
60	1	5.27916	-3.04346	-1.20357
61	1	5.40836	-4.36440	-0.05030
62	1	4.83389	-4.68435	-1.68067
63	6	5.69485	-1.68370	1.20197
64	1	5.27100	-2.64235	1.50745
65	1	6.53011	-1.89752	0.52738
66	1	6.12866	-1.22077	2.09697
67	6	5.75673	1.46869	1.21092
68	1	6.61086	1.63945	0.53618
69	1	5.38242	2.45687	1.49793
70	1	6.16705	1.00279	2.11053
71	6	2.76643	6.00442	-0.81819
72	1	1.82205	6.51381	-1.01949
73	1	3.26928	6.54799	-0.00524
74	1	3.39504	6.13122	-1.70899
75	6	4.98721	3.75776	-0.89721
76	1	5.63451	4.14043	-0.09701
77	1	5.41876	2.80975	-1.23160
78	1	5.05816	4.47121	-1.72738
79	6	2.44958	-6.07015	-0.78032

80	1	2.85327	-6.63594	0.06853
81	1	1.48066	-6.51321	-1.03388
82	1	3.12332	-6.24868	-1.62685
83	8	0.13215	-0.09552	1.77753
84	8	-0.14244	-0.09190	-1.79244
85	94	-0.00416	-0.09610	-0.00731

UO_2L2

E (CAM-B3LYP) = -2315.65275156 Hartree
Zero-point correction= 0.676786 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2314.975966 Hartree
Sum of electronic and thermal Enthalpies= -2314.931962 Hartree
Sum of electronic and thermal Free Energies= -2315.052294 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.011956	2.934507	-0.165079
2	6	-1.991119	3.876613	-0.627904
3	6	-3.134079	3.145143	-0.855113
4	6	-2.824513	1.779701	-0.530124
5	7	-1.516229	1.681775	-0.145305
6	6	0.359060	3.068346	0.201665
7	6	1.122284	4.166243	0.724932
8	7	1.110790	1.949297	0.123667
9	6	2.390263	3.673857	0.931128
10	6	2.369271	2.292787	0.533518
11	6	-1.805777	5.331909	-0.937714
12	1	-1.973985	5.978940	-0.070429
13	1	-0.798002	5.533671	-1.307699
14	1	-2.506011	5.646578	-1.716186
15	6	0.641576	5.534097	1.106922
16	1	0.667957	6.245312	0.274760
17	1	-0.384175	5.504398	1.481446
18	1	1.266017	5.946060	1.904188
19	6	-4.440152	3.640937	-1.399583
20	6	-4.580768	3.413871	-2.910612
21	1	-4.546135	4.708067	-1.179852
22	1	-5.271085	3.147369	-0.882108
23	1	-5.544536	3.783243	-3.275447
24	1	-3.787527	3.931869	-3.458395
25	1	-4.506661	2.349749	-3.153796
26	6	3.564917	4.397616	1.518356
27	6	3.742848	4.127120	3.018282
28	1	3.451153	5.473660	1.352845
29	1	4.481225	4.111228	0.989138
30	1	3.886298	3.059160	3.207570
31	1	4.609559	4.665761	3.414528
32	1	2.858444	4.444233	3.579448
33	6	-3.741077	0.745871	-0.458910
34	1	-4.770641	1.021401	-0.662566

35	6	-3.555963	-0.570681	-0.057320
36	6	-4.667626	-1.409576	0.301721
37	7	-2.362603	-1.238455	0.124029
38	6	-4.136907	-2.591287	0.740165
39	6	-2.708391	-2.469263	0.575076
40	6	-1.886736	-3.610276	0.690991
41	1	-2.404000	-4.503057	1.023189
42	6	-0.623531	-3.888748	0.270699
43	6	-0.077144	-5.178778	0.039150
44	8	0.298917	-2.948059	-0.175443
45	6	1.104784	-5.028243	-0.608749
46	1	-0.581138	-6.097720	0.302649
47	1	1.777143	-5.799010	-0.957739
48	6	1.384798	-3.639344	-0.703227
49	6	2.567582	-3.076406	-1.068766
50	1	3.254634	-3.810604	-1.473597
51	6	3.140450	-1.809472	-0.828927
52	6	4.566494	-1.631719	-0.946249
53	7	2.542411	-0.708263	-0.311285
54	6	4.837332	-0.403464	-0.409844
55	6	3.477997	1.472295	0.432091
56	6	3.571790	0.170734	-0.044093
57	1	4.426784	1.937432	0.679100
58	6	6.172005	0.257898	-0.255491
59	1	6.242544	1.176907	-0.847549
60	1	6.371707	0.526420	0.787896
61	1	6.978618	-0.403694	-0.579820
62	6	5.549797	-2.634852	-1.476293
63	6	6.054941	-3.615620	-0.409987
64	1	6.405472	-2.103244	-1.905942
65	1	5.108588	-3.193185	-2.309689
66	1	6.767053	-4.329652	-0.836284
67	1	6.554781	-3.080181	0.402923
68	1	5.227866	-4.180360	0.031351
69	6	-4.864071	-3.782726	1.290738
70	6	-4.756501	-3.901634	2.816365
71	1	-4.493664	-4.704589	0.825972
72	1	-5.920350	-3.721190	1.010805
73	1	-5.300041	-4.778625	3.182373
74	1	-3.713030	-3.989929	3.134190
75	1	-5.172461	-3.014376	3.302960
76	6	-6.109007	-1.009319	0.237692
77	1	-6.765223	-1.859366	0.437628
78	1	-6.347992	-0.232213	0.972265
79	1	-6.376185	-0.617472	-0.749612
80	92	0.015656	-0.264388	-0.078173
81	8	-0.070738	-0.283878	-1.822682
82	8	0.115428	-0.381632	1.661947

NpO_2L2

E (CAM-B3LYP) = -2353.09020516 Hartree
Zero-point correction= 0.674264 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2352.415941 Hartree
Sum of electronic and thermal Enthalpies= -2352.371427 Hartree
Sum of electronic and thermal Free Energies= -2352.493878 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.166368	2.875186	-0.293526
2	6	-2.202981	3.787900	-0.773366
3	6	-3.317421	3.021203	-0.936463
4	6	-2.941834	1.661804	-0.564242
5	7	-1.609919	1.633192	-0.209190
6	6	0.229720	3.098898	0.029046
7	6	0.933979	4.279472	0.515462
8	7	1.035692	2.053152	-0.063943
9	6	2.233414	3.892062	0.666079
10	6	2.292410	2.487113	0.289135
11	6	-2.057046	5.232175	-1.139126
12	1	-2.194318	5.903578	-0.285723
13	1	-1.071033	5.436605	-1.563936
14	1	-2.801500	5.509753	-1.890450
15	6	0.358444	5.605928	0.909387
16	1	0.272066	6.301042	0.068286
17	1	-0.637190	5.492917	1.346190
18	1	0.990091	6.084306	1.662335
19	6	-4.678264	3.454477	-1.388355
20	6	-5.593046	3.855252	-0.222829
21	1	-5.151540	2.653536	-1.966459
22	1	-4.581470	4.302380	-2.074873
23	1	-6.578540	4.162056	-0.586874
24	1	-5.730550	3.022493	0.473756
25	1	-5.162661	4.688533	0.340490
26	6	3.378560	4.699224	1.198514
27	6	3.643145	4.447407	2.689147
28	1	3.181016	5.763723	1.037792
29	1	4.286830	4.476053	0.626434
30	1	3.863677	3.392286	2.875275
31	1	4.490641	5.043300	3.042301
32	1	2.767211	4.709868	3.290159
33	6	-3.794577	0.599064	-0.507075
34	1	-4.832427	0.822902	-0.732119
35	6	-3.558302	-0.757054	-0.146014
36	6	-4.670485	-1.648591	0.151932
37	7	-2.377703	-1.380175	-0.040707
38	6	-4.117819	-2.851008	0.459343
39	6	-2.675851	-2.678316	0.299335
40	6	-1.823431	-3.760372	0.368128
41	1	-2.318113	-4.698299	0.598355
42	6	-0.467016	-3.984587	0.113891
43	6	0.139093	-5.234993	0.004174
44	8	0.475571	-3.017944	-0.139407

