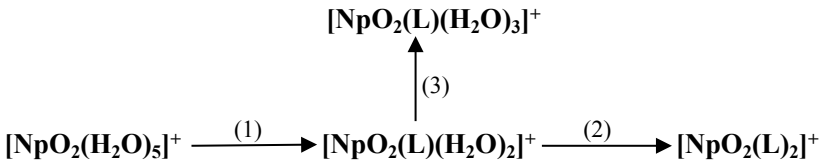
$[NpO_2(H_2O)_5]^+ \rightarrow [NpO_2(H_2O)_6]^+$ (kcal/mol)

GAS：ΔH = -11.7，TΔS = -12.5，ΔG = 0.8

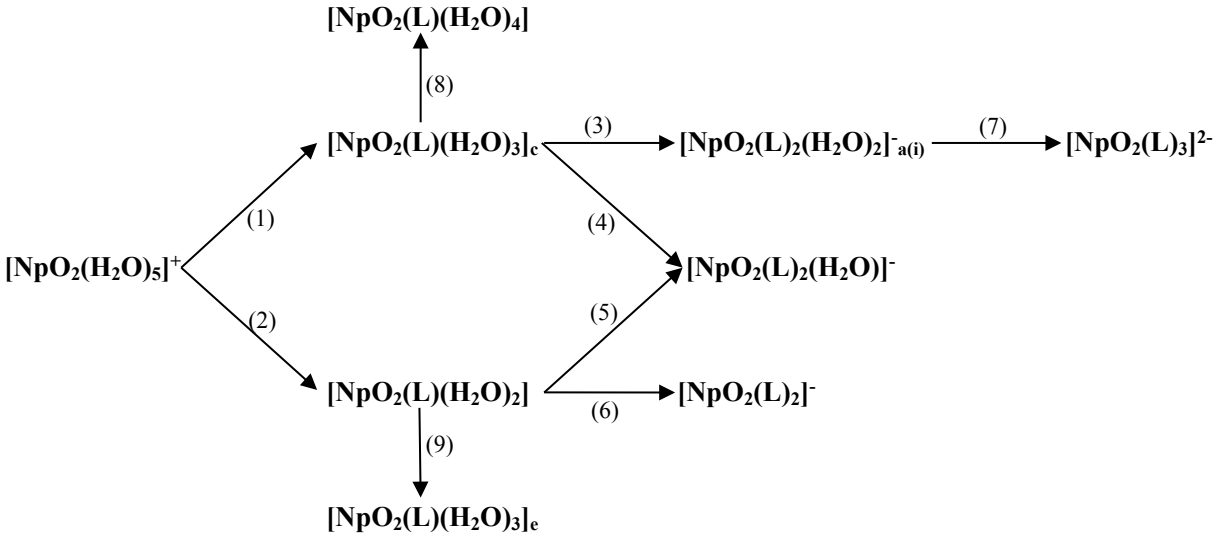
SMD：ΔH = -14.8，TΔS = -11.0，ΔG = -3.7

L = TMOGA：



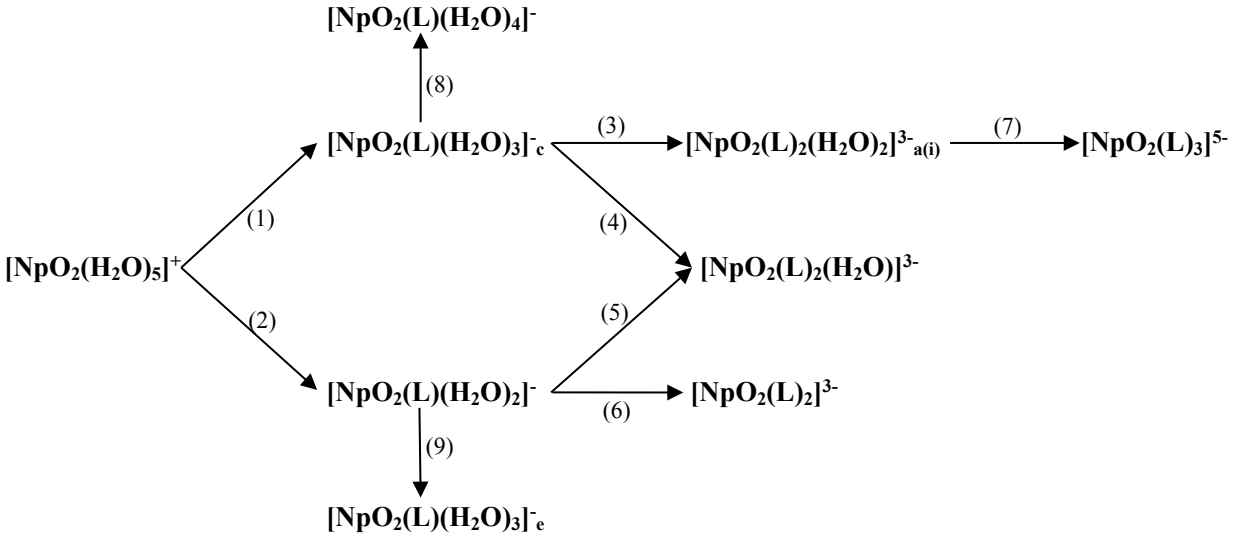
	GAS			SMD		
(kcal/mol)	ΔH	TΔS	ΔG	ΔH	TΔS	ΔG
(1)	-5.5	18.1	-23.6	3.4	17.3	-13.9
(2)	-15.8	4.2	-20.0	3.2	3.1	0.1
(3)	-9.6	-13.9	4.3	-16.0	-13.1	-2.9

L = DMOGA$^-$：



	GAS			SMD		
(kcal/mol)	ΔH	*T*ΔS	ΔG	ΔH	*T*ΔS	ΔG
(1)	-111.3	6.5	-117.8	-2.2	6.7	-8.9
(2)	-101.0	13.9	-114.9	-3.9	14.9	-18.7
(3)	-30.5(-34.4)	-1.1(-2.0)	-29.4(-32.4)	-9.5(-10.5)	-3.9(-4.0)	-5.6(-6.5)
(4)	-26.3	5.6	-31.9	-13.6	2.3	-15.9
(5)	-36.6	-1.8	-34.8	-11.9	-5.9	-6.0
(6)	-28.4	4.6	-33.0	-9.0	5.9	-14.9
(7)	52.4(56.3)	7.0(7.8)	45.4(48.5)	2.4(3.4)	6.6(6.7)	-4.2(-3.3)
(8)	-5.5	-10.5	5.0	-19.1	-10.8	-8.3
(9)	-18.4	-11. 5	-6.9	-11.5	-10.8	-0.6

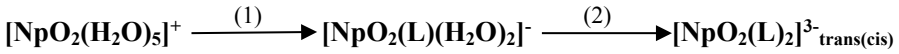
L = ODA^{2-}:



	GAS			SMD		
(kcal/mol)	ΔH	*T*ΔS	ΔG	ΔH	*T*ΔS	ΔG
(1)	-174.6	5.7	-180.3	-11.5	7.5	-19.0
(2)	-202.9	12.8	-215.6	-18.8	15.1	-33.8
(3)	13.6(11.1)	-0.3 (-0.9)	13.9 (12.0)	-3.1(-2.9)	-7.6(-5.9)	4.5(3.0)
(4)	20.8	5.7	15.0	-12.2	3.2	-15.4
(5)	49.0	-1.3	50.3	-4.9	-4.3	-0.6
(6)	80.9	7.7	73.2	-2.4	4.3	-6.7
(7)	200.8(203.3)	10.9(11.5)	189.9(191.8)	4.5(4.3)	10.9(9.1)	-6.3(-4.8)
(8)	-47.3	-14.3	-33.0	-13.6	-15.3	1.6

(9)	-26.3	-11.3	-15.1	-8.2	-10.9	2.7

L = MIDA^{2-}:



	GAS			SMD		
(kcal/mol)	ΔH	*T*ΔS	ΔG	ΔH	*T*ΔS	ΔG
(1)	-200.8	12.6	-213.3	-17.2	16.4	-33.5
(2)	88.3(96.5)	8.9(8.8)	79.4(87.7)	1.0(7.8)	5.0(3.6)	-4.1(4.2)

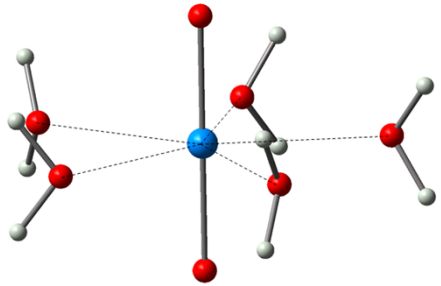
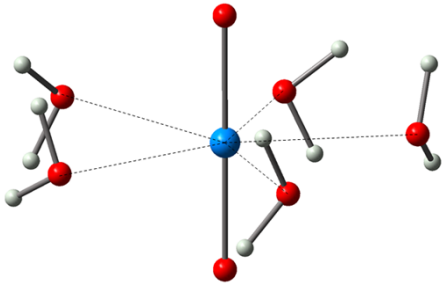
Np-O$_{*\text{-}n}$: yl — the oxygen of the neptunyl
water — the oxygen of the water
carb — the oxygen of the carboxyl of the ligand
amide — the oxygen of the amido of the ligand
ether — the oxygen of the ether of the ligand
n — the serial number of the atom

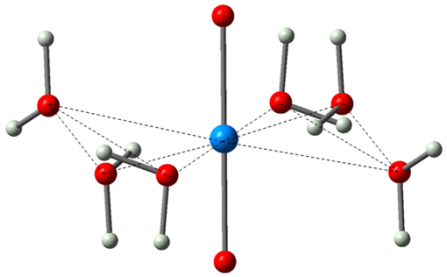
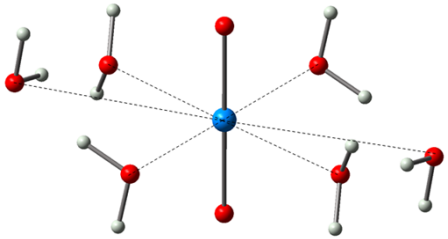
d, d_1/d_2 — Å

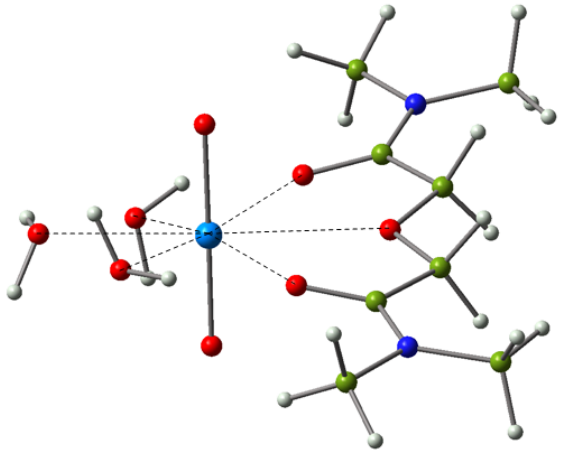
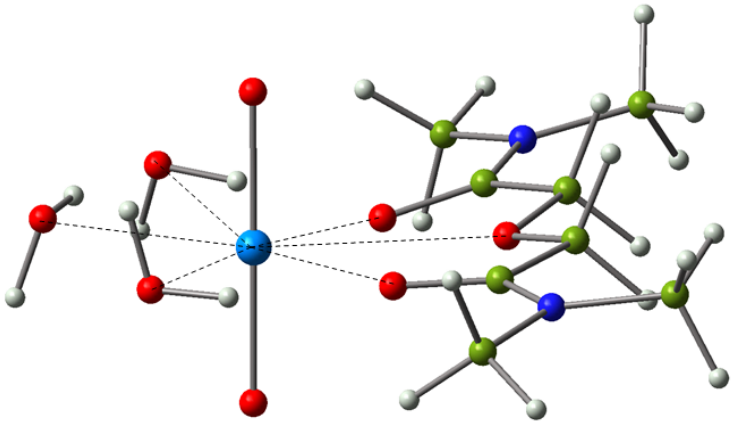
ρ_b — e$^-$/bohr^3

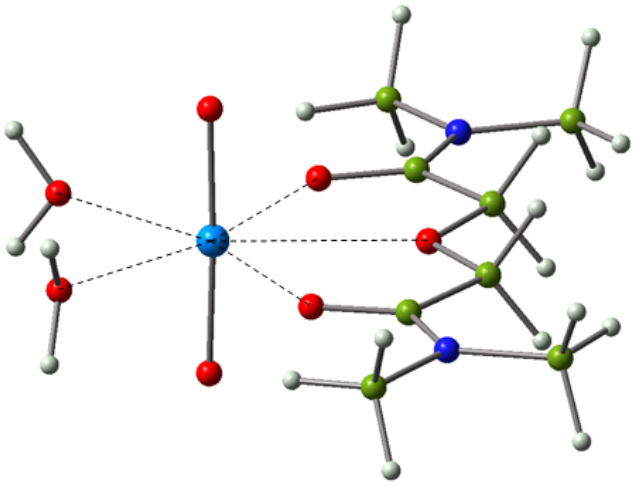
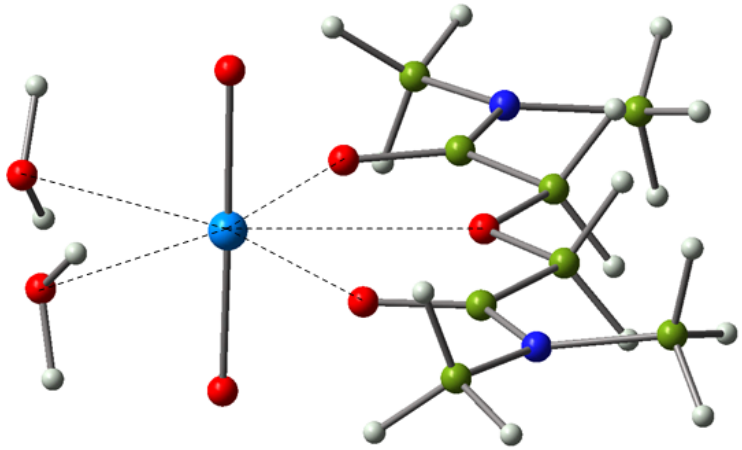
$\nabla^2\rho_b$ — e$^-$/bohr^5

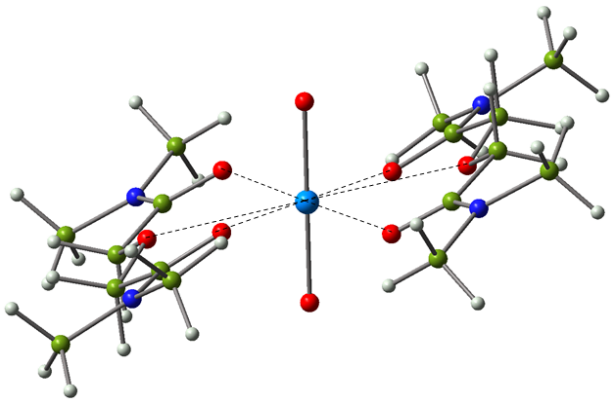
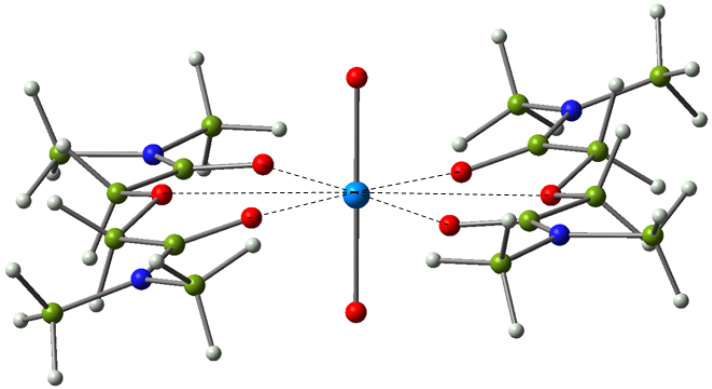
H_b — a.u.