45	6	1.458030	-5.028403	-0.348920
46	1	-0.368772	-6.176668	0.154286
47	1	2.223018	-5.770821	-0.524410
48	6	1.664033	-3.651004	-0.416691
49	6	2.891496	-3.024561	-0.644497
50	1	3.648330	-3.764251	-0.883929
51	6	3.377808	-1.734332	-0.543908
52	6	4.806116	-1.463774	-0.669525
53	7	2.692525	-0.589798	-0.226955
54	6	4.961226	-0.147302	-0.369756
55	6	3.432405	1.733077	0.228036
56	6	3.626392	0.369486	-0.110374
57	1	4.351697	2.269660	0.441589
58	6	6.225676	0.652010	-0.320981
59	1	6.191145	1.508996	-1.002459
60	1	6.420018	1.043459	0.684508
61	1	7.088095	0.043417	-0.603069
62	6	5.873208	-2.467518	-0.991508
63	6	6.376992	-3.231850	0.240066
64	1	6.717386	-1.953757	-1.462933
65	1	5.509195	-3.178355	-1.742125
66	1	7.151640	-3.954233	-0.036207
67	1	6.800293	-2.542504	0.976649
68	1	5.563099	-3.774699	0.730475
69	6	-4.811481	-4.104520	0.900818
70	6	-4.721194	-4.337274	2.414861
71	1	-4.399982	-4.972642	0.372085
72	1	-5.864609	-4.056595	0.606893
73	1	-5.236867	-5.259461	2.700723
74	1	-3.680172	-4.411474	2.743200
75	1	-5.178080	-3.506855	2.961085
76	6	-6.115518	-1.259628	0.136503
77	1	-6.757870	-2.112466	0.367316
78	1	-6.332979	-0.477626	0.872686
79	1	-6.422215	-0.877153	-0.843810
80	8	0.027619	-0.366350	-1.924948
81	8	0.106074	-0.359234	1.645779
82	93	0.060108	-0.317519	-0.139780

PuO_2L2

E (CAM-B3LYP) = -2392.53250985 Hartree
Zero-point correction= 0.674534 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2391.857976 Hartree
Sum of electronic and thermal Enthalpies= -2391.813579 Hartree
Sum of electronic and thermal Free Energies= -2391.936105 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.177001	2.862081	-0.300810
2	6	-2.211949	3.769010	-0.796591

3	6	-3.320765	2.996704	-0.969394
4	6	-2.942803	1.640536	-0.585838
5	7	-1.615414	1.619937	-0.214991
6	6	0.215324	3.091432	0.035246
7	6	0.906710	4.274223	0.534932
8	7	1.027085	2.050769	-0.053993
9	6	2.206107	3.893330	0.700128
10	6	2.277063	2.490805	0.315919
11	6	-2.067260	5.212832	-1.164518
12	1	-2.217427	5.885811	-0.314466
13	1	-1.076784	5.420123	-1.577579
14	1	-2.803599	5.485769	-1.925539
15	6	0.317429	5.595821	0.924613
16	1	0.236648	6.291916	0.083724
17	1	-0.682915	5.475116	1.348579
18	1	0.936281	6.077202	1.686251
19	6	-4.678385	3.421423	-1.438702
20	6	-5.606983	3.827721	-0.286118
21	1	-5.142651	2.614244	-2.015471
22	1	-4.577446	4.264431	-2.130731
23	1	-6.589667	4.128173	-0.662890
24	1	-5.748983	2.999767	0.415298
25	1	-5.185600	4.666819	0.275380
26	6	3.340815	4.703638	1.249778
27	6	3.591879	4.442990	2.741203
28	1	3.138549	5.768070	1.094468
29	1	4.256251	4.489791	0.685550
30	1	3.817054	3.387934	2.922113
31	1	4.432088	5.041491	3.107169
32	1	2.708271	4.695896	3.335042
33	6	-3.789555	0.573396	-0.528735
34	1	-4.827121	0.788014	-0.764173
35	6	-3.545899	-0.777227	-0.151397
36	6	-4.653757	-1.669482	0.160557
37	7	-2.362138	-1.393445	-0.039416
38	6	-4.095203	-2.864696	0.485017
39	6	-2.654587	-2.687638	0.318855
40	6	-1.796942	-3.765071	0.392903
41	1	-2.284202	-4.703907	0.635031
42	6	-0.442266	-3.981379	0.124906
43	6	0.169111	-5.228611	0.006346
44	8	0.490711	-3.008842	-0.140803
45	6	1.481044	-5.014373	-0.366860
46	1	-0.331592	-6.173055	0.163080
47	1	2.247805	-5.752051	-0.554269
48	6	1.678121	-3.635496	-0.435370
49	6	2.899620	-3.002344	-0.673543
50	1	3.657662	-3.736074	-0.927100
51	6	3.379476	-1.710641	-0.562645
52	6	4.806243	-1.432707	-0.690223
53	7	2.689953	-0.574353	-0.226748

54	6	4.957150	-0.120651	-0.369639
55	6	3.421413	1.744420	0.256738
56	6	3.620861	0.386097	-0.098916
57	1	4.337103	2.282441	0.482076
58	6	6.218406	0.683188	-0.312070
59	1	6.178575	1.550307	-0.980334
60	1	6.413818	1.060278	0.698704
61	1	7.082638	0.082564	-0.605574
62	6	5.876281	-2.427032	-1.031265
63	6	6.389587	-3.206087	0.187049
64	1	6.715873	-1.902882	-1.499505
65	1	5.511875	-3.129079	-1.789928
66	1	7.165994	-3.921227	-0.102881
67	1	6.813531	-2.525099	0.931016
68	1	5.580439	-3.759180	0.673849
69	6	-4.781749	-4.115166	0.945735
70	6	-4.681906	-4.329243	2.461908
71	1	-4.369902	-4.988208	0.425357
72	1	-5.836730	-4.074740	0.657335
73	1	-5.192750	-5.249599	2.762035
74	1	-3.638708	-4.396007	2.784885
75	1	-5.138391	-3.493739	3.000680
76	6	-6.100533	-1.287087	0.141629
77	1	-6.738850	-2.139463	0.385079
78	1	-6.320560	-0.495818	0.867077
79	1	-6.410190	-0.919555	-0.843485
80	8	0.025095	-0.345275	-1.899722
81	8	0.099492	-0.336820	1.624128
82	94	0.059088	-0.315081	-0.138017

UO_2L2^-

E (CAM-B3LYP) = -2315.70603278 Hartree
Zero-point correction= 0.672735 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2315.033298 Hartree
Sum of electronic and thermal Enthalpies= -2314.988988 Hartree
Sum of electronic and thermal Free Energies= -2315.110278 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.011956	2.934507	-0.165079
2	6	-1.991119	3.876613	-0.627904
3	6	-3.134079	3.145143	-0.855113
4	6	-2.824513	1.779701	-0.530124
5	7	-1.516229	1.681775	-0.145305
6	6	0.359060	3.068346	0.201665
7	6	1.122284	4.166243	0.724932
8	7	1.110790	1.949297	0.123667
9	6	2.390263	3.673857	0.931128
10	6	2.369271	2.292787	0.533518
11	6	-1.805777	5.331909	-0.937714

12	1	-1.973985	5.978940	-0.070429
13	1	-0.798002	5.533671	-1.307699
14	1	-2.506011	5.646578	-1.716186
15	6	0.641576	5.534097	1.106922
16	1	0.667957	6.245312	0.274760
17	1	-0.384175	5.504398	1.481446
18	1	1.266017	5.946060	1.904188
19	6	-4.440152	3.640937	-1.399583
20	6	-4.580768	3.413871	-2.910612
21	1	-4.546135	4.708067	-1.179852
22	1	-5.271085	3.147369	-0.882108
23	1	-5.544536	3.783243	-3.275447
24	1	-3.787527	3.931869	-3.458395
25	1	-4.506661	2.349749	-3.153796
26	6	3.564917	4.397616	1.518356
27	6	3.742848	4.127120	3.018282
28	1	3.451153	5.473660	1.352845
29	1	4.481225	4.111228	0.989138
30	1	3.886298	3.059160	3.207570
31	1	4.609559	4.665761	3.414528
32	1	2.858444	4.444233	3.579448
33	6	-3.741077	0.745871	-0.458910
34	1	-4.770641	1.021401	-0.662566
35	6	-3.555963	-0.570681	-0.057320
36	6	-4.667626	-1.409576	0.301721
37	7	-2.362603	-1.238455	0.124029
38	6	-4.136907	-2.591287	0.740165
39	6	-2.708391	-2.469263	0.575076
40	6	-1.886736	-3.610276	0.690991
41	1	-2.404000	-4.503057	1.023189
42	6	-0.623531	-3.888748	0.270699
43	6	-0.077144	-5.178778	0.039150
44	8	0.298917	-2.948059	-0.175443
45	6	1.104784	-5.028243	-0.608749
46	1	-0.581138	-6.097720	0.302649
47	1	1.777143	-5.799010	-0.957739
48	6	1.384798	-3.639344	-0.703227
49	6	2.567582	-3.076406	-1.068766
50	1	3.254634	-3.810604	-1.473597
51	6	3.140450	-1.809472	-0.828927
52	6	4.566494	-1.631719	-0.946249
53	7	2.542411	-0.708263	-0.311285
54	6	4.837332	-0.403464	-0.409844
55	6	3.477997	1.472295	0.432091
56	6	3.571790	0.170734	-0.044093
57	1	4.426784	1.937432	0.679100
58	6	6.172005	0.257898	-0.255491
59	1	6.242544	1.176907	-0.847549
60	1	6.371707	0.526420	0.787896
61	1	6.978618	-0.403694	-0.579820
62	6	5.549797	-2.634852	-1.476293

63	6	6.054941	-3.615620	-0.409987
64	1	6.405472	-2.103244	-1.905942
65	1	5.108588	-3.193185	-2.309689
66	1	6.767053	-4.329652	-0.836284
67	1	6.554781	-3.080181	0.402923
68	1	5.227866	-4.180360	0.031351
69	6	-4.864071	-3.782726	1.290738
70	6	-4.756501	-3.901634	2.816365
71	1	-4.493664	-4.704589	0.825972
72	1	-5.920350	-3.721190	1.010805
73	1	-5.300041	-4.778625	3.182373
74	1	-3.713030	-3.989929	3.134190
75	1	-5.172461	-3.014376	3.302960
76	6	-6.109007	-1.009319	0.237692
77	1	-6.765223	-1.859366	0.437628
78	1	-6.347992	-0.232213	0.972265
79	1	-6.376185	-0.617472	-0.749612
80	92	0.015656	-0.264388	-0.078173
81	8	-0.070738	-0.283878	-1.822682
82	8	0.115428	-0.381632	1.661947

NpO_2L2^-

E (CAM-B3LYP) = -2353.18742456 Hartree
Zero-point correction= 0.674730 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2352.512695 Hartree
Sum of electronic and thermal Enthalpies= -2352.468433 Hartree
Sum of electronic and thermal Free Energies= -2352.590600 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.048701	2.960685	-0.249484
2	6	-2.078315	3.909768	-0.611154
3	6	-3.241888	3.183025	-0.683639
4	6	-2.890235	1.816287	-0.386114
5	7	-1.548849	1.724040	-0.152305
6	6	0.366821	3.121893	-0.038542
7	6	1.156954	4.272692	0.341932
8	7	1.131246	2.030181	-0.144154
9	6	2.452840	3.824978	0.409972
10	6	2.416936	2.416267	0.100472
11	6	-1.926137	5.352240	-0.990332
12	1	-1.993639	6.038554	-0.138546
13	1	-0.966081	5.533980	-1.479690
14	1	-2.711076	5.643450	-1.696280
15	6	0.690724	5.640041	0.747432
16	1	0.589542	6.335314	-0.093684
17	1	-0.279200	5.594664	1.249150
18	1	1.398363	6.088770	1.451679
19	6	-4.616620	3.691735	-0.999890
20	6	-5.401469	4.113384	0.249472

21	1	-5.185050	2.927485	-1.541796
22	1	-4.545332	4.549015	-1.680044
23	1	-6.401902	4.478335	-0.010784
24	1	-5.512245	3.270739	0.938955
25	1	-4.875618	4.909117	0.786499
26	6	3.664515	4.605682	0.826491
27	6	4.011790	4.427081	2.310468
28	1	3.506682	5.669776	0.617545
29	1	4.528346	4.308972	0.219104
30	1	4.194637	3.373096	2.538956
31	1	4.904974	5.000854	2.584152
32	1	3.183698	4.758802	2.944940
33	6	-3.797146	0.772332	-0.307887
34	1	-4.834833	1.071309	-0.427895
35	6	-3.630081	-0.592122	-0.079454
36	6	-4.763502	-1.466734	0.096672
37	7	-2.456464	-1.299764	-0.007484
38	6	-4.253946	-2.721540	0.283718
39	6	-2.814954	-2.579358	0.193003
40	6	-1.983189	-3.729673	0.229891
41	1	-2.533516	-4.655258	0.365198
42	6	-0.659405	-3.983722	0.055416
43	6	-0.072571	-5.283014	-0.024628
44	8	0.350860	-3.054476	-0.129613
45	6	1.246582	-5.135772	-0.282156
46	1	-0.634904	-6.199479	0.088425
47	1	1.993747	-5.906141	-0.413395
48	6	1.537713	-3.738856	-0.333280
49	6	2.774067	-3.198521	-0.496321
50	1	3.514687	-3.977321	-0.647203
51	6	3.329269	-1.892936	-0.440800
52	6	4.764273	-1.710773	-0.510655
53	7	2.690751	-0.724212	-0.260367
54	6	4.977852	-0.372546	-0.331699
55	6	3.532984	1.599313	0.029579
56	6	3.675718	0.229050	-0.182850
57	1	4.477788	2.122796	0.150931
58	6	6.287661	0.354369	-0.299334
59	1	6.338410	1.139977	-1.061897
60	1	6.463689	0.836298	0.670122
61	1	7.123740	-0.328060	-0.477045
62	6	5.794619	-2.788663	-0.683715
63	6	6.170151	-3.489098	0.628957
64	1	6.700102	-2.357740	-1.126459
65	1	5.445785	-3.536750	-1.406069
66	1	6.920798	-4.271464	0.465851
67	1	6.576625	-2.768609	1.345703
68	1	5.291627	-3.948342	1.092466
69	6	-5.008481	-3.989689	0.556759
70	6	-5.007851	-4.389743	2.038054
71	1	-4.598673	-4.814757	-0.039472