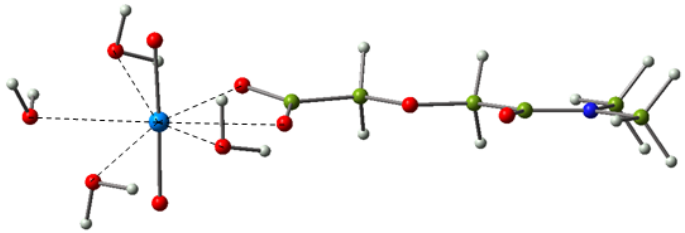
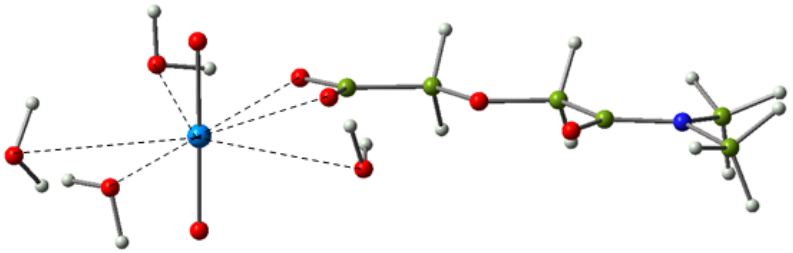
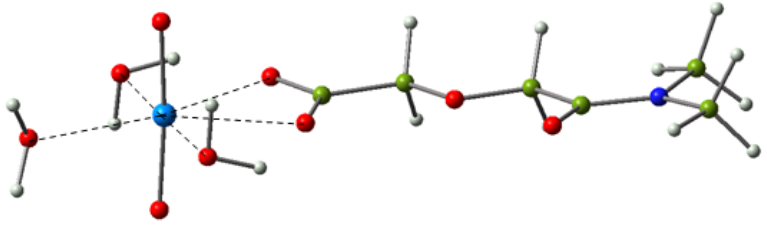
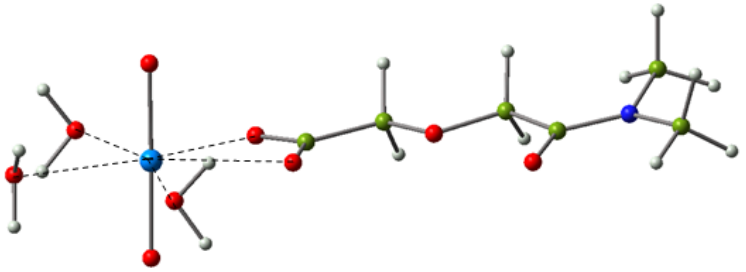
$[NpO_2]^+$																
	GAS								SMD							
																
∠O-Np-O	179.2								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-1}	1.736	0.965/0.771	2.25	2.97	0.336	0.117	-0.35	1.174	1.818	1.006/0.812	2.02	2.80	0.269	0.238	-0.22	1.464
Np-O_{yl-2}	1.736	0.962/0.772	2.25	2.97	0.335	0.117	-0.35	1.174	1.818	1.006/0.812	2.02	2.80	0.269	0.238	-0.22	1.463
$[NpO_2(H_2O)_5]^+$																
	GAS								SMD							
																
∠O-Np-O	180.0								179.8							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-1}	1.781	0.982/0.799	2.19	2.86	0.294	0.189	-0.27	1.331	1.824	1.005/0.818	2.04	2.76	0.262	0.245	-0.21	1.490
Np-O_{yl-2}	1.781	0.982/0.799	2.19	2.86	0.294	0.189	-0.27	1.331	1.824	1.005/0.818	2.04	2.76	0.262	0.243	-0.21	1.486

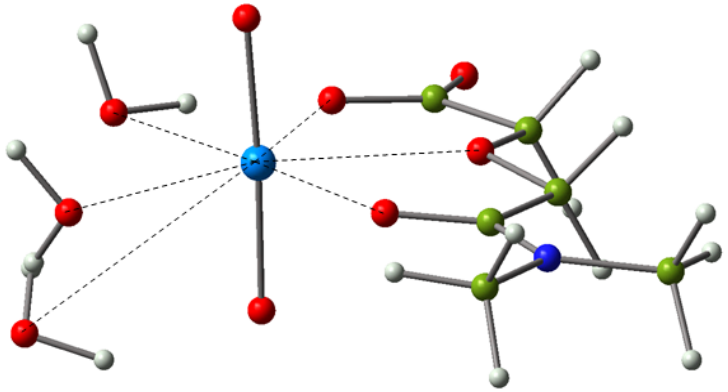
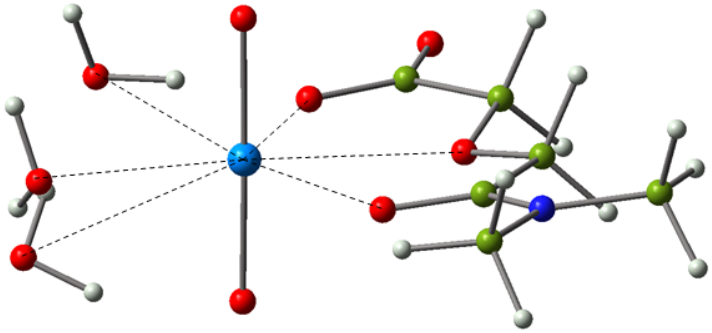
Np-$O_{water-4}$	2.566	1.396/1.170	0.29	0.85	0.040	0.164	1.05×10^{-3}	4.559	2.686	1.442/1.244	0.27	0.75	0.031	0.116	0.69×10^{-3}	4.266
Np-$O_{water-7}$	2.565	1.396/1.170	0.29	0.86	0.040	0.164	1.07×10^{-3}	4.564	2.752	1.471/1.281	0.27	0.69	0.027	0.098	0.59×10^{-3}	4.270
Np-$O_{water-10}$	2.566	1.397/1.170	0.29	0.86	0.040	0.164	1.07×10^{-3}	4.566	2.702	1.449/1.253	0.29	0.75	0.030	0.111	0.61×10^{-3}	4.246
Np-$O_{water-13}$	2.566	1.396/1.170	0.29	0.86	0.040	0.164	1.06×10^{-3}	4.564	2.643	1.422/1.221	0.29	0.79	0.034	0.130	0.95×10^{-3}	4.286
Np-$O_{water-16}$	2.566	1.397/1.171	0.29	0.85	0.040	0.164	1.05×10^{-3}	4.560	2.759	1.474/1.285	0.27	0.69	0.027	0.096	0.48×10^{-3}	4.267
$[NpO_2(H_2O)_6]^+$																
	GAS								SMD							
																
∠O-Np-O	180.0								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-1}	1.788	0.986/0.801	2.16	2.82	0.289	0.197	-0.26	1.352	1.827	1.007/0.820	2.03	2.76	0.260	0.248	-0.21	1.500
Np-O_{yl-2}	1.788	0.986/0.801	2.16	2.82	0.289	0.197	-0.26	1.352	1.827	1.007/0.820	2.03	2.76	0.260	0.248	-0.21	1.501
Np-$O_{water-4}$	2.655	1.438/1.218	0.28	0.74	0.035	0.129	-0.07×10^{-3}	4.374	2.639	1.426/1.214	0.22	0.78	0.033	0.132	1.69×10^{-3}	4.639
Np-$O_{water-7}$	2.647	1.435/1.214	0.28	0.75	0.036	0.131	-0.08×10^{-3}	4.364	3.748		0.07	0.07				
Np-$O_{water-10}$	2.649	1.435/1.215	0.28	0.75	0.035	0.131	-0.06×10^{-3}	4.368	2.587	1.394/1.193	0.35	0.86	0.039	0.150	0.75×10^{-3}	4.195
Np-$O_{water-13}$	2.655	1.438/1.218	0.28	0.74	0.035	0.129	-0.07×10^{-3}	4.374	2.639	1.426/1.214	0.22	0.78	0.033	0.132	1.69×10^{-3}	4.639
Np-$O_{water-16}$	2.647	1.435/1.214	0.28	0.75	0.036	0.131	-0.08×10^{-3}	4.364	3.748		0.07	0.07				
Np-$O_{water-19}$	2.649	1.435/1.215	0.28	0.75	0.035	0.131	-0.06×10^{-3}	4.368	2.587	1.394/1.193	0.35	0.86	0.039	0.150	0.75×10^{-3}	4.195
$[NpO_2(TMOGA)(H_2O)_3]^+$																

	GAS								SMD							
																
∠O-Np-O	179.0								179.5							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}30}$	1.780	0.983/0.798	2.16	2.86	0.294	0.190	-0.27	1.326	1.834	1.014/0.820	2.01	2.77	0.257	0.268	-0.20	1.554
Np-$O_{yl\text{-}31}$	1.788	0.986/0.802	2.15	2.83	0.288	0.201	-0.26	1.359	1.835	1.014/0.820	2.01	2.76	0.257	0.268	-0.20	1.554
Np-$O_{water\text{-}39}$	2.700	1.459/1.242	0.27	0.68	0.032	0.116	-0.28×10^{-3}	4.263	3.520		0.08	0.13				
Np-$O_{water\text{-}36}$	2.605	1.409/1.196	0.28	0.80	0.038	0.145	0.38×10^{-3}	4.017	2.636	1.421/1.216	0.34	0.80	0.036	0.133	0.31×10^{-3}	4.323
Np-$O_{water\text{-}33}$	2.608	1.411/1.198	0.29	0.79	0.038	0.144	0.04×10^{-3}	3.983	2.743	1.472/1.272	0.29	0.69	0.028	0.102	0.37×10^{-3}	4.172
Np-$O_{amide\text{-}8}$	2.573	1.406/1.169	0.25	0.87	0.038	0.157	1.52×10^{-3}	4.471	2.749	1.491/1.261	0.22	0.74	0.025	0.097	1.11×10^{-3}	4.633
Np-$O_{ether\text{-}4}$	2.774	1.505/1.269	0.13	0.66	0.023	0.096	1.28×10^{-3}	5.112	2.951	1.583/1.369	0.12	0.55	0.016	0.061	0.97×10^{-3}	5.166
Np-$O_{amide\text{-}9}$	2.599	1.420/1.181	0.24	0.85	0.036	0.147	1.39×10^{-3}	4.546	2.675	1.454/1.223	0.22	0.80	0.030	0.118	1.46×10^{-3}	4.737
$[NpO_2(TMOGA)(H_2O)_2]^+$																

																
∠O-Np-O	177.2								178.9							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}30}$	1.784	0.984/0.800	2.16	2.85	0.291	0.197	-0.26	1.347	1.822	1.004/0.818	2.03	2.77	0.263	0.243	-0.21	1.485
Np-$O_{yl\text{-}31}$	1.783	0.984/0.800	2.16	2.85	0.292	0.196	-0.26	1.346	1.822	1.004/0.818	2.03	2.77	0.263	0.243	-0.21	1.487
Np-$O_{water\text{-}36}$	2.523	1.381/1.143	0.27	0.91	0.042	0.186	2.08×10^{-3}	5.053	2.740	1.467/1.274	0.29	0.73	0.027	0.101	0.75×10^{-3}	4.349
Np-$O_{water\text{-}33}$	2.546	1.389/1.157	0.28	0.88	0.041	0.175	1.61×10^{-3}	4.806	2.740	1.466/1.274	0.29	0.73	0.028	0.101	0.75×10^{-3}	4.333
Np-$O_{amide\text{-}8}$	2.498	1.368/1.132	0.30	0.98	0.045	0.193	1.55×10^{-3}	4.440	2.563	1.395/1.170	0.31	0.94	0.039	0.157	1.82×10^{-3}	4.338
Np-$O_{ether\text{-}4}$	2.701	1.470/1.231	0.14	0.71	0.028	0.116	1.50×10^{-3}	4.919	2.718	1.472/1.246	0.16	0.71	0.026	0.107	1.65×10^{-3}	4.810
Np-$O_{amide\text{-}9}$	2.482	1.359/1.124	0.30	0.99	0.047	0.202	1.52×10^{-3}	4.455	2.574	1.400/1.175	0.30	0.93	0.038	0.153	1.80×10^{-3}	4.348
$[NpO_2(TMOGA)_2]^+$																
	GAS								SMD							

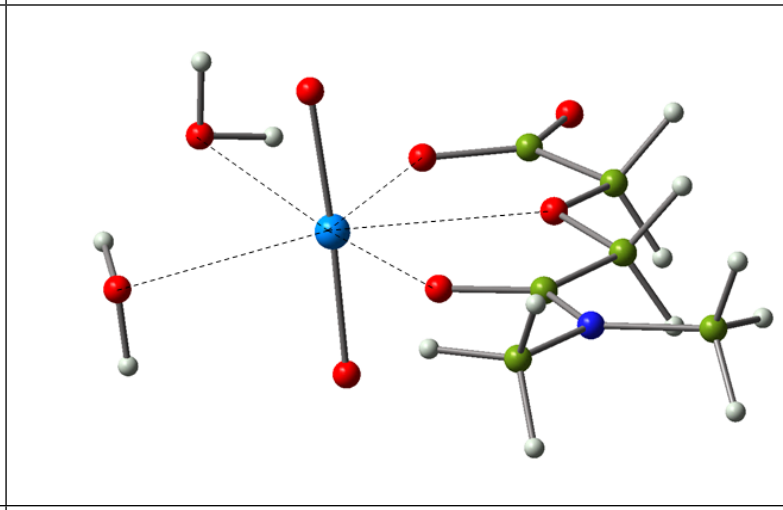
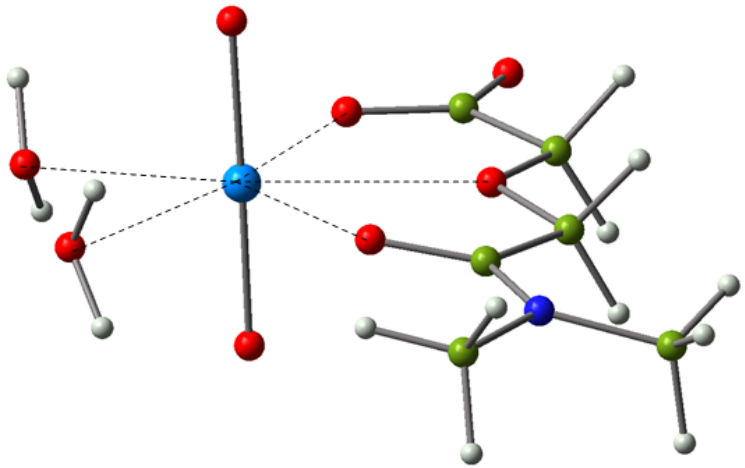
																
∠O-Np-O	180.0								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}59}$	1.795	0.993/0.802	2.12	2.84	0.285	0.226	-0.25	1.414	1.829	1.009/0.821	2.01	2.77	0.258	0.251	-0.20	1.513
Np-$O_{yl\text{-}60}$	1.795	0.993/0.802	2.12	2.84	0.285	0.226	-0.25	1.415	1.829	1.009/0.821	2.01	2.77	0.258	0.251	-0.20	1.513
Np-$O_{amide\text{-}37}$	2.568	1.408/1.162	0.26	0.89	0.039	0.161	1.30×10^{-3}	4.425	2.586	1.409/1.179	0.29	0.91	0.036	0.148	2.14×10^{-3}	4.475
Np-$O_{ether\text{-}33}$	2.821	1.523/1.299	0.13	0.61	0.022	0.088	0.68×10^{-3}	6.502	2.980	1.584/1.397	0.12	0.53	0.014	0.059	1.08×10^{-3}	6.591
Np-$O_{amide\text{-}38}$	2.567	1.408/1.162	0.26	0.89	0.039	0.161	1.33×10^{-3}	4.425	2.660	1.444/1.218	0.27	0.85	0.030	0.121	1.71×10^{-3}	4.495
Np-$O_{amide\text{-}8}$	2.568	1.408/1.162	0.26	0.89	0.039	0.161	1.32×10^{-3}	4.425	2.586	1.409/1.179	0.29	0.92	0.036	0.148	2.14×10^{-3}	4.475
Np-$O_{ether\text{-}4}$	2.820	1.523/1.299	0.13	0.61	0.022	0.088	0.69×10^{-3}	6.502	2.979	1.584/1.397	0.12	0.53	0.014	0.059	1.08×10^{-3}	6.582
Np-$O_{amide\text{-}9}$	2.567	1.408/1.162	0.26	0.89	0.039	0.161	1.33×10^{-3}	4.426	2.660	1.444/1.218	0.27	0.85	0.030	0.121	1.71×10^{-3}	4.495
$[NpO_2(DMOGA)(H_2O)_4]$																
	GAS								SMD							