72	1	-6.045432	-3.875674	0.220869
73	1	-5.565629	-5.319263	2.202246
74	1	-3.986732	-4.533497	2.404222
75	1	-5.464194	-3.603741	2.647826
76	6	-6.201354	-1.045559	0.092192
77	1	-6.868255	-1.909111	0.167613
78	1	-6.435772	-0.379400	0.931044
79	1	-6.466382	-0.509274	-0.826539
80	8	-0.038262	-0.368653	-1.932047
81	8	0.131954	-0.332739	1.646725
82	93	0.040261	-0.300185	-0.142993

PuO_2L2^-

E (CAM-B3LYP) = -2392.6285451 Hartree
Zero-point correction= 0.674895 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2391.953650 Hartree
Sum of electronic and thermal Enthalpies= -2391.909478 Hartree
Sum of electronic and thermal Free Energies= -2392.031759 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-1.06427	2.94860	-0.25246
2	6	-2.09472	3.89241	-0.62774
3	6	-3.25318	3.15943	-0.71243
4	6	-2.89665	1.79504	-0.40743
5	7	-1.55814	1.71059	-0.15800
6	6	0.34861	3.11684	-0.02891
7	6	1.12777	4.27145	0.36284
8	7	1.11992	2.03053	-0.13267
9	6	2.42568	3.83169	0.44056
10	6	2.40084	2.42410	0.12436
11	6	-1.94503	5.33528	-1.00635
12	1	-2.02490	6.02184	-0.15577
13	1	-0.98030	5.52119	-1.48499
14	1	-2.72348	5.62260	-1.72110
15	6	0.64823	5.63423	0.76823
16	1	0.55259	6.33221	-0.07136
17	1	-0.32740	5.58076	1.25801
18	1	1.34458	6.08470	1.48262
19	6	-4.62715	3.65946	-1.04516
20	6	-5.42698	4.08342	0.19390
21	1	-5.18609	2.88949	-1.58888
22	1	-4.55336	4.51376	-1.72889
23	1	-6.42655	4.44204	-0.07831
24	1	-5.54055	3.24367	0.88646
25	1	-4.91057	4.88446	0.73222
26	6	3.62934	4.61801	0.86947
27	6	3.97025	4.43113	2.35388
28	1	3.46484	5.68247	0.66752
29	1	4.49860	4.33204	0.26458

30	1	4.15953	3.37684	2.57563
31	1	4.85786	5.00928	2.63644
32	1	3.13647	4.75227	2.98637
33	6	-3.79668	0.74563	-0.33170
34	1	-4.83576	1.03564	-0.46166
35	6	-3.61987	-0.61557	-0.09011
36	6	-4.74846	-1.49414	0.09681
37	7	-2.44163	-1.31487	-0.00835
38	6	-4.23181	-2.74302	0.30270
39	6	-2.79382	-2.59356	0.20927
40	6	-1.95630	-3.73890	0.25462
41	1	-2.50013	-4.66660	0.40154
42	6	-0.63252	-3.98487	0.07022
43	6	-0.03870	-5.28072	-0.01325
44	8	0.36848	-3.04893	-0.12916
45	6	1.27566	-5.12544	-0.28976
46	1	-0.59381	-6.20040	0.10928
47	1	2.02630	-5.89097	-0.42936
48	6	1.55669	-3.72660	-0.34582
49	6	2.78836	-3.17926	-0.51899
50	1	3.53209	-3.95295	-0.68074
51	6	3.33584	-1.87101	-0.45634
52	6	4.76951	-1.68063	-0.53153
53	7	2.69135	-0.70847	-0.25836
54	6	4.97685	-0.34381	-0.33538
55	6	3.52238	1.61554	0.05258
56	6	3.67205	0.24832	-0.17351
57	1	4.46379	2.14346	0.18131
58	6	6.28293	0.38974	-0.30034
59	1	6.32736	1.18272	-1.05567
60	1	6.45955	0.86362	0.67299
61	1	7.12203	-0.28665	-0.48695
62	6	5.80458	-2.75046	-0.72536
63	6	6.19411	-3.46532	0.57543
64	1	6.70437	-2.30902	-1.16941
65	1	5.45451	-3.49147	-1.45440
66	1	6.94798	-4.24120	0.39675
67	1	6.60191	-2.75166	1.29825
68	1	5.32180	-3.93558	1.03967
69	6	-4.97883	-4.01125	0.59530
70	6	-4.97200	-4.39042	2.08206
71	1	-4.56635	-4.84259	0.00964
72	1	-6.01735	-3.90741	0.26091
73	1	-5.52437	-5.32045	2.26114
74	1	-3.94906	-4.52356	2.44721
75	1	-5.43075	-3.59818	2.68191
76	6	-6.18874	-1.08128	0.08625
77	1	-6.85073	-1.94784	0.17035
78	1	-6.42820	-0.40728	0.91741
79	1	-6.45592	-0.55667	-0.83859
80	8	-0.03455	-0.34220	-1.90614

81	8	0.12162	-0.31015	1.62527
82	94	0.03980	-0.29621	-0.14070

UO_2L3^-

E (CAM-B3LYP) = -2617.67183683 Hartree
Zero-point correction= 0.765974 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2616.905863 Hartree
Sum of electronic and thermal Enthalpies= -2616.854987 Hartree
Sum of electronic and thermal Free Energies= -2616.990501 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.401455	-1.450393	-0.254803
2	7	-0.044921	-2.555216	0.155205
3	7	2.326887	-1.396722	-0.012390
4	6	-4.144181	0.096594	-1.024777
5	6	-3.557068	-3.411332	-0.569645
6	6	-2.360455	-2.781350	-0.103933
7	6	-1.110336	-3.342620	0.360948
8	6	-0.729395	-4.548323	1.008819
9	6	0.658492	-4.473277	1.165466
10	6	1.040856	-3.228934	0.625024
11	6	2.289559	-2.600748	0.464773
12	6	3.542171	-0.806053	-0.340739
13	6	4.691312	-1.513015	-0.729992
14	6	5.862086	-0.849320	-1.055843
15	6	-3.837868	-4.879247	-0.679605
16	6	-1.604703	-5.648795	1.534842
17	6	1.555966	-5.466460	1.845438
18	6	1.709888	-5.207229	3.349965
19	1	2.373129	-5.943893	3.818782
20	1	2.122732	-4.209411	3.526837
21	1	0.739402	-5.251299	3.854223
22	8	7.015897	-1.458942	-1.458696
23	6	7.004979	-2.859497	-1.560405
24	1	1.171214	-6.482025	1.692268
25	1	-4.258927	-5.312477	0.235753
26	1	6.794037	-3.337061	-0.594235
27	1	-2.927369	-5.438506	-0.911782
28	1	-4.556115	-5.074468	-1.483348
29	1	-1.155462	-6.106991	2.422598
30	1	-1.776085	-6.456315	0.811830
31	1	2.549577	-5.449863	1.379970
32	1	3.208257	-3.131012	0.735813
33	1	4.639589	-2.590993	-0.810079
34	1	-2.585685	-5.267987	1.831117
35	1	8.003891	-3.149025	-1.891809
36	1	6.266568	-3.209581	-2.293650
37	1	-5.143037	0.133236	-1.451064
38	7	-2.330948	1.510328	-0.165445

39	7	0.076550	2.477730	0.298033
40	7	2.389316	1.220449	0.052860
41	6	-3.579731	1.323371	-0.721464
42	6	-4.249818	2.580056	-0.859067
43	6	-3.394489	3.538388	-0.354004
44	6	-2.227632	2.826132	0.066374
45	6	-0.950690	3.300980	0.554020
46	6	-0.512670	4.448988	1.265740
47	6	0.871570	4.299732	1.412088
48	6	1.193686	3.072530	0.799692
49	6	2.410679	2.392911	0.603015
50	6	3.575639	0.588993	-0.304883
51	6	4.757416	1.259887	-0.658077
52	6	5.895806	0.559125	-1.019247
53	6	-5.627883	2.794226	-1.410577
54	1	-5.841224	2.055961	-2.192122
55	1	-5.676627	3.772645	-1.903993
56	6	-6.723311	2.724213	-0.338690
57	1	-7.717059	2.892545	-0.769990
58	1	-6.554523	3.478044	0.436772
59	1	-6.722783	1.745033	0.150313
60	6	-3.606689	5.021774	-0.371589
61	6	-1.334207	5.549253	1.870347
62	6	1.821975	5.252397	2.075400
63	6	2.129602	6.492669	1.227420
64	1	2.826056	7.166780	1.740016
65	1	2.573513	6.203942	0.269341
66	1	1.214203	7.051513	1.009176
67	8	7.077790	1.133187	-1.391421
68	6	7.133663	2.536066	-1.420075
69	1	1.410458	5.577216	3.040560
70	1	-2.670466	5.551229	-0.568363
71	1	6.413651	2.958566	-2.133205
72	1	-4.009090	5.415826	0.569601
73	1	-4.313254	5.300252	-1.161036
74	1	-0.859161	5.920265	2.786060
75	1	-2.331953	5.196132	2.143967
76	1	2.760030	4.736239	2.311488
77	1	3.354085	2.856658	0.908071
78	1	4.756462	2.341850	-0.682378
79	1	-1.466998	6.414977	1.209022
80	1	8.145613	2.794617	-1.737223
81	1	6.944480	2.972225	-0.430114
82	6	-3.637866	-1.171638	-0.799790
83	6	-4.364811	-2.384977	-1.015983
84	6	-5.748583	-2.500809	-1.582357
85	1	-5.839278	-3.442816	-2.136898
86	1	-5.924616	-1.705849	-2.316120
87	6	-6.844843	-2.448853	-0.510313
88	1	-7.843128	-2.543353	-0.953464
89	1	-6.714711	-3.257537	0.215777

90	1	-6.801832	-1.503865	0.040194
91	92	-0.146236	-0.026923	-0.048351
92	8	-0.185284	-0.076470	1.700896
93	8	-0.060970	0.020651	-1.797596

NpO_2L3^-

E (CAM-B3LYP) = -2655.10539136 Hartree
Zero-point correction= 0.763302 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2654.342089 Hartree
Sum of electronic and thermal Enthalpies= -2654.290946 Hartree
Sum of electronic and thermal Free Energies= -2654.427357 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.466065	-1.488469	-0.211215
2	7	-0.062173	-2.610204	0.008983
3	7	2.376362	-1.423270	-0.069263
4	6	-4.273377	0.091255	-0.731765
5	6	-3.670124	-3.443327	-0.516155
6	6	-2.391542	-2.826817	-0.144813
7	6	-1.131687	-3.419709	0.177401
8	6	-0.712520	-4.682924	0.720402
9	6	0.667222	-4.592777	0.857176
10	6	1.019136	-3.290935	0.399309
11	6	2.293972	-2.643285	0.325689
12	6	3.611438	-0.802067	-0.262084
13	6	4.794409	-1.501391	-0.555692
14	6	5.989972	-0.841779	-0.777447
15	6	-3.959372	-4.901016	-0.687768
16	6	-1.543376	-5.840969	1.191340
17	6	1.601500	-5.608631	1.449543
18	6	1.821407	-5.418372	2.956249
19	1	2.516883	-6.164629	3.358558
20	1	2.225571	-4.423054	3.164664
21	1	0.875231	-5.503530	3.499992
22	8	7.172357	-1.452004	-1.082367
23	6	7.167813	-2.852402	-1.190999
24	1	1.221019	-6.620376	1.265444
25	1	-4.190952	-5.403454	0.257314
26	1	6.874359	-3.333320	-0.248440
27	1	-3.104233	-5.419933	-1.128731
28	1	-4.817038	-5.048596	-1.351349
29	1	-0.983307	-6.441640	1.914695
30	1	-1.848873	-6.516812	0.383806
31	1	2.572436	-5.561268	0.940340
32	1	3.184074	-3.211745	0.621727
33	1	4.751504	-2.578627	-0.646324
34	1	-2.455161	-5.504619	1.693680
35	1	8.190952	-3.142283	-1.437115
36	1	6.494301	-3.197471	-1.986346