																
∠O-Np-O	177.5								179.2							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}22}$	1.802	0.993/0.809	2.13	2.80	0.278	0.222	-0.24	1.414	1.835	1.015/0.820	2.02	2.76	0.257	0.269	-0.20	1.554
Np-$O_{yl\text{-}23}$	1.786	0.986/0.800	2.15	2.84	0.290	0.197	-0.26	1.339	1.834	1.014/0.820	2.00	2.76	0.257	0.265	-0.20	1.547
Np-$O_{water\text{-}34}$	2.727	1.471/1.258	0.28	0.63	0.030	0.109	-0.41×10^{-3}	4.418	2.647	1.424/1.224	0.35	0.80	0.035	0.129	0.18×10^{-3}	4.463
Np-$O_{water\text{-}31}$	2.630	1.422/1.209	0.29	0.78	0.036	0.137	0.20×10^{-3}	4.075	3.228	1.696/1.537	0.16	0.23	0.009	0.038	1.07×10^{-3}	6.176
Np-$O_{water\text{-}28}$	2.624	1.420/1.205	0.32	0.77	0.038	0.139	-0.16×10^{-3}	4.119	2.839	1.512/1.327	0.29	0.61	0.023	0.080	0.12×10^{-3}	4.335
Np-$O_{water\text{-}25}$	2.738	1.474/1.265	0.27	0.63	0.030	0.105	-0.42×10^{-3}	4.358	3.214	1.670/1.545	0.21	0.35	0.009	0.037	0.86×10^{-3}	5.741
Np-$O_{carb\text{-}8}$	2.526	1.370/1.157	0.35	0.93	0.048	0.171	-1.35×10^{-3}	3.732	2.569	1.401/1.171	0.30	0.91	0.039	0.155	1.21×10^{-3}	4.480
Np-$O_{carb\text{-}1}$	2.583	1.398/1.185	0.33	0.88	0.042	0.148	-1.05×10^{-3}	3.866	3.801		0.03	0.07				
$[NpO_2(DMOGA)(H_2O)_3]_c$																
	GAS								SMD							
																

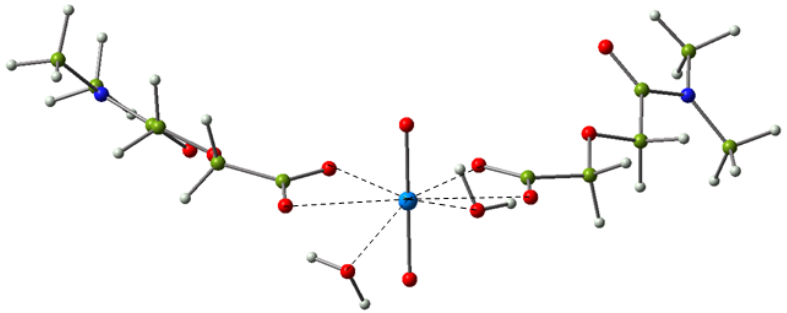
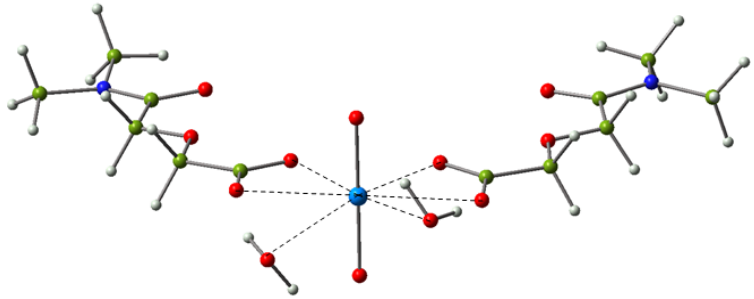
∠O-Np-O	175.0								179.1							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-22}	1.800	0.996/0.804	2.14	2.83	0.282	0.230	-0.24	1.426	1.831	1.009/0.822	2.03	2.76	0.257	0.255	-0.20	1.523
Np-O_{yl-23}	1.800	0.996/0.805	2.14	2.83	0.282	0.231	-0.24	1.426	1.833	1.010/0.823	2.03	2.75	0.256	0.257	-0.20	1.532
Np-$O_{water-31}$	2.607	1.409/1.199	0.32	0.79	0.039	0.151	-0.05×10^{-3}	5.078	2.598	1.402/1.196	0.31	0.84	0.037	0.147	1.17×10^{-3}	4.341
Np-$O_{water-28}$	2.585	1.417/1.169	0.26	0.84	0.039	0.160	1.04×10^{-3}	4.549	2.698	1.450/1.248	0.29	0.74	0.030	0.113	0.84×10^{-3}	4.271
Np-$O_{water-25}$	2.620	1.416/1.205	0.32	0.78	0.038	0.146	-0.03×10^{-3}	5.053	2.690	1.444/1.246	0.30	0.75	0.031	0.115	0.72×10^{-3}	4.268
Np-O_{carb-8}	2.495	1.357/1.138	0.37	0.97	0.051	0.189	-1.97×10^{-3}	3.896	2.598	1.404/1.195	0.34	0.90	0.039	0.141	-0.12×10^{-3}	3.872
Np-O_{carb-1}	2.555	1.387/1.168	0.35	0.91	0.045	0.163	-1.36×10^{-3}	4.065	2.612	1.410/1.202	0.34	0.90	0.038	0.136	-0.11×10^{-3}	3.906
$[NpO_2(DMOGA)(H_2O)_3]_e$																
	GAS								SMD							
																
∠O-Np-O	176.6								178.9							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-22}	1.789	0.987/0.801	2.16	2.84	0.288	0.201	-0.26	1.358	1.829	1.009/0.820	2.02	2.77	0.259	0.250	-0.20	1.508
Np-O_{yl-23}	1.808	0.996/0.812	2.02	2.77	0.273	0.237	-0.23	1.445	1.840	1.014/0.826	1.92	2.71	0.252	0.260	-0.19	1.543

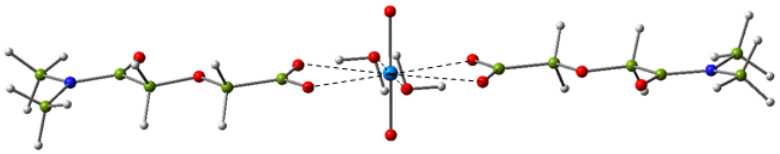
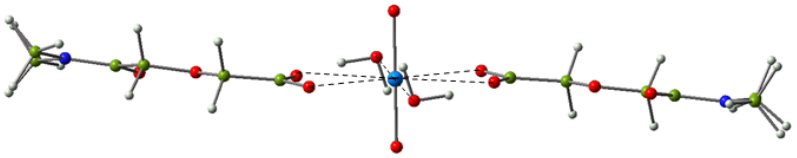
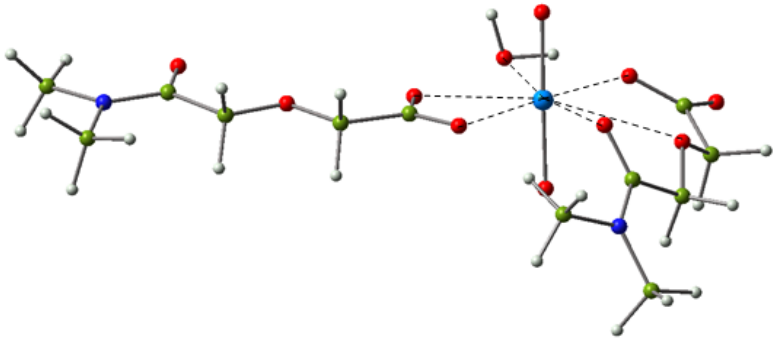
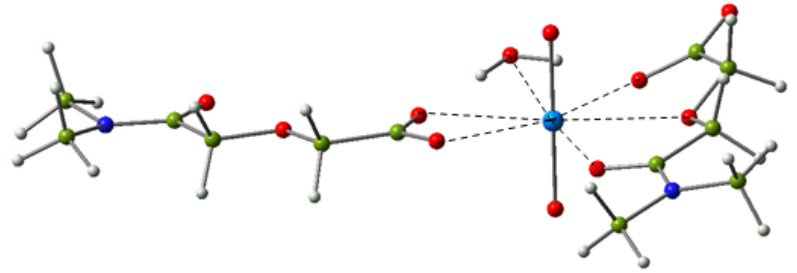
Np-$O_{water-25}$	2.698	1.454/1.245	0.29	0.68	0.032	0.116	-0.03×10^{-3}	4.228	3.714		0.09	0.10				
Np-$O_{water-28}$	3.581		0.09	0.09					3.421		0.11	0.14				
Np-$O_{water-31}$	2.515	1.368/1.147	0.37	0.94	0.046	0.187	0.41×10^{-3}	4.585	2.680	1.436/1.244	0.34	0.76	0.032	0.117	0.45×10^{-3}	4.293
Np-$O_{amide-9}$	2.500	1.367/1.135	0.29	0.97	0.045	0.193	1.54×10^{-3}	4.516	2.522	1.374/1.150	0.32	0.98	0.042	0.175	1.87×10^{-3}	4.360
Np-$O_{ether-4}$	2.628	1.433/1.196	0.17	0.78	0.033	0.138	1.58×10^{-3}	4.566	2.755	1.485/1.270	0.17	0.70	0.025	0.097	1.24×10^{-3}	4.810
Np-O_{carb-8}	2.398	1.312/1.088	0.40	1.12	0.060	0.240	-1.67×10^{-3}	3.954	2.510	1.366/1.146	0.33	1.01	0.045	0.178	1.05×10^{-3}	4.135

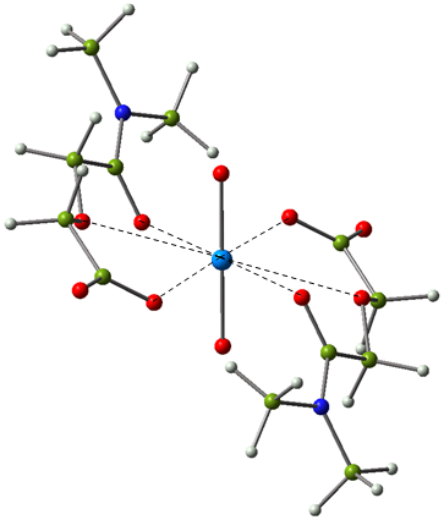
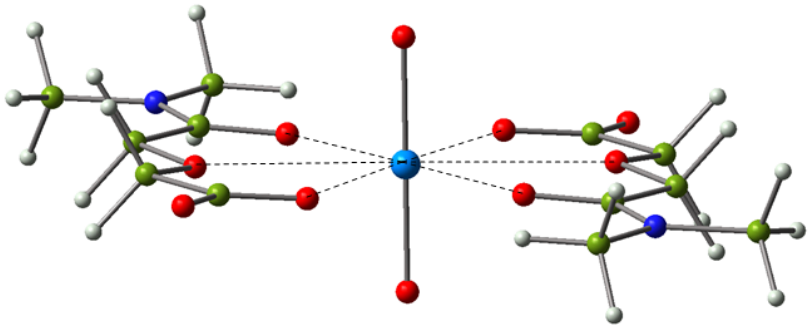
$[NpO_2(DMOGA)(H_2O)_2]$

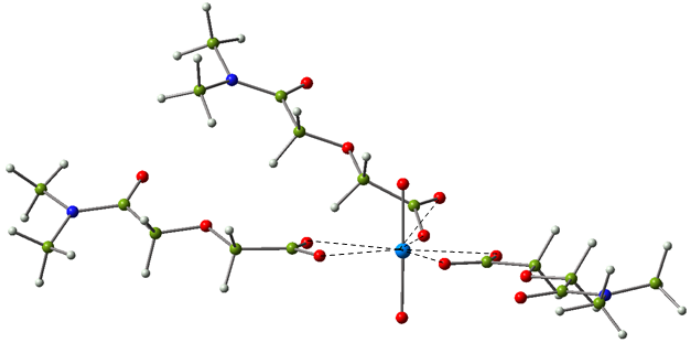
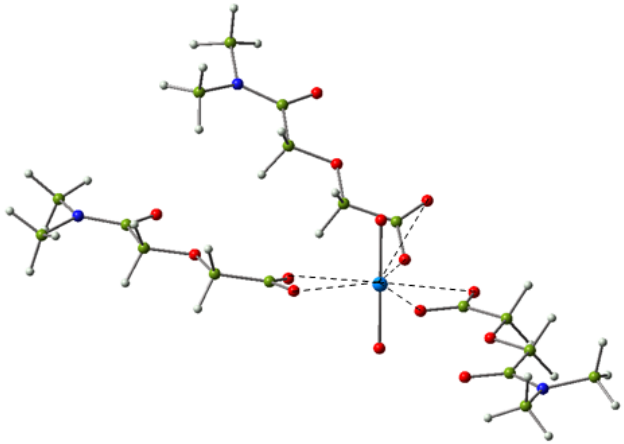
	GAS	SMD
		
∠O-Np-O	176.6	179.1

	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-22}	1.791	0.988/0.803	2.14	2.83	0.286	0.204	-0.25	1.368	1.834	1.011/0.823	2.02	2.75	0.255	0.258	-0.20	1.535
Np-O_{yl-23}	1.793	0.989/0.804	2.14	2.83	0.284	0.211	-0.25	1.382	1.832	1.010/0.822	2.02	2.75	0.256	0.258	-0.20	1.535
Np-$O_{water-25}$	2.754	1.485/1.271	0.29	0.60	0.029	0.101	-0.68×10^{-3}	4.319	2.681	1.441/1.240	0.29	0.77	0.031	0.118	0.95×10^{-3}	4.397
Np-$O_{water-28}$	2.612	1.414/1.199	0.33	0.79	0.039	0.146	-0.22×10^{-3}	4.361	2.716	1.457/1.259	0.29	0.73	0.029	0.108	0.75×10^{-3}	4.298

Np-$O_{amide-9}$	2.503	1.368/1.136	0.29	0.97	0.045	0.191	1.44×10^{-3}	4.500	2.539	1.383/1.157	0.31	0.95	0.041	0.169	1.76×10^{-3}	4.334
Np-$O_{ether-4}$	2.610	1.423/1.187	0.17	0.80	0.035	0.145	1.61×10^{-3}	4.520	2.670	1.450/1.221	0.18	0.76	0.030	0.121	1.62×10^{-3}	4.638
Np-O_{carb-8}	2.372	1.297/1.077	0.43	1.16	0.064	0.255	-2.49×10^{-3}	3.924	2.476	1.350/1.128	0.42	1.08	0.049	0.195	0.79×10^{-3}	4.126
$[NpO_2(DMOGA)_2(H_2O)_2]^-_a$																
	GAS								SMD							
																
∠O-Np-O	175.4								178.4							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-44}	1.811	1.001/0.810	2.07	2.79	0.273	0.248	-0.23	1.478	1.844	1.020/0.824	2.00	2.75	0.252	0.286	-0.19	1.607
Np-O_{yl-43}	1.811	1.001/0.810	2.07	2.79	0.273	0.248	-0.23	1.479	1.843	1.020/0.823	1.99	2.75	0.252	0.284	-0.19	1.602
Np-$O_{carb-29}$	2.553	1.389/1.165	0.35	0.93	0.045	0.161	-0.93×10^{-3}	3.779	2.649	1.430/1.220	0.32	0.86	0.035	0.128	-0.07×10^{-3}	4.601
Np-$O_{carb-22}$	2.665	1.441/1.224	0.30	0.78	0.035	0.123	-0.88×10^{-3}	4.469	2.689	1.445/1.244	0.28	0.78	0.032	0.113	-0.05×10^{-3}	4.715
Np-$O_{water-46}$	2.781	1.499/1.282	0.31	0.59	0.028	0.095	-0.61×10^{-3}	4.592	3.183	1.669/1.517	0.22	0.31	0.010	0.041	0.93×10^{-3}	8.420
Np-$O_{water-49}$	2.774	1.494/1.281	0.31	0.60	0.028	0.098	-0.56×10^{-3}	4.765	3.183	1.668/1.517	0.21	0.32	0.010	0.041	0.92×10^{-3}	8.087
Np-O_{carb-1}	2.665	1.442/1.224	0.30	0.79	0.035	0.123	-0.88×10^{-3}	4.429	2.718	1.459/1.259	0.27	0.75	0.030	0.106	0.01×10^{-3}	4.783
Np-O_{carb-8}	2.551	1.388/1.164	0.35	0.94	0.045	0.162	-0.96×10^{-3}	3.800	2.589	1.400/1.190	0.34	0.92	0.040	0.150	-0.14×10^{-3}	4.529
$[NpO_2(DMOGA)_2(H_2O)_2]^-_i$																
	GAS								SMD							