37	1	-5.314760	0.123778	-1.036694
38	7	-2.396919	1.549930	-0.113457
39	7	0.055839	2.547102	0.175558
40	7	2.436103	1.260757	0.015244
41	6	-3.680019	1.330060	-0.510202
42	6	-4.392760	2.599070	-0.650361
43	6	-3.507745	3.572728	-0.305142
44	6	-2.262028	2.874638	0.034897
45	6	-0.976753	3.389829	0.395871
46	6	-0.507305	4.593259	1.021316
47	6	0.868240	4.433277	1.156677
48	6	1.165377	3.152600	0.611981
49	6	2.408170	2.450838	0.499689
50	6	3.642384	0.598152	-0.215915
51	6	4.855882	1.261914	-0.463990
52	6	6.021315	0.565718	-0.730470
53	6	-5.819324	2.756090	-1.082228
54	1	-6.055021	2.026771	-1.865989
55	1	-5.957636	3.742485	-1.539409
56	6	-6.817617	2.598088	0.072479
57	1	-7.849976	2.712103	-0.276802
58	1	-6.633324	3.348120	0.847882
59	1	-6.721457	1.613206	0.539788
60	6	-3.724940	5.050437	-0.391693
61	6	-1.291216	5.748583	1.569720
62	6	1.846570	5.404637	1.749778
63	6	2.266182	6.516173	0.779531
64	1	2.983400	7.204540	1.242385
65	1	2.728050	6.091886	-0.117745
66	1	1.396711	7.097112	0.455652
67	8	7.230027	1.141580	-0.995555
68	6	7.288406	2.544976	-1.010182
69	1	1.418649	5.864249	2.650335
70	1	-2.835147	5.554168	-0.778185
71	1	6.632945	2.972315	-1.780228
72	1	-3.958664	5.504429	0.577220
73	1	-4.556877	5.279203	-1.065070
74	1	-0.728386	6.242781	2.368900
75	1	-2.241885	5.422907	2.001197
76	1	2.741121	4.869246	2.089289
77	1	3.322142	2.950213	0.843066
78	1	4.860547	2.343650	-0.483663
79	1	-1.520160	6.517470	0.821687
80	1	8.324079	2.804488	-1.236980
81	1	7.014506	2.974400	-0.037394
82	6	-3.736879	-1.186886	-0.585054
83	6	-4.509568	-2.409822	-0.796183
84	6	-5.944624	-2.472827	-1.224230
85	1	-6.133546	-3.422766	-1.737077
86	1	-6.149765	-1.688523	-1.962184
87	6	-6.927005	-2.335197	-0.053421

88	1	-7.965865	-2.378386	-0.399389
89	1	-6.774519	-3.137757	0.674878
90	1	-6.780000	-1.385481	0.470084
91	8	-0.070240	-0.074762	1.679121
92	8	-0.177870	0.029418	-1.901494
93	93	-0.138557	-0.020937	-0.110813

PuO_2L3^-

E (CAM-B3LYP) = -2694.52435856 Hartree
Zero-point correction= 0.765863 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2693.758495 Hartree
Sum of electronic and thermal Enthalpies= -2693.707634 Hartree
Sum of electronic and thermal Free Energies= -2693.844284 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.408498	-1.440522	-0.252267
2	7	-0.046868	-2.531501	0.169681
3	7	2.335414	-1.391015	-0.021250
4	6	-4.150005	0.094775	-1.039464
5	6	-3.550327	-3.409243	-0.573296
6	6	-2.361608	-2.768843	-0.098371
7	6	-1.111266	-3.320781	0.376387
8	6	-0.730759	-4.523201	1.028407
9	6	0.657616	-4.447138	1.185625
10	6	1.039458	-3.205192	0.641398
11	6	2.292609	-2.587254	0.470416
12	6	3.550187	-0.803990	-0.352690
13	6	4.698788	-1.510907	-0.743197
14	6	5.868135	-0.845951	-1.072603
15	6	-3.820267	-4.879270	-0.683196
16	6	-1.606645	-5.621648	1.557768
17	6	1.554662	-5.439788	1.867019
18	6	1.709259	-5.178794	3.371185
19	1	2.370738	-5.916267	3.841292
20	1	2.124747	-4.181751	3.546497
21	1	0.738659	-5.219840	3.875537
22	8	7.022044	-1.454928	-1.477148
23	6	7.012307	-2.855543	-1.576649
24	1	1.168759	-6.455244	1.715706
25	1	-4.250906	-5.313482	0.227375
26	1	6.804223	-3.331947	-0.609271
27	1	-2.903156	-5.433341	-0.901579
28	1	-4.526476	-5.081179	-1.496049
29	1	-1.165861	-6.066798	2.456512
30	1	-1.765550	-6.439069	0.842948
31	1	2.548310	-5.425082	1.401577
32	1	3.208334	-3.121101	0.746434
33	1	4.647724	-2.589302	-0.819770
34	1	-2.592936	-5.242077	1.837387

35	1	8.010678	-3.144654	-1.910128
36	1	6.272382	-3.207649	-2.307441
37	1	-5.145216	0.131062	-1.474596
38	7	-2.340249	1.498169	-0.163618
39	7	0.070500	2.453959	0.310261
40	7	2.396073	1.218249	0.041889
41	6	-3.584950	1.319469	-0.729956
42	6	-4.248677	2.579777	-0.871037
43	6	-3.392636	3.532314	-0.357074
44	6	-2.232917	2.811059	0.071185
45	6	-0.956550	3.277808	0.567512
46	6	-0.520180	4.422910	1.282961
47	6	0.864709	4.274038	1.429633
48	6	1.187643	3.049846	0.813488
49	6	2.410312	2.382106	0.606534
50	6	3.582827	0.591472	-0.317780
51	6	4.763230	1.263431	-0.673011
52	6	5.901007	0.562592	-1.036900
53	6	-5.621276	2.801088	-1.433276
54	1	-5.831893	2.064458	-2.217204
55	1	-5.661849	3.780324	-1.926021
56	6	-6.725806	2.734907	-0.370508
57	1	-7.715452	2.908070	-0.809442
58	1	-6.559801	3.487173	0.407101
59	1	-6.733402	1.755214	0.117416
60	6	-3.596063	5.017007	-0.374016
61	6	-1.343572	5.519747	1.891343
62	6	1.813970	5.226696	2.094628
63	6	2.119142	6.469522	1.249467
64	1	2.814287	7.143999	1.763431
65	1	2.563565	6.183677	0.290748
66	1	1.202590	7.026943	1.032432
67	8	7.082358	1.137055	-1.411516
68	6	7.137621	2.539859	-1.439979
69	1	1.402164	5.548860	3.060630
70	1	-2.655005	5.541477	-0.561321
71	1	6.415631	2.962375	-2.151142
72	1	-4.004712	5.412441	0.564011
73	1	-4.293885	5.300954	-1.169405
74	1	-0.875837	5.880009	2.815224
75	1	-2.344869	5.166964	2.152037
76	1	2.753139	4.711857	2.329277
77	1	3.350426	2.849879	0.917335
78	1	4.761572	2.345574	-0.695117
79	1	-1.467796	6.392782	1.237902
80	1	8.148677	2.798957	-1.759612
81	1	6.950704	2.975848	-0.449497
82	6	-3.641317	-1.171170	-0.808553
83	6	-4.360221	-2.389165	-1.029090
84	6	-5.738247	-2.513766	-1.607498
85	1	-5.818448	-3.456266	-2.163045

86	1	-5.913034	-1.719564	-2.342482
87	6	-6.844355	-2.468877	-0.545286
88	1	-7.838282	-2.569345	-0.997012
89	1	-6.715541	-3.276936	0.181765
90	1	-6.811800	-1.523776	0.005761
91	8	-0.195886	-0.074167	1.673314
92	8	-0.069009	0.019728	-1.759933
93	94	-0.144482	-0.026665	-0.042829