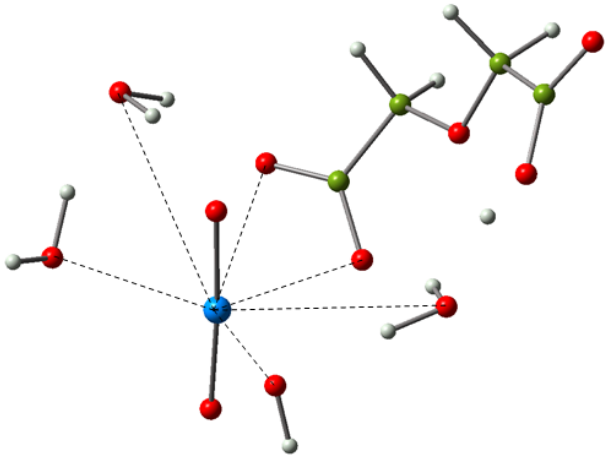
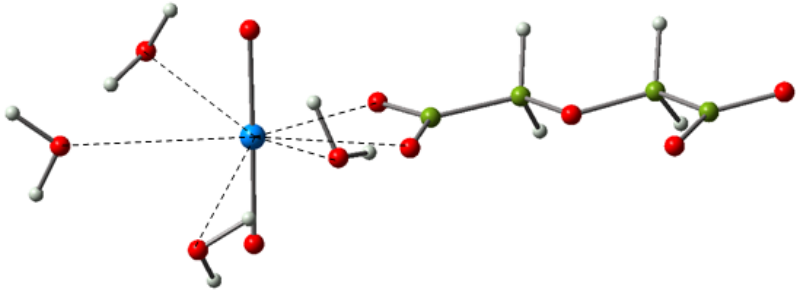
																
∠O-Np-O	180.0								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-43}	1.810	1.001/0.809	2.10	2.80	0.274	0.247	-0.23	1.467	1.839	1.017/0.823	2.01	2.75	0.254	0.277	-0.19	1.581
Np-O_{yl-44}	1.810	1.001/0.809	2.10	2.80	0.274	0.247	-0.23	1.469	1.839	1.017/0.823	2.01	2.76	0.254	0.277	-0.19	1.581
Np-$O_{water-49}$	2.692	1.449/1.243	0.32	0.69	0.032	0.120	-0.26×10^{-3}	5.003	2.834	1.509/1.326	0.27	0.60	0.023	0.082	0.32×10^{-3}	4.716
Np-$O_{carb-29}$	2.699	1.457/1.242	0.28	0.74	0.033	0.114	-0.66×10^{-3}	4.350	2.765	1.484/1.280	0.25	0.71	0.027	0.095	-0.07×10^{-3}	4.484
Np-$O_{carb-22}$	2.571	1.397/1.174	0.35	0.92	0.043	0.155	-0.86×10^{-3}	4.180	2.638	1.425/1.213	0.33	0.88	0.036	0.129	-0.26×10^{-3}	4.254
Np-$O_{water-46}$	2.692	1.449/1.243	0.32	0.69	0.032	0.120	-0.26×10^{-3}	5.004	2.833	1.509/1.325	0.27	0.60	0.023	0.082	0.32×10^{-3}	4.717
Np-O_{carb-8}	2.700	1.458/1.243	0.28	0.74	0.033	0.113	-0.66×10^{-3}	4.349	2.767	1.486/1.282	0.25	0.71	0.027	0.094	-0.07×10^{-3}	4.488
Np-O_{carb-1}	2.571	1.397/1.174	0.35	0.92	0.043	0.155	-0.86×10^{-3}	4.185	2.636	1.424/1.212	0.33	0.88	0.036	0.129	-0.26×10^{-3}	4.246
$[NpO_2(DMOGA)_2(H_2O)]^-$																
	GAS								SMD							
																
∠O-Np-O	179.0								179.6							

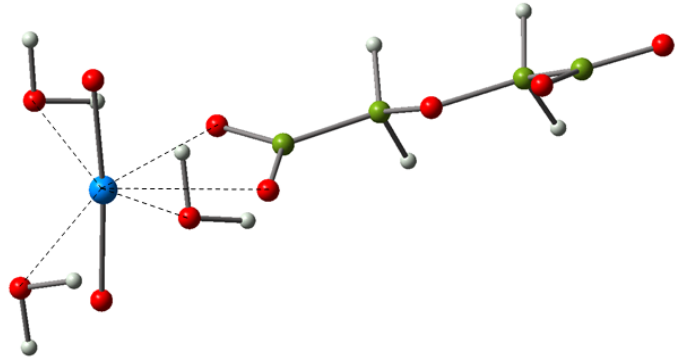
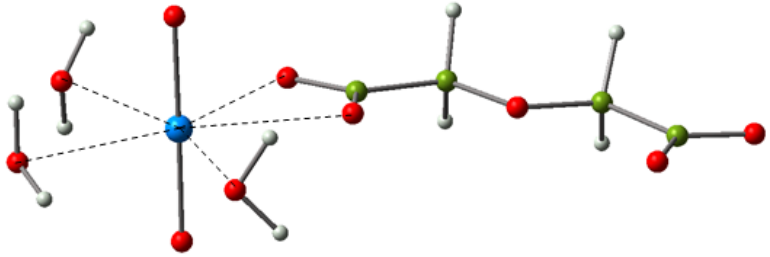
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}43}$	1.805	0.999/0.806	2.11	2.81	0.278	0.242	-0.24	1.454	1.841	1.017/0.823	2.00	2.76	0.253	0.280	-0.19	1.590
Np-$O_{yl\text{-}44}$	1.817	1.004/0.813	2.04	2.80	0.269	0.260	-0.22	1.508	1.840	1.017/0.823	2.00	2.75	0.253	0.277	-0.19	1.584
Np-$O_{water\text{-}46}$	2.669	1.438/1.232	0.33	0.72	0.034	0.127	-0.27×10^{-3}	4.849	3.380		0.16	0.16				
Np-$O_{carb\text{-}29}$	2.569	1.394/1.175	0.36	0.92	0.043	0.156	-0.78×10^{-3}	4.258	2.809	1.503/1.306	0.23	0.67	0.025	0.086	0.08×10^{-3}	4.980
Np-$O_{carb\text{-}22}$	2.604	1.413/1.191	0.32	0.89	0.040	0.143	-0.72×10^{-3}	4.004	2.593	1.406/1.187	0.34	0.93	0.040	0.144	-0.31×10^{-3}	3.952
Np-$O_{amide\text{-}9}$	2.618	1.436/1.184	0.24	0.82	0.034	0.140	1.31×10^{-3}	4.749	2.605	1.419/1.188	0.30	0.91	0.036	0.142	1.40×10^{-3}	4.270
Np-$O_{ether\text{-}4}$	2.911	1.569/1.346	0.12	0.54	0.019	0.071	0.18×10^{-3}	6.258	2.738	1.480/1.258	0.17	0.71	0.026	0.103	1.06×10^{-3}	5.077
Np-$O_{carb\text{-}8}$	2.525	1.382/1.146	0.35	0.96	0.045	0.176	0.11×10^{-3}	4.519	2.559	1.394/1.167	0.32	0.95	0.041	0.159	0.76×10^{-3}	4.384
$[NpO_2(DMOGA)_2]^-$																
	GAS								SMD							
																
∠O-Np-O	180.0								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε

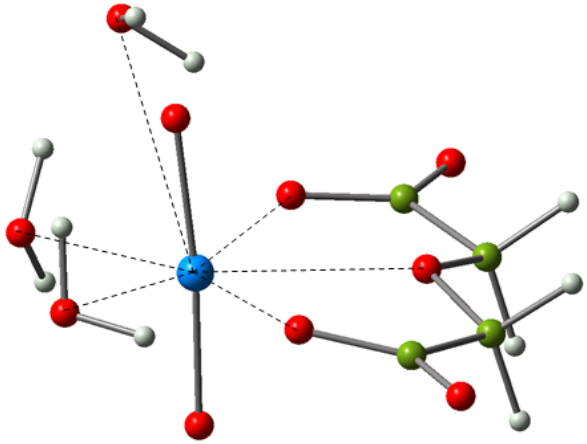
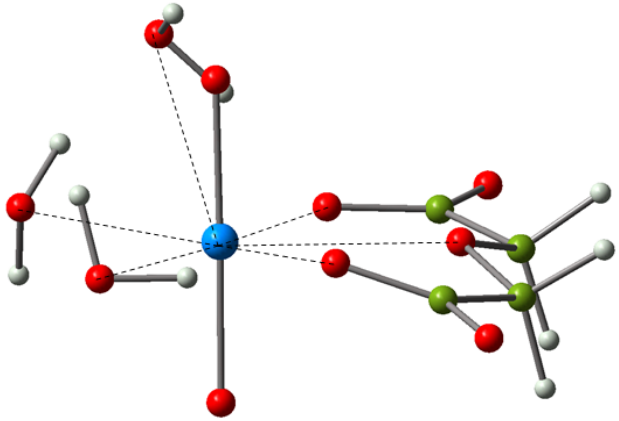
Np-O_{yl-43}	1.814	1.002/0.811	2.04	2.80	0.271	0.256	-0.23	1.495	1.840	1.017/0.823	2.00	2.76	0.254	0.276	-0.19	1.581
Np-O_{yl-44}	1.814	1.002/0.811	2.04	2.80	0.271	0.256	-0.23	1.495	1.840	1.017/0.823	2.00	2.76	0.254	0.276	-0.19	1.581
Np-$O_{amide-30}$	2.599	1.426/1.174	0.26	0.84	0.036	0.147	1.12×10^{-3}	4.535	2.735	1.484/1.255	0.25	0.79	0.026	0.100	1.23×10^{-3}	4.789
Np-$O_{ether-25}$	2.877	1.549/1.332	0.14	0.57	0.021	0.077	0.13×10^{-3}	6.420	2.948	1.578/1.371	0.14	0.56	0.016	0.062	0.98×10^{-3}	5.509
Np-$O_{carb-29}$	2.464	1.351/1.115	0.41	1.09	0.052	0.206	-0.24×10^{-3}	4.267	2.590	1.412/1.180	0.36	0.97	0.037	0.146	1.15×10^{-3}	4.573
Np-$O_{amide-9}$	2.599	1.426/1.174	0.26	0.84	0.036	0.147	1.12×10^{-3}	4.535	2.735	1.484/1.255	0.25	0.79	0.026	0.100	1.23×10^{-3}	4.789
Np-$O_{ether-4}$	2.877	1.549/1.332	0.14	0.57	0.021	0.077	0.13×10^{-3}	6.419	2.948	1.578/1.371	0.14	0.56	0.016	0.062	0.98×10^{-3}	5.509
Np-O_{carb-8}	2.464	1.350/1.115	0.41	1.09	0.052	0.207	-0.24×10^{-3}	4.267	2.590	1.412/1.180	0.36	0.97	0.037	0.146	1.15×10^{-3}	4.573
$[NpO_2(DMOGA)_3]^{2-}$																
	GAS								SMD							
																
∠O-Np-O	178.7								179.7							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-64}	1.813	1.002/0.811	2.07	2.81	0.272	0.256	-0.23	1.501	1.844	1.019/0.825	1.98	2.75	0.251	0.284	-0.19	1.608
Np-O_{yl-65}	1.813	1.002/0.811	2.09	2.81	0.272	0.254	-0.23	1.494	1.844	1.019/0.825	2.00	2.75	0.251	0.283	-0.19	1.608
Np-$O_{carb-50}$	2.693	1.458/1.235	0.28	0.79	0.033	0.115	-0.29×10^{-3}	4.184	2.647	1.430/1.216	0.31	0.87	0.036	0.126	-0.19×10^{-3}	4.106

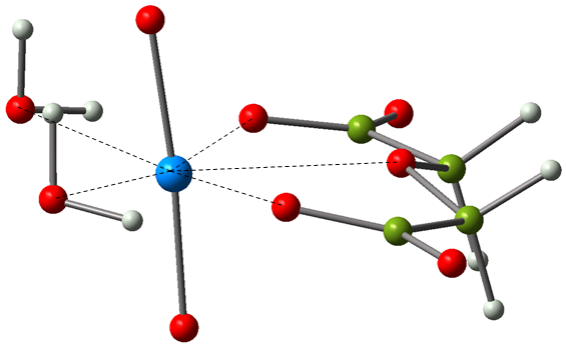
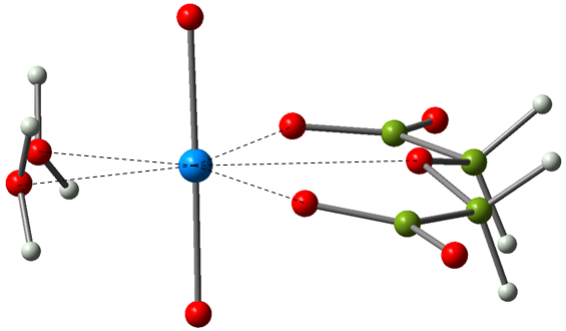
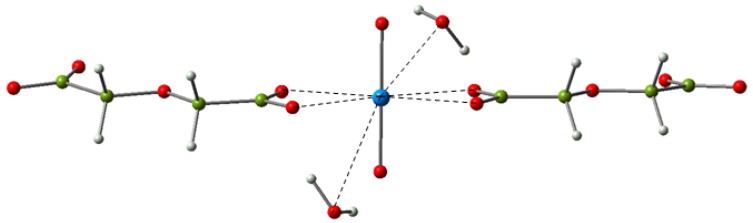
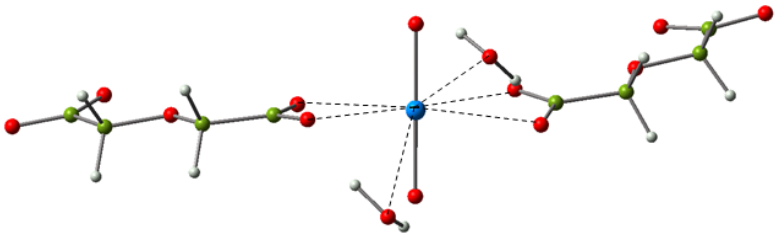
Np-$O_{carb-43}$	2.633	1.429/1.204	0.31	0.86	0.037	0.134	-0.31×10^{-3}	4.229	2.753	1.479/1.275	0.29	0.78	0.028	0.097	-0.05×10^{-3}	4.532
Np-O_{carb-8}	2.717	1.472/1.245	0.29	0.78	0.031	0.109	-0.22×10^{-3}	4.561	2.723	1.468/1.255	0.30	0.81	0.030	0.104	-0.14×10^{-3}	3.992
Np-O_{carb-1}	2.588	1.406/1.182	0.33	0.91	0.041	0.149	-0.52×10^{-3}	3.981	2.701	1.456/1.245	0.31	0.83	0.032	0.109	-0.19×10^{-3}	4.128
Np-$O_{carb-22}$	2.405	1.325/1.081	0.49	1.19	0.057	0.245	-0.14×10^{-3}	4.707	2.465	1.353/1.113	0.43	1.12	0.049	0.208	1.26×10^{-3}	4.450
Np-$O_{carb-29}$	4.617		0.03	0.04					4.546		0.03	0.04				

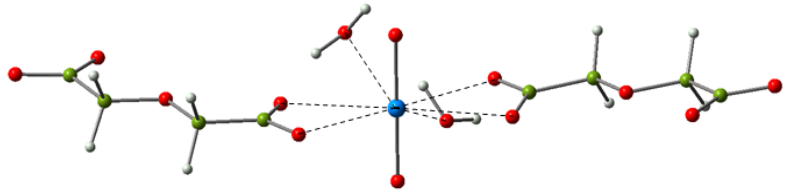
$[NpO_2(ODA)(H_2O)_4]^-$

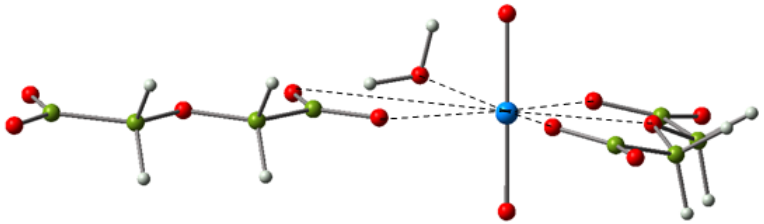
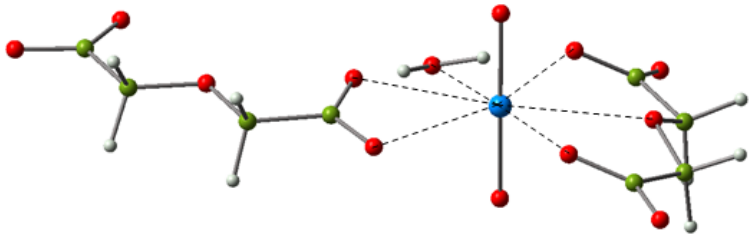
	GAS								SMD							
																
∠O-Np-O	175.8								179.1							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-14}	1.831	1.011/0.820	1.93	2.72	0.259	0.284	-0.20	1.585	1.825	1.006/0.819	2.00	2.76	0.261	0.241	-0.21	1.484
Np-O_{yl-15}	1.804	0.999/0.805	2.13	2.84	0.279	0.235	-0.24	1.436	1.827	1.007/0.819	1.99	2.75	0.260	0.244	-0.21	1.490
Np-$O_{water-26}$	3.604		0.08	0.08					3.144	1.650/1.498	0.23	0.35	0.011	0.042	0.74×10^{-3}	5.190
Np-$O_{water-23}$	2.646	1.433/1.213	0.32	0.80	0.036	0.136	-0.21×10^{-3}	4.908	3.134	1.655/1.480	0.12	0.41	0.009	0.042	1.30×10^{-3}	6.368

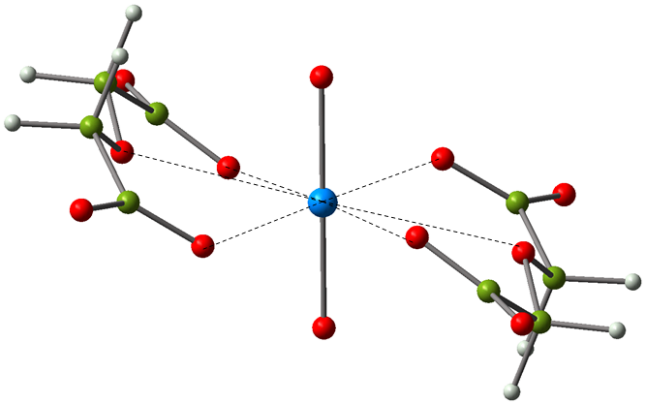
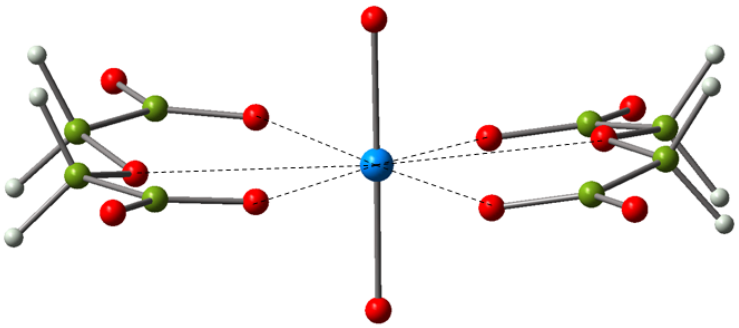
Np-$O_{water-20}$	2.234	1.221/1.014	0.84	1.57	0.093	0.359	-0.01	3.731	3.164	1.676/1.501	0.24	0.34	0.011	0.042	0.65×10^{-3}	5.002
Np-$O_{water-17}$	3.749		0.08	0.07					3.408		0.12	0.17				
Np-O_{carb-8}	2.460	1.345/1.115	0.36	1.02	0.053	0.209	-1.38×10^{-3}	4.217	2.599	1.402/1.197	0.30	0.86	0.039	0.141	-0.05×10^{-3}	3.905
Np-O_{carb-1}	2.931		0.21	0.56					2.582	1.395/1.187	0.35	0.93	0.041	0.146	-0.14×10^{-3}	3.827
$[NpO_2(ODA)(H_2O)_3]^-_c$																
	GAS								SMD							
																
∠O-Np-O	174.3								179.2							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-14}	1.806	0.999/0.807	2.11	2.81	0.278	0.238	-0.24	1.452	1.838	1.016/0.822	2.02	2.75	0.255	0.274	-0.20	1.574
Np-O_{yl-15}	1.799	0.996/0.803	2.13	2.83	0.283	0.229	-0.25	1.413	1.836	1.015/0.821	2.02	2.76	0.256	0.271	-0.20	1.563
Np-$O_{water-23}$	2.612	1.419/1.196	0.33	0.78	0.039	0.146	-0.49×10^{-3}	4.466	2.617	1.416/1.202	0.30	0.82	0.036	0.142	0.92×10^{-3}	4.305
Np-$O_{water-20}$	2.630	1.425/1.206	0.33	0.77	0.038	0.141	-0.36×10^{-3}	4.428	2.835	1.516/1.319	0.26	0.64	0.023	0.081	0.39×10^{-3}	4.162
Np-$O_{water-17}$	2.836	1.516/1.321	0.25	0.53	0.024	0.086	-0.53×10^{-3}	5.514	2.740	1.470/1.270	0.28	0.71	0.028	0.103	0.48×10^{-3}	4.312
Np-O_{carb-8}	2.408	1.310/1.098	0.43	1.09	0.063	0.231	-4.38×10^{-3}	3.673	2.614	1.414/1.200	0.34	0.90	0.038	0.137	-0.30×10^{-3}	4.089
Np-O_{carb-1}	2.546	1.382/1.164	0.37	0.93	0.046	0.165	-1.79×10^{-3}	4.029	2.702	1.455/1.248	0.32	0.82	0.031	0.110	-0.18×10^{-3}	4.325
$[NpO_2(ODA)(H_2O)_3]^-_e$																

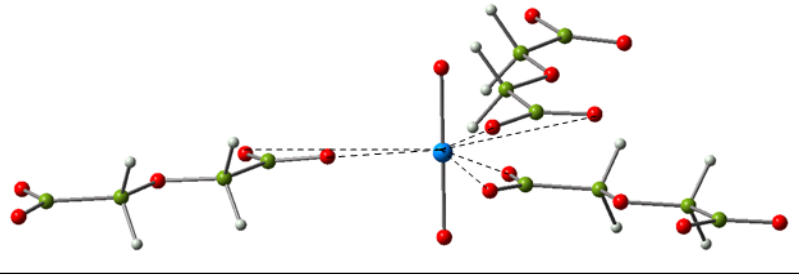
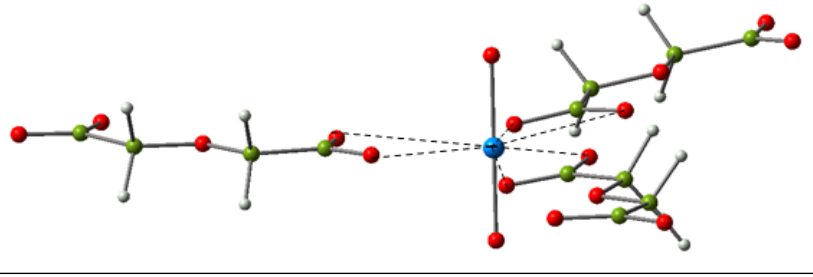
	GAS								SMD							
																
∠O-Np-O	174.3								178.8							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}14}$	1.836	1.015/0.821	1.97	2.72	0.257	0.288	-0.20	1.597	1.853	1.025/0.828	1.91	2.70	0.246	0.295	-0.18	1.641
Np-$O_{yl\text{-}15}$	1.809	1.002/0.806	2.12	2.83	0.276	0.250	-0.23	1.479	1.841	1.019/0.822	2.00	2.76	0.254	0.283	-0.19	1.597
Np-$O_{water\text{-}17}$	3.584		0.08	0.08					3.540		0.09	0.09				
Np-$O_{water\text{-}20}$	2.592	1.414/1.178	0.36	0.85	0.042	0.152	-0.69×10^{-3}	4.162	2.698	1.459/1.238	0.32	0.75	0.032	0.114	-0.03×10^{-3}	3.920
Np-$O_{water\text{-}23}$	2.692	1.455/1.239	0.33	0.70	0.033	0.118	-0.54×10^{-3}	4.405	3.232	1.672/1.560	0.20	0.34	0.009	0.038	1.06×10^{-3}	8.212
Np-$O_{carb\text{-}9}$	2.435	1.329/1.107	0.39	1.08	0.055	0.224	-0.94×10^{-3}	4.782	2.528	1.374/1.155	0.33	0.98	0.043	0.173	0.97×10^{-3}	4.827
Np-$O_{ether\text{-}4}$	2.570	1.399/1.173	0.21	0.85	0.038	0.166	1.13×10^{-3}	5.619	2.710	1.461/1.250	0.19	0.74	0.028	0.111	1.12×10^{-3}	5.831
Np-$O_{carb\text{-}8}$	2.442	1.332/1.111	0.41	1.09	0.054	0.223	-0.78×10^{-3}	5.160	2.558	1.388/1.173	0.33	0.96	0.040	0.163	0.99×10^{-3}	5.402
$[NpO_2(ODA)(H_2O)_2]^-$																

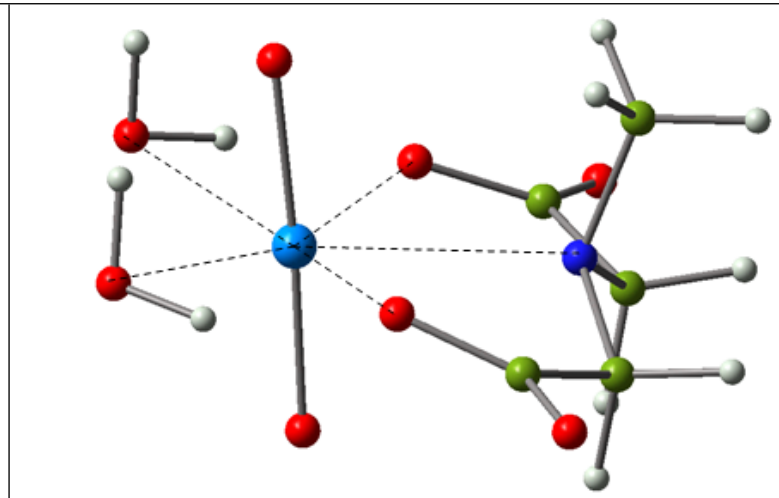
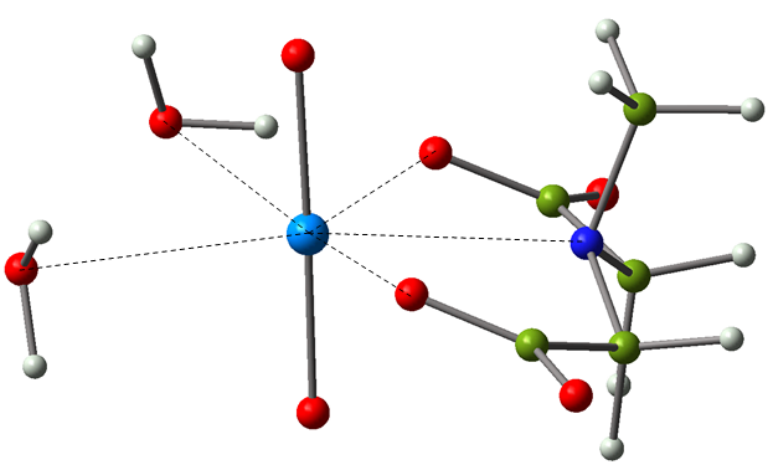
																
∠O-Np-O	175.2								179.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-14}	1.815	0.999/0.815	2.08	2.76	0.268	0.243	-0.22	1.476	1.845	1.019/0.825	2.01	2.74	0.250	0.283	-0.19	1.609
Np-O_{yl-15}	1.794	0.990/0.804	2.14	2.84	0.284	0.211	-0.25	1.386	1.844	1.019/0.825	2.01	2.75	0.250	0.284	-0.19	1.610
Np-$O_{water-17}$	2.680	1.451/1.231	0.34	0.70	0.034	0.122	-0.51×10^{-3}	4.269	2.632	1.425/1.207	0.29	0.80	0.035	0.136	0.75×10^{-3}	4.272
Np-$O_{water-20}$	2.675	1.448/1.228	0.34	0.70	0.034	0.123	-0.49×10^{-3}	4.269	2.653	1.435/1.219	0.29	0.79	0.034	0.129	0.68×10^{-3}	4.094
Np-O_{carb-9}	2.422	1.323/1.101	0.40	1.09	0.057	0.227	-1.31×10^{-3}	3.953	2.533	1.380/1.155	0.39	1.03	0.043	0.171	0.91×10^{-3}	4.548
Np-$O_{ether-4}$	2.571	1.400/1.173	0.21	0.85	0.039	0.158	0.93×10^{-3}	4.199	2.734	1.479/1.255	0.18	0.72	0.027	0.103	0.93×10^{-3}	4.556
Np-O_{carb-8}	2.420	1.322/1.099	0.40	1.10	0.058	0.228	-1.32×10^{-3}	3.954	2.538	1.384/1.156	0.39	1.01	0.043	0.169	0.90×10^{-3}	4.436
$[NpO_2(ODA)_2(H_2O)_2]^{3-}{}_a$																
	GAS								SMD							
																