UO_2L3^{2-}

E (CAM-B3LYP) = -2617.60619876 Hartree
Zero-point correction= 0.760872 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2616.845327 Hartree
Sum of electronic and thermal Enthalpies= -2616.794151 Hartree
Sum of electronic and thermal Free Energies= -2616.930400 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.409724	-1.456020	-0.255676
2	7	-0.022196	-2.560573	0.121456
3	7	2.381817	-1.395295	-0.044603
4	6	-4.176183	0.094334	-1.017643
5	6	-3.530236	-3.438485	-0.535284
6	6	-2.348922	-2.817601	-0.094030
7	6	-1.080354	-3.353733	0.331663
8	6	-0.677079	-4.563163	0.976626
9	6	0.708116	-4.478721	1.120292
10	6	1.081609	-3.227024	0.582035
11	6	2.325665	-2.602897	0.434841
12	6	3.598748	-0.809270	-0.343516
13	6	4.759774	-1.509105	-0.706071
14	6	5.942346	-0.844413	-1.005930
15	6	-3.812250	-4.906286	-0.667488
16	6	-1.551538	-5.651694	1.527279
17	6	1.616375	-5.464017	1.797808
18	6	1.783416	-5.193834	3.299436
19	1	2.457780	-5.920747	3.771468
20	1	2.187628	-4.190001	3.460560
21	1	0.816674	-5.240163	3.811021
22	8	7.112501	-1.467017	-1.378432
23	6	7.084611	-2.862962	-1.480052
24	1	1.234304	-6.483662	1.657787
25	1	-4.299319	-5.349993	0.212967
26	1	6.843066	-3.342131	-0.520865
27	1	-2.892970	-5.472511	-0.843309
28	1	-4.476959	-5.095977	-1.519833
29	1	-1.112979	-6.084350	2.435375
30	1	-1.722235	-6.484274	0.830581
31	1	2.607234	-5.446152	1.325424
32	1	3.237314	-3.136447	0.733482

33	1	4.709827	-2.587964	-0.780920
34	1	-2.535347	-5.256405	1.796151
35	1	8.087611	-3.169629	-1.788128
36	1	6.358405	-3.207947	-2.229002
37	1	-5.181632	0.129847	-1.426607
38	7	-2.341127	1.513010	-0.166171
39	7	0.096103	2.484165	0.265260
40	7	2.442919	1.223965	0.017429
41	6	-3.594313	1.334885	-0.693862
42	6	-4.252326	2.588933	-0.815371
43	6	-3.369628	3.557824	-0.321282
44	6	-2.218099	2.857810	0.077661
45	6	-0.925176	3.310640	0.526755
46	6	-0.467439	4.460484	1.238254
47	6	0.914003	4.303658	1.373321
48	6	1.229264	3.071687	0.760023
49	6	2.443299	2.397616	0.575575
50	6	3.632033	0.595832	-0.308313
51	6	4.824454	1.258706	-0.635265
52	6	5.975362	0.556019	-0.969937
53	6	-5.640519	2.807401	-1.336679
54	1	-5.847074	2.113751	-2.162327
55	1	-5.726706	3.816089	-1.765161
56	6	-6.730674	2.635502	-0.268530
57	1	-7.738564	2.791127	-0.678747
58	1	-6.580666	3.346406	0.551358
59	1	-6.683366	1.628852	0.158118
60	6	-3.582745	5.042469	-0.362684
61	6	-1.290223	5.544899	1.868224
62	6	1.873154	5.252004	2.029820
63	6	2.192858	6.483315	1.172252
64	1	2.895359	7.159803	1.676936
65	1	2.633537	6.178826	0.217457
66	1	1.280313	7.044501	0.947055
67	8	7.173781	1.141604	-1.311327
68	6	7.210844	2.540699	-1.341533
69	1	1.464765	5.592265	2.992209
70	1	-2.637406	5.574472	-0.503812
71	1	6.502456	2.956770	-2.071198
72	1	-4.050255	5.453396	0.543935
73	1	-4.236051	5.315325	-1.201179
74	1	-0.827109	5.888650	2.802848
75	1	-2.290774	5.177436	2.113693
76	1	2.807679	4.730126	2.269167
77	1	3.378699	2.862796	0.911928
78	1	4.823923	2.341211	-0.655032
79	1	-1.422924	6.434613	1.236544
80	1	8.227399	2.815854	-1.634552
81	1	6.990443	2.981058	-0.358934
82	6	-3.652019	-1.188939	-0.771156
83	6	-4.366204	-2.401917	-0.969237

84	6	-5.761547	-2.524666	-1.502615
85	1	-5.892204	-3.499868	-1.992883
86	1	-5.934767	-1.772529	-2.283541
87	6	-6.845230	-2.370370	-0.425252
88	1	-7.858200	-2.453259	-0.843986
89	1	-6.730051	-3.137707	0.348101
90	1	-6.752680	-1.395867	0.064015
91	92	-0.260726	-0.023652	-0.077740
92	8	-0.273681	-0.074104	1.677591
93	8	-0.150268	0.023505	-1.830429

NpO_2L3^{2-}

E (CAM-B3LYP) = -2655.09426284 Hartree
Zero-point correction= 0.761727 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2654.332536 Hartree
Sum of electronic and thermal Enthalpies= -2654.281127 Hartree
Sum of electronic and thermal Free Energies= -2654.419400 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.488554	-1.498794	-0.181829
2	7	-0.041313	-2.629782	-0.056787
3	7	2.408552	-1.424798	-0.113522
4	6	-4.297282	0.083866	-0.699787
5	6	-3.635610	-3.448705	-0.541996
6	6	-2.398423	-2.827067	-0.150592
7	6	-1.100092	-3.409747	0.176952
8	6	-0.696955	-4.631765	0.794217
9	6	0.693988	-4.554760	0.914467
10	6	1.057653	-3.294969	0.378726
11	6	2.314717	-2.644770	0.304537
12	6	3.637092	-0.809246	-0.295399
13	6	4.828836	-1.503630	-0.569002
14	6	6.030700	-0.845005	-0.773401
15	6	-3.893076	-4.909131	-0.762469
16	6	-1.560278	-5.734766	1.335841
17	6	1.607701	-5.549252	1.572193
18	6	1.791572	-5.298972	3.075584
19	1	2.471157	-6.031714	3.531762
20	1	2.195989	-4.296863	3.246564
21	1	0.830063	-5.351591	3.596471
22	8	7.224000	-1.467510	-1.059854
23	6	7.202389	-2.863774	-1.162990
24	1	1.225323	-6.568179	1.424426
25	1	-4.252019	-5.435725	0.132142
26	1	6.887252	-3.341658	-0.224890
27	1	-2.981851	-5.420254	-1.087622
28	1	-4.650328	-5.058310	-1.542466
29	1	-1.074001	-6.230316	2.184950
30	1	-1.792749	-6.519834	0.602322