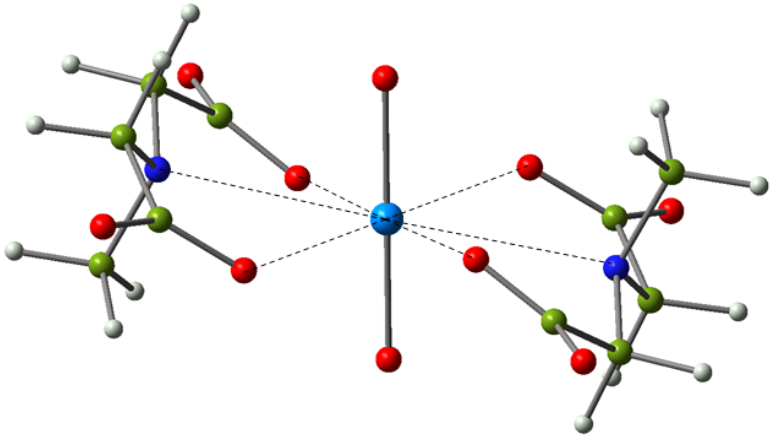
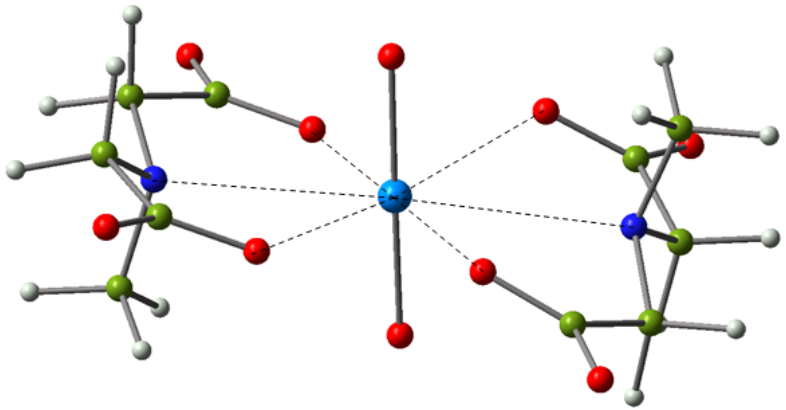
∠O-Np-O	179.8								179.6							
	d	d_1/d_2(Å)	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-27}	1.812	1.002/0.810	2.01	2.78	0.273	0.253	-0.23	1.472	1.851	1.023/0.825	1.92	2.71	0.249	0.288	-0.19	1.612
Np-O_{yl-28}	1.812	1.002/0.810	2.01	2.78	0.273	0.253	-0.23	1.471	1.848	1.024/0.827	1.91	2.70	0.248	0.290	-0.18	1.620
Np-O_{carb-8}	2.545	1.382/1.163	0.40	0.96	0.046	0.166	-1.37×10^{-3}	4.216	2.598	1.406/1.200	0.34	0.90	0.038	0.140	-0.11×10^{-3}	4.768
Np-O_{carb-1}	2.503	1.361/1.143	0.38	1.00	0.051	0.184	-1.92×10^{-3}	3.987	2.702	1.456/1.250	0.26	0.76	0.031	0.110	-0.09×10^{-3}	4.965
Np-$O_{water-33}$	3.700		0.12	0.10					3.341		0.18	0.20				
Np-$O_{water-30}$	3.717		0.12	0.10					3.329		0.18	0.20				
Np-$O_{carb-14}$	2.498	1.357/1.141	0.38	1.01	0.051	0.187	-1.91×10^{-3}	4.099	2.706	1.453/1.249	0.26	0.77	0.031	0.111	-0.07×10^{-3}	5.044
Np-$O_{carb-21}$	2.546	1.383/1.163	0.40	0.96	0.046	0.165	-1.36×10^{-3}	4.183	2.606	1.402/1.196	0.34	0.91	0.039	0.143	-0.11×10^{-3}	4.816
$[NpO_2(ODA)_2(H_2O)_2]^{3-}{}_i$																
	GAS								SMD							
																
∠O-Np-O	179.8								180.0							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-27}	1.831	1.011/0.820	2.02	2.73	0.259	0.277	-0.21	1.558	1.839	1.016/0.822	1.97	2.74	0.254	0.273	-0.20	1.569
Np-O_{yl-28}	1.802	0.998/0.804	2.11	2.84	0.280	0.233	-0.24	1.426	1.834	1.014/0.820	2.01	2.77	0.258	0.268	-0.20	1.548
Np-$O_{water-30}$	2.764	1.496/1.269	0.31	0.61	0.029	0.098	-0.74×10^{-3}	4.159	3.218	1.688/1.534	0.20	0.30	0.009	0.037	0.87×10^{-3}	5.871
Np-O_{carb-8}	2.728	1.468/1.260	0.30	0.73	0.031	0.106	-0.90×10^{-3}	4.733	2.743	1.473/1.270	0.25	0.74	0.029	0.099	-0.14×10^{-3}	4.450
Np-O_{carb-1}	2.544	1.382/1.162	0.38	0.96	0.046	0.163	-1.35×10^{-3}	3.920	2.714	1.461/1.253	0.31	0.82	0.031	0.105	-0.20×10^{-3}	4.221
Np-$O_{water-33}$	2.751	1.483/1.268	0.31	0.62	0.029	0.103	-0.48×10^{-3}	4.841	3.237		0.20	0.28				

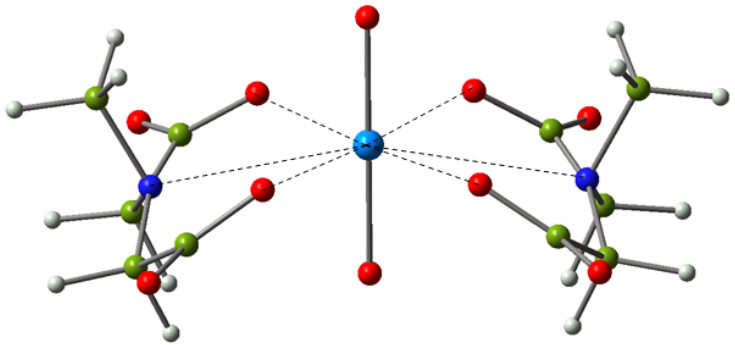
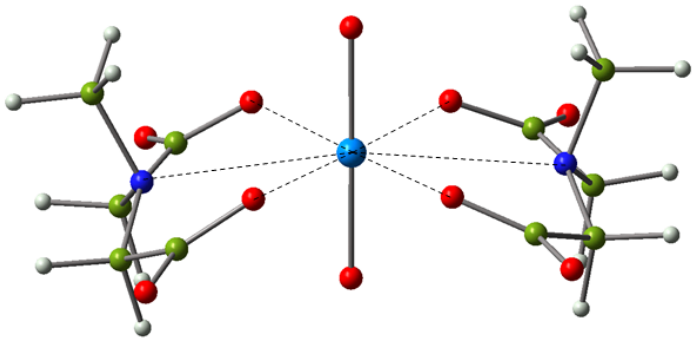
Np-$O_{carb-21}$	2.668	1.440/1.229	0.32	0.79	0.035	0.122	-0.94×10^{-3}	4.500	2.735	1.470/1.265	0.26	0.75	0.029	0.101	-0.17×10^{-3}	4.293
Np-$O_{carb-14}$	2.547	1.385/1.163	0.38	0.96	0.046	0.162	-1.34×10^{-3}	3.861	2.727	1.468/1.259	0.30	0.81	0.030	0.102	-0.21×10^{-3}	4.197
$[NpO_2(ODA)_2(H_2O)]^{3-}$																
	GAS								SMD							
																
∠O-Np-O	178.0								179.7							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-O_{yl-27}	1.817	1.001/0.816	2.07	2.77	0.266	0.250	-0.22	1.493	1.843	1.019/0.825	2.00	2.75	0.251	0.283	-0.19	1.606
Np-O_{yl-28}	1.807	0.997/0.811	2.10	2.81	0.273	0.236	-0.23	1.450	1.844	1.019/0.825	2.00	2.75	0.250	0.284	-0.19	1.607
Np-$O_{water-30}$	2.645	1.432/1.213	0.35	0.78	0.037	0.131	-0.42×10^{-3}	4.120	3.427		0.15	0.15				
Np-$O_{carb-21}$	3.992		0.03	0.04					2.742	1.475/1.268	0.25	0.74	0.029	0.100	-0.12×10^{-3}	4.206
Np-$O_{carb-14}$	2.474	1.356/1.120	0.41	1.08	0.048	0.200	1.06×10^{-3}	4.459	2.690	1.452/1.238	0.31	0.84	0.033	0.112	-0.22×10^{-3}	4.172
Np-O_{carb-9}	2.476	1.352/1.126	0.41	1.08	0.049	0.199	0.43×10^{-3}	4.307	2.480	1.356/1.126	0.41	1.08	0.049	0.197	0.56×10^{-3}	4.158
Np-$O_{ether-4}$	2.712	1.472/1.242	0.16	0.71	0.028	0.111	1.03×10^{-3}	4.721	2.771	1.493/1.279	0.18	0.69	0.025	0.095	0.71×10^{-3}	5.067
Np-O_{carb-8}	2.496	1.363/1.134	0.40	1.05	0.047	0.188	0.52×10^{-3}	4.225	2.567	1.399/1.169	0.32	0.94	0.040	0.157	0.81×10^{-3}	4.337
$[NpO_2(ODA)_2]^{3-}$																
	GAS								SMD							

																
∠O-Np-O	180.0								179.4							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}27}$	1.818	1.005/0.813	2.05	2.80	0.268	0.264	-0.22	1.525	1.847	1.021/0.827	1.99	2.74	0.248	0.288	-0.19	1.625
Np-$O_{yl\text{-}28}$	1.818	1.005/0.813	2.05	2.80	0.268	0.264	-0.22	1.524	1.848	1.021/0.827	1.99	2.74	0.248	0.288	-0.18	1.625
Np-$O_{carb\text{-}22}$	2.602	1.420/1.184	0.37	0.94	0.038	0.142	0.42×10^{-3}	4.236	2.619	1.429/1.192	0.35	0.93	0.035	0.136	1.19×10^{-3}	4.289
Np-$O_{ether\text{-}17}$	2.900	1.554/1.348	0.14	0.56	0.019	0.072	0.36×10^{-3}	6.431	2.999	1.598/1.404	0.13	0.53	0.014	0.057	0.89×10^{-3}	6.320
Np-$O_{carb\text{-}21}$	2.604	1.421/1.185	0.37	0.94	0.038	0.141	0.40×10^{-3}	4.233	2.606	1.422/1.187	0.35	0.95	0.036	0.140	1.24×10^{-3}	4.369
Np-$O_{carb\text{-}9}$	2.601	1.420/1.184	0.37	0.94	0.038	0.142	0.42×10^{-3}	4.237	2.579	1.407/1.174	0.36	0.97	0.039	0.151	1.04×10^{-3}	4.312
Np-$O_{ether\text{-}4}$	2.904	1.556/1.349	0.14	0.56	0.019	0.072	0.36×10^{-3}	6.442	2.833	1.523/1.310	0.16	0.64	0.021	0.082	0.97×10^{-3}	5.738
Np-$O_{carb\text{-}8}$	2.603	1.421/1.185	0.37	0.94	0.038	0.141	0.41×10^{-3}	4.234	2.577	1.405/1.174	0.36	0.97	0.039	0.152	1.11×10^{-3}	4.362
$[NpO_2(ODA)_3]^{5-}$																
	GAS								SMD							

																
∠O-Np-O	180.0								179.9							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}40}$	1.810	1.001/0.809	2.09	2.82	0.274	0.251	-0.23	1.481	1.845	1.020/0.825	2.00	2.75	0.250	0.285	-0.19	1.611
Np-$O_{yl\text{-}41}$	1.810	1.001/0.809	2.09	2.82	0.274	0.251	-0.23	1.482	1.845	1.020/0.825	1.99	2.75	0.250	0.284	-0.19	1.606
Np-$O_{carb\text{-}34}$	4.307		0.06	0.06					3.329		0.16	0.37				
Np-$O_{carb\text{-}27}$	2.416	1.337/1.081	0.48	1.20	0.053	0.242	1.39×10^{-3}	5.147	2.518	1.369/1.150	0.38	1.04	0.046	0.175	-0.14×10^{-3}	3.931
Np-$O_{carb\text{-}8}$	4.320		0.06	0.05					3.279		0.16	0.40				
Np-$O_{carb\text{-}1}$	2.416	1.336/1.081	0.48	1.20	0.053	0.243	1.47×10^{-3}	4.962	2.531	1.374/1.158	0.38	1.02	0.045	0.170	-0.08×10^{-3}	4.230
Np-$O_{carb\text{-}21}$	4.327		0.05	0.05					3.261		0.17	0.42				
Np-$O_{carb\text{-}14}$	2.416	1.336/1.081	0.48	1.20	0.053	0.243	1.55×10^{-3}	4.799	2.540	1.379/1.162	0.38	1.01	0.044	0.165	-0.08×10^{-3}	3.943
$[NpO_2(MIDA)(H_2O)_2]^-$																
	GAS								SMD							

																
∠O-Np-O	176.7								178.6							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}19}$	1.818	1.001/0.817	2.07	2.76	0.266	0.248	-0.22	0.005	1.850	1.024/0.827	1.99	2.74	0.248	0.295	-0.18	0.003
Np-$O_{yl\text{-}18}$	1.798	0.992/0.806	2.12	2.83	0.281	0.218	-0.24	0.003	1.848	1.023/0.826	1.99	2.75	0.249	0.294	-0.19	0.003
Np-$O_{water\text{-}24}$	2.688	1.456/1.234	0.34	0.69	0.034	0.119	-0.55×10^{-3}	0.192	3.281	1.699/1.582	0.20	0.30	0.008	0.035	1.08×10^{-3}	1.129
Np-$O_{water\text{-}21}$	2.690	1.457/1.235	0.34	0.69	0.034	0.119	-0.56×10^{-3}	0.190	2.950	1.574/1.377	0.25	0.57	0.018	0.063	0.21×10^{-3}	0.256
Np-$O_{carb\text{-}8}$	2.423	1.323/1.101	0.41	1.10	0.058	0.226	-1.64×10^{-3}	0.331	2.469	1.343/1.127	0.43	1.10	0.050	0.203	0.17×10^{-3}	0.063
Np-$N_{ether\text{-}4}$	2.643	1.401/1.242	0.23	0.81	0.044	0.132	-2.00×10^{-3}	0.275	2.737	1.438/1.299	0.22	0.75	0.035	0.109	-1.00×10^{-3}	0.022
Np-$O_{carb\text{-}9}$	2.424	1.323/1.102	0.41	1.09	0.058	0.225	-1.62×10^{-3}	0.332	2.498	1.358/1.141	0.34	1.00	0.047	0.188	0.51×10^{-3}	0.107
$[NpO_2(MIDA)_2]^{3-}{}_{trans}$																
	GAS								SMD							

																
∠O-Np-O	180.0								179.3							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}35}$	1.820	1.006/0.814	2.05	2.80	0.266	0.266	-0.22	0.004	1.848	1.021/0.827	1.99	2.74	0.248	0.290	-0.18	0.001
Np-$O_{yl\text{-}36}$	1.820	1.006/0.814	2.05	2.80	0.266	0.266	-0.22	0.004	1.846	1.020/0.826	1.98	2.75	0.249	0.289	-0.19	0.002
Np-$O_{carb\text{-}9}$	2.637	1.435/1.204	0.36	0.91	0.035	0.128	0.23×10^{-3}	0.262	2.571	1.402/1.171	0.37	0.99	0.040	0.154	0.88×10^{-3}	0.292
Np-$N_{ether\text{-}4}$	2.955	1.545/1.410	0.12	0.56	0.022	0.068	0.13×10^{-3}	0.038	2.976	1.548/1.428	0.16	0.59	0.022	0.061	-0.12×10^{-3}	0.026
Np-$O_{carb\text{-}8}$	2.636	1.435/1.204	0.36	0.91	0.035	0.129	0.24×10^{-3}	0.262	2.597	1.414/1.187	0.36	0.95	0.038	0.143	0.67×10^{-3}	0.240
Np-$O_{carb\text{-}25}$	2.637	1.435/1.204	0.36	0.91	0.035	0.129	0.23×10^{-3}	0.263	2.608	1.419/1.191	0.36	0.94	0.037	0.139	0.60×10^{-3}	0.251
Np-$N_{ether\text{-}21}$	2.954	1.544/1.410	0.12	0.56	0.022	0.068	0.13×10^{-3}	0.036	2.955	1.538/1.417	0.17	0.61	0.023	0.064	-0.16×10^{-3}	0.052
Np-$O_{carb\text{-}26}$	2.637	1.435/1.204	0.36	0.91	0.035	0.129	0.24×10^{-3}	0.262	2.792	1.504/1.290	0.31	0.79	0.025	0.086	0.21×10^{-3}	0.260
$\mathbf{[NpO_2(MIDA)_2]^{3-}_{cis}}$																
	GAS								SMD							

																
∠O-Np-O	179.9								179.6							
	d	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε	*d*	d_1/d_2	*MBO*	*DI*	ρ_b	$\nabla^2\rho_b$	H_b	ε
Np-$O_{yl\text{-}35}$	1.808	0.997/0.811	2.09	2.81	0.273	0.237	-0.23	0.010	1.837	1.012/0.825	2.00	2.74	0.252	0.267	-0.19	0.003
Np-$O_{yl\text{-}36}$	1.819	1.002/0.817	2.04	2.79	0.265	0.254	-0.22	0.002	1.840	1.013/0.826	1.99	2.75	0.251	0.272	-0.19	0.001
Np-$O_{carb\text{-}8}$	2.604	1.416/1.191	0.37	0.94	0.037	0.139	0.58×10^{-3}	0.290	2.580	1.402/1.180	0.37	0.97	0.039	0.148	0.80×10^{-3}	0.285
Np-$N_{ether\text{-}4}$	3.001	1.572/1.430	0.11	0.53	0.020	0.060	0.10×10^{-3}	0.035	2.958	1.544/1.415	0.16	0.60	0.023	0.063	-0.27×10^{-3}	0.094
Np-$O_{carb\text{-}9}$	2.613	1.421/1.195	0.37	0.93	0.036	0.135	0.56×10^{-3}	0.291	2.582	1.403/1.181	0.37	0.97	0.039	0.147	0.82×10^{-3}	0.288
Np-$O_{carb\text{-}25}$	2.607	1.417/1.192	0.37	0.94	0.037	0.138	0.58×10^{-3}	0.289	2.596	1.410/1.188	0.37	0.95	0.037	0.141	0.90×10^{-3}	0.306
Np-$N_{ether\text{-}21}$	2.995	1.568/1.427	0.11	0.54	0.020	0.061	0.09×10^{-3}	0.042	2.991	1.553/1.438	0.16	0.58	0.021	0.058	-0.06×10^{-3}	0.130
Np-$O_{carb\text{-}26}$	2.617	1.422/1.197	0.36	0.93	0.036	0.134	0.54×10^{-3}	0.292	2.602	1.413/1.191	0.37	0.95	0.037	0.139	0.87×10^{-3}	0.308

$[NpO_2(H_2O)_5]^+$

GAS： H = -1046.934284 Hartree

G = -1047.001016 Hartree

S = 140.448 Cal/Mol-Kelvin

O	-0.00191500	0.00065500	-1.78115800
O	-0.00053800	0.00234100	1.78068400
Np	-0.00149900	0.00136300	-0.00023700
O	2.03903700	-1.55424600	0.00015900
H	2.62022400	-1.48522900	0.77624300
H	2.61920900	-1.48555500	-0.77671900
O	-0.84883900	-2.41950200	0.00069400
H	-0.60454000	-2.95158900	0.77661600
H	-0.60732700	-2.95082500	-0.77662600
O	-2.56687100	0.06050800	0.00022000
H	-2.99819100	-0.33459100	0.77655200
H	-2.99853400	-0.33329100	-0.77658000
O	-0.73298200	2.46063000	-0.00075500
H	-1.24086800	2.74824300	0.77653400
H	-1.24291000	2.74824800	-0.77669700
O	2.11288400	1.45576200	-0.00154100
H	2.23014300	2.02711000	0.77605500
H	2.22646900	2.03076100	-0.77699200

SMD： H = -1047.101669 Hartree

G = -1047.165072 Hartree

S = 133.443 Cal/Mol-Kelvin

O	-0.10500300	0.12848700	-1.79772000
O	0.12157400	-0.09187000	1.83630200
Np	0.00997300	0.02123200	0.01929900
O	-1.07070600	-2.42854600	-0.19852100
H	-1.47144500	-2.56805600	0.67770100
H	-1.83502600	-2.26825800	-0.77875000
O	-2.73858300	0.12210000	0.10002600
H	-2.95971100	-0.68820500	0.59178200
H	-2.94691100	-0.10341800	-0.82327900
O	-0.63927000	2.64369600	0.06676700
H	-1.35197800	2.68348900	0.72832700
H	-1.10782900	2.71235200	-0.78359700
O	2.31942400	1.29975400	-0.10391300
H	2.90321500	0.77847700	0.47511800
H	2.62664300	1.08152000	-1.00162400
O	2.11336100	-1.76386700	-0.03532000
H	2.49779800	-1.56592100	0.83626900
H	2.71137700	-1.31462500	-0.65775900

$[NpO_2(H_2O)_6]^+$

GAS： H = -1123.33686 Hartree

G = -1123.405797 Hartree

S = 145.089 Cal/Mol-Kelvin

O	1.25652000	-0.02858500	-0.10958400
O	-2.30222800	-0.31452400	0.07802300
Np	-0.52285500	-0.17155400	-0.01578100
O	-0.84442000	-0.91991600	2.51107300
H	-1.81392900	-0.92178800	2.60080000
H	-0.53869900	-0.18031200	3.06700700
O	0.21838600	-2.63889800	0.59317100
H	-0.05649300	-2.79026100	1.51586000
H	1.18785700	-2.55462200	0.62707600
O	-0.97461300	-2.01983500	-1.85878600
H	-1.93170000	-2.17292800	-1.76526800
H	-0.55392500	-2.84057000	-1.54407500
O	-0.20128800	0.57680500	-2.54263500
H	-0.50700700	-0.16280200	-3.09856600
H	0.76822200	0.57867800	-2.63236000
O	-1.26409500	2.29578900	-0.62473500
H	-2.23356500	2.21151500	-0.65864000
H	-0.98921500	2.44715200	-1.54742400
O	-0.07109700	1.67672700	1.82722100
H	0.88599000	1.82982000	1.73370400
H	-0.49178500	2.49746100	1.51250800

SMD： H = -1123.522501 Hartree

G = -1123.589779 Hartree

S = 141.598 Cal/Mol-Kelvin

O	1.29455700	-0.29469700	0.12086700
O	-2.34027600	-0.04839000	-0.15245600
Np	-0.52285900	-0.17154300	-0.01579600
O	-0.65929100	-1.44225600	2.29353600
H	-1.51339100	-1.40023300	2.75807800
H	0.00762600	-1.17448800	2.94971800
O	0.11366100	-3.75040700	0.89773300
H	-0.17100400	-3.01247400	1.48497900
H	1.08404800	-3.68226800	0.89851800
O	-0.53600000	-2.38944500	-1.34681800
H	-1.47817500	-2.57564500	-1.50136300
H	-0.28732500	-2.98262600	-0.58024700
O	-0.38646700	1.09914100	-2.32515200
H	-1.05338000	0.83135000	-2.98133000
H	0.46763200	1.05714400	-2.78969900
O	-1.15953000	3.40730800	-0.92906600
H	-2.12991400	3.33911400	-0.92992300
H	-0.87477500	2.66942600	-1.51633000
O	-0.50963000	2.04639000	1.31513100
H	0.43255400	2.23244400	1.46979100
H	-0.75799800	2.63950900	0.54842000

$[NpO_2(TMOGA)(H_2O)_3]^+$

GAS： H = -1543.568065 Hartree

G = -1543.660518 Hartree

S = 194.583 Cal/Mol-Kelvin

N	-1.69494100	-1.49483300	0.22379900
C	-0.60294300	-2.24949600	0.03614500
C	0.77372400	-1.59066800	0.13952300
O	1.74540300	-2.61427300	0.03668600
C	3.06453900	-2.10838900	-0.03509000
C	4.01948700	-3.30270100	-0.05114100
N	5.32685700	-3.08151300	-0.24712800
O	-0.67163700	-3.46786700	-0.21834000
O	3.55910100	-4.44968200	0.11499800
C	6.23727400	-4.23095900	-0.31427800
C	5.94559900	-1.75844000	-0.34876600
C	-3.01856400	-2.12609700	0.17098800
C	-1.68429300	-0.04471500	0.42281400
H	0.89941800	-0.86211400	-0.67572500
H	0.88217500	-1.05991100	1.09588000
H	3.18858000	-1.50241200	-0.94368400
H	3.27771600	-1.47081100	0.83635700
H	6.51623400	-4.57057400	0.68957700
H	5.76041200	-5.04909000	-0.85559700
H	7.13907300	-3.92810200	-0.84971300
H	6.73571200	-1.66502100	0.40357400
H	6.38757700	-1.62361900	-1.34179700
H	5.22184100	-0.96276000	-0.17773400
H	-3.70265400	-1.55237800	0.80009500
H	-3.40449900	-2.14059600	-0.85471300

H	-2.95459500	-3.14568100	0.55061400
H	-2.30386400	0.43492700	-0.34233600
H	-2.09062000	0.20259700	1.40942400
H	-0.67774900	0.36416300	0.34738700
O	1.40258300	-5.29860500	-1.83525500
O	0.84757700	-5.35203400	1.68897200
Np	1.11575700	-5.31298700	-0.07818900
O	-1.30870500	-6.04402300	-0.70299300
H	-1.72543400	-5.17019600	-0.80607900
H	-1.20951800	-6.40292700	-1.60132700
O	0.63076400	-7.86692900	-0.23977800
H	0.02697600	-8.15608600	0.46420600
H	1.49262100	-8.27863300	-0.04923200
O	3.05301800	-7.02292000	0.70545600
H	2.89523400	-6.86207100	1.65287300
H	3.81481100	-6.45771400	0.48206500

SMD： H = -1543.736443 Hartree

G = -1543.822998 Hartree

S = 182.17 Cal/Mol-Kelvin

N	-1.78325600	-1.29599300	0.13701800
C	-0.74785600	-2.14338100	0.04901200
C	0.65726900	-1.54968500	-0.01143800
O	1.59135100	-2.60383900	0.14029000
C	2.92827400	-2.16723800	-0.01670400

C	3.84408100	-3.38292200	0.08682600
N	5.16023700	-3.20417700	-0.06846200
O	-0.91278800	-3.38483700	0.01494100
O	3.36171400	-4.52182500	0.31214600
C	6.04609500	-4.36894200	0.05210000
C	5.80925600	-1.90157500	-0.23794500
C	-3.14172100	-1.82853800	0.26919700
C	-1.66061600	0.16394300	0.09210600
H	0.80038800	-1.04627500	-0.97915900
H	0.79458100	-0.80354200	0.78178500
H	3.06085200	-1.68386800	-0.99472400
H	3.18698900	-1.43650000	0.76211500
H	6.05935000	-4.74449100	1.08038400
H	5.71932700	-5.17037000	-0.61347700
H	7.05464700	-4.06419800	-0.22871300
H	6.47055600	-1.70580700	0.61242000
H	6.40629300	-1.90610900	-1.15494400
H	5.08041000	-1.09679400	-0.30505100
H	-3.74119400	-1.11208400	0.83487600
H	-3.60262700	-1.98038300	-0.71352500
H	-3.12180300	-2.77748500	0.80524200
H	-2.47498900	0.56222100	-0.51872600
H	-1.73264600	0.59303700	1.09769600
H	-0.72070500	0.47131300	-0.36488900
O	1.00432300	-5.29197600	-1.88374100
O	0.77373200	-5.64750100	1.76049500

Np	0.88587300	-5.46226800	-0.06130700
O	-1.77837300	-6.06182500	-0.31667400
H	-1.94514300	-5.10228100	-0.21980100
H	-1.82533800	-6.20598000	-1.27764800
O	1.27491600	-8.04367500	-0.42764300
H	1.09258200	-8.43489700	0.44415500
H	2.26044500	-7.89846900	-0.42784400
O	3.89547400	-7.27035800	-0.31412900
H	4.19749900	-7.65377300	0.52750000
H	3.77758600	-6.31779200	-0.10622600

$[NpO_2(TMOGA)(H_2O)_2]^+$

GAS: H = -1467.168798 Hartree

G = -1467.261334 Hartree

S = 194.758 Cal/Mol-Kelvin

N	3.59613300	1.93962400	-0.00831100
C	2.35450600	1.42679500	-0.00449400
C	1.16752000	2.39638600	0.01661000
O	-0.01309700	1.61787600	-0.00563100
C	-1.20057300	2.38945000	0.01531400
C	-2.37781000	1.40799500	-0.00478000
N	-3.62620500	1.90209200	-0.00266400
O	2.13417300	0.20144100	-0.01816100
O	-2.14039500	0.18688900	-0.02168800
C	-4.77408900	0.99097200	-0.02734200

C	-3.96174100	3.32449200	0.01186400
C	4.75940400	1.05008100	-0.03656000
C	3.91037100	3.36753500	0.01274500
H	1.19701700	3.01662600	0.92443400
H	1.20040200	3.06151300	-0.85839600
H	-1.23361700	3.00984600	0.92261100
H	-1.23674600	3.05271100	-0.86075800
H	-4.41668000	-0.03622400	-0.04403700
H	-5.39113600	1.15283900	0.86294700
H	-5.37894800	1.18579900	-0.91946200
H	-4.51868000	3.58602600	-0.89494300
H	-4.58998600	3.54608900	0.88153300
H	-3.07268400	3.95128400	0.06391400
H	5.36225400	1.19947400	0.86574800
H	4.41996700	0.01801200	-0.08312100
H	5.37323600	1.27569900	-0.91505300
H	4.53290900	3.59499300	0.88506700
H	4.46580200	3.64000800	-0.89164400
H	3.01202400	3.98058600	0.06457000
O	0.00207100	-1.10283200	1.78486600
O	0.00619600	-1.14771500	-1.78052300
Np	-0.00849300	-1.08312500	0.00140100
O	1.70501000	-2.96541700	0.03141600
H	2.27409600	-3.08194200	-0.74626300
H	2.26631800	-3.06056100	0.81761700
O	-1.57593600	-3.06027300	0.00552000

H	-1.73253500	-3.60542500	-0.78134500
H	-1.74236900	-3.61075400	0.78659100

SMD： H = -1467.313655 Hartree

G = -1467.399562 Hartree

S = 180.807 Cal/Mol-Kelvin

N	3.58779200	2.01100700	-0.09310700
C	2.36018300	1.47450000	-0.04885900
C	1.15778500	2.40589300	-0.00845200
O	-0.01451000	1.60431100	-0.02340900
C	-1.19573100	2.39204800	-0.00210300
C	-2.38683100	1.44567600	0.02732900
N	-3.61858600	1.97033500	0.09450100
O	2.18885900	0.23229800	-0.05338700
O	-2.20232200	0.20548500	0.00038900
C	-4.76962200	1.06354500	0.02994600
C	-3.89921800	3.39794700	-0.08732800
C	4.74369200	1.11062100	-0.02753800
C	3.85398600	3.43776500	0.11520700
H	1.18477900	3.01808700	0.90318600
H	1.16401400	3.08047300	-0.87474300
H	-1.19988200	3.04106700	0.88373000
H	-1.23851000	3.03097400	-0.89445100
H	-4.95616400	0.73610100	-0.99938200
H	-4.59065000	0.18793500	0.65485200

H	-5.64885200	1.59414800	0.39837400
H	-4.74332400	3.67478400	0.54824300
H	-3.04496500	4.00960600	0.19961100
H	-4.15876900	3.61081600	-1.13090600
H	5.62738400	1.65719100	-0.36004900
H	4.90732100	0.75523700	0.99641300
H	4.58625000	0.25146300	-0.68069000
H	4.70575300	3.72960000	-0.50327100
H	2.99962000	4.04708700	-0.17664200
H	4.09491900	3.63840300	1.16562500
O	0.07445100	-1.09627100	1.82163700
O	-0.05775100	-1.16495800	-1.81933700
Np	0.00788900	-1.11299400	0.00089200
O	1.81631900	-3.17134100	0.01145100
H	2.23253700	-3.06142200	-0.86110500
H	2.48147600	-2.82806100	0.63328500
O	-1.74318400	-3.22036100	0.04078200
H	-2.36005100	-2.96715000	-0.66780300
H	-2.24135700	-3.04860000	0.85877200

$[NpO_2(TMOGA)_2]^+$

GAS： H = -1963.803653 Hartree

G = -1963.921952 Hartree

S = 248.979 Cal/Mol-Kelvin

N	-1.62968400	-1.17622200	0.20175300

C	-0.51349300	-1.93281600	0.23707800
C	0.82811300	-1.25936200	-0.06129100
O	1.83405600	-2.18082800	0.30348200
C	3.13226900	-1.74947500	-0.04690100
C	4.07971900	-2.91064700	0.26289700
N	5.40674800	-2.66906000	0.26259400
O	-0.53526300	-3.14547800	0.49295900
O	3.60401400	-4.03160400	0.49489400
C	6.33857100	-3.74239500	0.60702000
C	6.00946600	-1.36616800	-0.00786000
C	-2.92248400	-1.77642600	0.52895700
C	-1.65228900	0.25260600	-0.09973700
H	0.89115000	-1.02139900	-1.13493600
H	0.94296800	-0.32715900	0.50884100
H	3.18438900	-1.50848200	-1.12056300
H	3.39952900	-0.84992000	0.52444200
H	6.94834100	-3.44198600	1.46670200
H	5.76906600	-4.63541000	0.85693200
H	7.00140100	-3.94953900	-0.24088300
H	6.89857600	-1.51075200	-0.62920700
H	5.32912000	-0.71435700	-0.55599700
H	6.31408300	-0.86854900	0.92154800
H	-3.59634100	-1.70615400	-0.33258400
H	-2.76866300	-2.82090100	0.79306000
H	-3.37427900	-1.24566100	1.37475400
H	-2.48821000	0.45953900	-0.77543600