31	1	2.594081	-5.528631	1.090173
32	1	3.204890	-3.199070	0.636159
33	1	4.784127	-2.581731	-0.654553
34	1	-2.517294	-5.344821	1.696299
35	1	8.225683	-3.171562	-1.393323
36	1	6.535149	-3.207781	-1.965243
37	1	-5.340691	0.116518	-1.009962
38	7	-2.420802	1.549614	-0.086950
39	7	0.075747	2.562030	0.104635
40	7	2.469291	1.260501	-0.038106
41	6	-3.717707	1.330325	-0.490086
42	6	-4.395096	2.587258	-0.652854
43	6	-3.477992	3.567262	-0.330143
44	6	-2.271320	2.868202	0.024168
45	6	-0.948735	3.373304	0.382355
46	6	-0.494426	4.540206	1.065168
47	6	0.892707	4.394907	1.181699
48	6	1.202206	3.153490	0.574654
49	6	2.429124	2.451468	0.462677
50	6	3.669165	0.600687	-0.253448
51	6	4.891268	1.255856	-0.486000
52	6	6.062528	0.557111	-0.731152
53	6	-5.821763	2.786809	-1.070043
54	1	-6.127386	1.997578	-1.767616
55	1	-5.917054	3.730124	-1.624278
56	6	-6.799201	2.810460	0.113133
57	1	-7.835499	2.961405	-0.217313
58	1	-6.540051	3.614744	0.809442
59	1	-6.748289	1.868565	0.668132
60	6	-3.668058	5.048534	-0.463112
61	6	-1.309204	5.639939	1.680557
62	6	1.852416	5.357284	1.817316
63	6	2.194720	6.557914	0.924869
64	1	2.898290	7.244530	1.414998
65	1	2.642437	6.218813	-0.014926
66	1	1.289976	7.120053	0.671076
67	8	7.283102	1.141110	-0.981316
68	6	7.324340	2.540589	-1.002542
69	1	1.439199	5.733339	2.764402
70	1	-2.731225	5.536554	-0.748229
71	1	6.674392	2.960526	-1.782519
72	1	-4.013312	5.535428	0.459041
73	1	-4.409073	5.278970	-1.238974
74	1	-0.806137	6.043286	2.568988
75	1	-2.288402	5.272464	2.002642
76	1	2.780624	4.837047	2.083976
77	1	3.341915	2.938107	0.835477
78	1	4.894800	2.338108	-0.507177
79	1	-1.492952	6.491155	1.009328
80	1	8.360751	2.815086	-1.215635
81	1	7.029578	2.976528	-0.037774

82	6	-3.774407	-1.197655	-0.566984
83	6	-4.507791	-2.410944	-0.802606
84	6	-5.942680	-2.520831	-1.225059
85	1	-6.081776	-3.425408	-1.832077
86	1	-6.213001	-1.679664	-1.874888
87	6	-6.918586	-2.568135	-0.041289
88	1	-7.961187	-2.651728	-0.375784
89	1	-6.695935	-3.422617	0.606138
90	1	-6.823478	-1.663486	0.567253
91	8	-0.147610	-0.078275	1.640187
92	8	-0.174305	0.031351	-1.950937
93	93	-0.181082	-0.022977	-0.153899

PuO_2L3^{2-}

E (CAM-B3LYP) = -2694.5306659 Hartree
Zero-point correction= 0.761892 (Hartree/Particle)
Sum of electronic and zero-point Energies= -2693.768774 Hartree
Sum of electronic and thermal Enthalpies= -2693.717472 Hartree
Sum of electronic and thermal Free Energies= -2693.855759 Hartree

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	7	-2.49505	-1.49411	-0.16684
2	7	-0.04469	-2.62003	-0.05002
3	7	2.40718	-1.42150	-0.11591
4	6	-4.30409	0.08362	-0.69328
5	6	-3.63242	-3.44669	-0.54942
6	6	-2.40080	-2.82171	-0.14527
7	6	-1.10181	-3.40222	0.18115
8	6	-0.69825	-4.62733	0.79226
9	6	0.69254	-4.55061	0.91124
10	6	1.05488	-3.28808	0.38084
11	6	2.31256	-2.64068	0.30383
12	6	3.63591	-0.80789	-0.30027
13	6	4.82747	-1.50237	-0.57443
14	6	6.02875	-0.84329	-0.78163
15	6	-3.88111	-4.90661	-0.78306
16	6	-1.56192	-5.73232	1.32927
17	6	1.60744	-5.54881	1.56169
18	6	1.79571	-5.30601	3.06578
19	1	2.47542	-6.04186	3.51677
20	1	2.20218	-4.30534	3.24042
21	1	0.83545	-5.35978	3.58888
22	8	7.22206	-1.46570	-1.06890
23	6	7.20099	-2.86209	-1.16990
24	1	1.22367	-6.56670	1.41028
25	1	-4.24296	-5.44230	0.10501
26	1	6.88753	-3.33877	-0.23062
27	1	-2.96517	-5.41057	-1.10635
28	1	-4.63272	-5.05354	-1.56900

29	1	-1.07891	-6.22769	2.18045
30	1	-1.78969	-6.51743	0.59424
31	1	2.59254	-5.52682	1.07711
32	1	3.20261	-3.19633	0.63387
33	1	4.78330	-2.58071	-0.65767
34	1	-2.52134	-5.34416	1.68523
35	1	8.22407	-3.16976	-1.40139
36	1	6.53265	-3.20767	-1.97058
37	1	-5.34566	0.11615	-1.00979
38	7	-2.42806	1.54505	-0.07313
39	7	0.07077	2.55526	0.10525
40	7	2.46690	1.25980	-0.04502
41	6	-3.72389	1.32889	-0.48125
42	6	-4.39734	2.58682	-0.65377
43	6	-3.47823	3.56549	-0.33340
44	6	-2.27564	2.86340	0.02949
45	6	-0.95227	3.36727	0.38427
46	6	-0.49747	4.53607	1.06373
47	6	0.88977	4.39178	1.17707
48	6	1.19799	3.14926	0.57148
49	6	2.42567	2.45007	0.45696
50	6	3.66746	0.60202	-0.26063
51	6	4.88882	1.25765	-0.49560
52	6	6.06008	0.55888	-0.74139
53	6	-5.82152	2.78824	-1.07859
54	1	-6.12556	1.99763	-1.77533
55	1	-5.91212	3.73021	-1.63596
56	6	-6.80491	2.81743	0.09955
57	1	-7.83923	2.96998	-0.23644
58	1	-6.54727	3.62298	0.79498
59	1	-6.75905	1.87691	0.65731
60	6	-3.66137	5.04673	-0.47628
61	6	-1.31260	5.63563	1.67895
62	6	1.85060	5.35606	1.80809
63	6	2.19145	6.55397	0.91141
64	1	2.89557	7.24232	1.39836
65	1	2.63794	6.21193	-0.02790
66	1	1.28621	7.11507	0.65708
67	8	7.28020	1.14307	-0.99393
68	6	7.32116	2.54252	-1.01524
69	1	1.43872	5.73518	2.75458
70	1	-2.72117	5.52883	-0.76060
71	1	6.67020	2.96240	-1.79443
72	1	-4.00795	5.54101	0.44150
73	1	-4.39838	5.27582	-1.25640
74	1	-0.81117	6.03779	2.56894
75	1	-2.29268	5.26823	1.99851
76	1	2.77934	4.83685	2.07497
77	1	3.33832	2.93787	0.82889
78	1	4.89184	2.33993	-0.51778
79	1	-1.49470	6.48782	1.00845

80	1	8.35727	2.81726	-1.22960
81	1	7.02743	2.97845	-0.05016
82	6	-3.77940	-1.19658	-0.55957
83	6	-4.50708	-2.41081	-0.80845
84	6	-5.93806	-2.52341	-1.24332
85	1	-6.06807	-3.42288	-1.85997
86	1	-6.20721	-1.67744	-1.88737
87	6	-6.92348	-2.58658	-0.06824
88	1	-7.96291	-2.67219	-0.41210
89	1	-6.70194	-3.44602	0.57301
90	1	-6.83804	-1.68720	0.54953
91	8	-0.10618	-0.07802	1.63677
92	8	-0.21099	0.03232	-1.91089
93	94	-0.17353	-0.02262	-0.13615