H	-1.78941500	0.84717200	0.81227500
H	-0.73825900	0.57271200	-0.59964100
N	4.12790300	-8.66701700	-0.19271300
C	3.01151000	-7.91127000	-0.23673600
C	1.66992000	-8.58140400	0.06914600
O	0.66419200	-7.66547800	-0.31008300
C	-0.63458300	-8.09278600	0.04329400
C	-1.58080000	-6.93363300	-0.27765000
N	-2.90782000	-7.17510200	-0.28157200
O	3.03289700	-6.70168700	-0.50711700
O	-1.10401200	-5.81406100	-0.51427600
C	-3.83803300	-6.10402000	-0.63726000
C	-3.51177700	-8.47620200	-0.00511200
C	5.42048000	-8.07035900	-0.52718100
C	4.15178700	-10.09126400	0.12958400
H	1.55638700	-9.52151100	-0.48810200
H	1.60525300	-8.80402000	1.14596000
H	-0.90179300	-8.99742400	-0.51989100
H	-0.68787400	-8.32356200	1.11915200
H	-3.26736200	-5.21319300	-0.89230000
H	-4.44508400	-6.41083700	-1.49659300
H	-4.50362100	-5.89006400	0.20679500
H	-4.40482900	-8.32718800	0.60947900
H	-3.81036500	-8.98102600	-0.93258400
H	-2.83471700	-9.12351700	0.55237700
H	5.87640500	-8.61754200	-1.36013700

H	5.26520200	-7.03192300	-0.81334100
H	6.09152900	-8.12113400	0.33797500
H	4.29258600	-10.69867700	-0.77334400
H	4.98598700	-10.28716600	0.81073300
H	3.23673700	-10.40552100	0.63127100
O	1.36569200	-4.37049100	-1.71189400
O	1.13377400	-5.47434300	1.69616700
Np	1.24955000	-4.92255800	-0.00805400

SMD： H = -1963.923262 Hartree

G = -1964.030463 Hartree

S = 225.624 Cal/Mol-Kelvin

N	-2.93741800	3.81919100	0.05316800
C	-2.52894100	2.54294400	-0.02155400
C	-3.60163800	1.45997400	-0.05951200
O	-2.95578900	0.22532700	-0.30074100
C	-3.77152900	-0.89216700	-0.00279600
C	-2.90424900	-2.13935200	-0.14199200
N	-3.49352000	-3.33627500	0.00715600
O	-1.31748000	2.22539100	-0.03707900
O	-1.68368000	-2.02191800	-0.39396800
C	-2.72083600	-4.56986100	-0.14123500
C	-4.90836700	-3.52733500	0.32978100
C	-1.96859800	4.91473300	0.01716400
C	-4.34547800	4.21642500	-0.01619400

H	-4.12932400	1.44182700	0.90517400
H	-4.33962200	1.66604000	-0.84532600
H	-4.16037900	-0.81833700	1.02295100
H	-4.62685100	-0.94225300	-0.68988200
H	-3.27826900	-5.26631200	-0.77470700
H	-1.75981000	-4.35294900	-0.60371100
H	-2.55751700	-5.03659200	0.83676700
H	-4.99051600	-4.24197500	1.15469900
H	-5.38156400	-2.59790700	0.64072500
H	-5.44514500	-3.93021000	-0.53612500
H	-2.14882500	5.58773700	0.86080600
H	-0.95824500	4.51578700	0.08083900
H	-2.07880900	5.48121800	-0.91442400
H	-4.46309700	5.15289100	0.53349700
H	-4.66214800	4.37567400	-1.05338800
H	-4.99282200	3.47326300	0.44943900
N	2.93733900	-3.81942800	-0.04960600
C	2.52889800	-2.54303800	0.02236900
C	3.60172700	-1.46021300	0.06037600
O	2.95584300	-0.22541600	0.30056200
C	3.77191400	0.89191900	0.00310600
C	2.90447900	2.13911300	0.14146600
N	3.49379500	3.33608600	-0.00701300
O	1.31746900	-2.22518500	0.03473800
O	1.68369200	2.02151700	0.39227800
C	2.72093800	4.56959800	0.14098300

C	4.90869600	3.52724800	-0.32942200
C	1.96852700	-4.91495000	-0.01320900
C	4.34531200	-4.21657400	0.02186200
H	4.33940800	-1.66577200	0.84658000
H	4.12979700	-1.44271400	-0.90414000
H	4.62664800	0.94214700	0.69092100
H	4.16164900	0.81789800	-1.02229200
H	1.75969800	4.35260400	0.60297500
H	3.27800400	5.26609300	0.77471900
H	2.55802700	5.03633300	-0.83708500
H	4.99086900	4.24138100	-1.15478100
H	5.44518500	3.93079900	0.53634100
H	5.38215600	2.59771100	-0.63963000
H	2.07967900	-5.48161300	0.91814400
H	0.95811200	-4.51600400	-0.07582600
H	2.14793500	-5.58778100	-0.85718100
H	4.66098400	-4.37374200	1.05968100
H	4.46340000	-5.15417000	-0.52580200
H	4.99308300	-3.47438900	-0.44474300
O	-0.20622200	-0.12099700	1.81273500
O	0.20618000	0.12139100	-1.81445600
Np	-0.00008900	0.00015800	-0.00086900

$[NpO_2(DMOGA)(H_2O)_4]$

GAS： H = -1560.881624 Hartree

G = -1560.974531 Hartree

S = 195.541 Cal/Mol-Kelvin

O	-2.80131300	3.36020000	-0.02600000
C	-1.57971200	3.02186600	0.04486100
C	-1.27592600	1.53368800	0.14685500
O	0.09896500	1.29562700	-0.01462600
C	0.42385400	-0.05840300	0.13452500
C	1.93411100	-0.22592400	-0.11020500
N	2.43296800	-1.50426200	0.01826100
O	-0.64983500	3.87264500	0.06038600
O	2.63509600	0.72884300	-0.40526500
C	3.85390400	-1.72726900	-0.20212700
C	1.66386800	-2.68522400	0.36802000
H	-1.63762000	1.19130500	1.13299500
H	-1.87747700	1.00704600	-0.61249200
H	0.16157500	-0.41588500	1.14627200
H	-0.14057300	-0.68252600	-0.58174200
H	4.00920200	-2.44268000	-1.02103800
H	4.31421700	-0.77399000	-0.45851700
H	4.32627000	-2.13154100	0.70342500
H	0.60937400	-2.45282700	0.51064400
H	2.04202200	-3.13257800	1.29813300
H	1.73983700	-3.44346500	-0.42401500
O	-2.14731200	6.01519600	-1.74476600
O	-2.26768700	5.80004800	1.83352500
Np	-2.19689100	5.87000200	0.05047800

O	0.49598000	6.23983300	-0.27608600
H	0.64132100	5.30293800	-0.02650600
H	0.42989600	6.21513900	-1.24672200
O	-1.18797400	8.24031100	0.55216700
H	-1.39688600	8.26650600	1.50167900
H	-0.25926600	7.94033700	0.49886500
O	-4.07060400	7.71517900	0.09461500
H	-4.81517500	7.09724900	-0.03673800
H	-3.99275500	8.21265300	-0.73597900
O	-4.73851000	5.10556000	-0.57665600
H	-4.51407700	4.21679200	-0.23015400
H	-4.47094800	5.05227100	-1.51180200

SMD： H = -1561.015307 Hartree

G = -1561.104132 Hartree

S = 186.949 Cal/Mol-Kelvin

O	-3.57101900	2.57351800	0.11150000
C	-2.32529000	2.49636500	-0.05650400
C	-1.73169100	1.09356900	0.03565800
O	-0.32390700	1.13056700	-0.10951600
C	0.24271200	-0.16213300	-0.03452100
C	1.76102100	-0.02698600	-0.15450600
N	2.47873600	-1.17637800	-0.07724100
O	-1.54548000	3.46845100	-0.30793100
O	2.28212600	1.08702200	-0.32213000

C	3.93779900	-1.11671800	-0.04495700
C	1.89717400	-2.47405000	0.26490200
H	-2.01922800	0.65806200	1.00431400
H	-2.19440200	0.47409200	-0.74818900
H	-0.01718600	-0.64423800	0.92016500
H	-0.14666700	-0.80176200	-0.84161200
H	4.35382000	-1.85674700	-0.73609600
H	4.26653200	-0.12196200	-0.34051700
H	4.31046000	-1.33479600	0.96378500
H	0.88297200	-2.57349600	-0.12296800
H	1.88417500	-2.63767400	1.35003400
H	2.50539900	-3.25828400	-0.19403700
O	-1.77357300	6.15558200	-1.83022300
O	-2.07218600	5.85224200	1.81405700
Np	-1.91500700	5.99291300	-0.00820500
O	0.97951100	4.59755800	0.03570400
H	0.21741200	3.98567600	-0.05996500
H	1.07229300	4.96623200	-0.85849600
O	-0.92803200	8.65221800	0.10542500
H	-1.89473700	8.83767500	0.21522100
H	-0.59073700	8.63843200	1.01729800
O	-3.69347600	8.66581500	0.32539800
H	-3.76014400	8.00569400	1.03847400
H	-3.87392200	8.14407400	-0.47682800
O	-4.36728000	5.08390000	-0.41677200
H	-4.11637200	4.13180100	-0.21930600

H	-4.41988700	5.11842700	-1.38714500

$[NpO_2(DMOGA)(H_2O)_3]_c$

GAS: H = -1484.488869 Hartree

G = -1484.576417 Hartree

S = 184.261 Cal/Mol-Kelvin

O	-0.36479900	1.75066500	0.14093300
C	0.55811000	0.89000500	-0.01018400
C	1.99069900	1.40517800	0.01520900
O	2.90568900	0.34132800	-0.04977500
C	4.23365900	0.78354800	-0.01920100
C	5.15834300	-0.44605100	-0.05242900
N	6.51242400	-0.18639000	-0.03363600
O	0.31568100	-0.33710200	-0.17765500
O	4.70448500	-1.57802000	-0.10101300
C	7.43846700	-1.30872100	0.00024300
C	7.11486200	1.12702300	0.11273400
H	2.11152300	2.10255400	-0.83246400
H	2.11738700	2.00056300	0.93523900
H	4.45044100	1.44099200	-0.88068000
H	4.43209800	1.37648000	0.89174200
H	7.98637500	-1.33513600	0.95267700
H	6.86568200	-2.22832300	-0.11208200
H	8.16825600	-1.22496200	-0.81543600
H	6.39762000	1.92343200	-0.08422800

H	7.93890800	1.23794400	-0.60359100
H	7.52565400	1.27313800	1.12315600
O	-2.09674400	-0.40674000	1.77557800
O	-2.35752600	0.20616600	-1.75932600
Np	-2.15775800	-0.06440000	0.00938100
O	-1.29723000	-2.53470900	-0.13955300
H	-0.41110400	-2.25922600	-0.45114500
H	-1.16589800	-2.67001700	0.81512800
O	-4.48547600	-1.18952300	-0.00958500
H	-4.71217700	-1.68265400	-0.81410300
H	-4.68883000	-1.76502000	0.74440800
O	-3.02445200	2.39008500	0.15794200
H	-3.18829700	2.56371100	-0.78465200
H	-2.10495100	2.69732900	0.30045600

SMD： H = -1484.587528 Hartree

G = -1484.672103 Hartree

S = 178.003 Cal/Mol-Kelvin

O	0.26248000	-1.75675500	-0.28046800
C	-0.66433900	-0.88864600	-0.22469200
C	-2.09249600	-1.40966500	-0.15365500
O	-3.01214500	-0.33300400	-0.13477100
C	-4.34332700	-0.78706200	0.01189400
C	-5.27437700	0.42299400	-0.08130300
N	-6.60451600	0.17358600	0.02413400

O	-0.43223900	0.35608800	-0.19640900
O	-4.81050200	1.55918400	-0.26510600
C	-7.55017000	1.28575600	0.04197300
C	-7.15552100	-1.12426100	0.41079900
H	-2.27168800	-2.07306700	-1.01317900
H	-2.18161700	-2.02493400	0.75514000
H	-4.59290200	-1.51224300	-0.77725200
H	-4.47674800	-1.29507600	0.97937000
H	-7.92031200	1.46497100	1.05956400
H	-7.05915700	2.18654700	-0.32207500
H	-8.40380700	1.05104600	-0.60157000
H	-6.52971100	-1.94516500	0.06093100
H	-8.14019400	-1.23746000	-0.05104700
H	-7.27385900	-1.20257700	1.49916400
O	1.97644500	-0.04391200	1.83356200
O	2.32862000	0.12655100	-1.80901300
Np	2.13807900	0.03792800	0.01162500
O	1.70289400	2.69212400	0.04308000
H	1.22631400	2.78416500	-0.80082500
H	0.99984900	2.75525600	0.71354000
O	4.60624300	1.07993500	0.33277900
H	4.69057200	1.57726300	-0.49951800
H	4.44168300	1.76747700	1.00166600
O	3.52116300	-2.16058500	0.03805900
H	4.20087800	-2.06154300	-0.65174800
H	4.01866700	-2.12873600	0.87394800

$[NpO_2(DMOGA)(H_2O)_3]_e$

GAS: H = -1484.501871 Hartree

G = -1484.582785 Hartree

S = 170.298 Cal/Mol-Kelvin

O	-3.35157600	3.54986700	0.09128100
C	-2.30571600	2.93803200	-0.05754500
C	-2.36512800	1.40168500	0.07017500
O	-1.07356000	0.82292200	-0.17486500
C	-0.99820900	-0.55964900	0.05370600
C	0.46918700	-0.97262100	-0.10090200
N	0.79006800	-2.27922600	0.00349600
O	-1.12930300	3.41681700	-0.31022700
O	1.32870800	-0.10087600	-0.31327800
C	2.18293800	-2.70119800	-0.13864700
C	-0.16447100	-3.35027000	0.26380400
H	-2.69750600	1.14390300	1.08464600
H	-3.09221400	1.00425400	-0.64911800
H	-1.34874700	-0.80516100	1.06920000
H	-1.63066300	-1.10548100	-0.66320800
H	2.26968600	-3.42240500	-0.95944500
H	2.79920300	-1.82990300	-0.35059400
H	2.52514600	-3.17681800	0.78784100
H	-1.17303400	-2.96580100	0.40649400
H	0.12640100	-3.89466300	1.17005200

H	-0.17697700	-4.05734100	-0.57458100
O	1.01915800	2.34703800	-2.17716800
O	1.14077300	2.46266900	1.41359100
Np	1.03216400	2.38069300	-0.38889200
O	0.82992500	5.07023400	-0.45522600
H	-0.13194100	4.85520400	-0.31049700
H	0.87726100	5.34168800	-1.38669100
O	2.86216700	4.73697700	1.59185100
H	2.31183900	4.00621900	1.94925100
H	2.20487500	5.24779600	1.07996300
O	3.44739100	3.08152400	-0.38634900
H	3.46593400	3.76627600	0.35119000
H	3.80446700	3.49101700	-1.18869000

SMD： H = -1484.608533 Hartree

G = -1484.688881 Hartree

S = 169.108 Cal/Mol-Kelvin

O	-3.11370300	3.57484700	0.02407900
C	-2.06308000	2.91138000	0.04822600
C	-2.21411700	1.38749100	0.12648600
O	-0.95196000	0.75708400	0.32331100
C	-0.97069900	-0.65102100	0.17972900
C	0.47892100	-1.12915500	0.13407600
N	0.71828300	-2.44406900	0.05687000
O	-0.87317100	3.39685800	-0.00892400

O	1.41102800	-0.28599300	0.15623700
C	2.08828100	-2.95103400	-0.03709000
C	-0.31589400	-3.47821100	0.03199800
H	-2.89848700	1.13759200	0.94687200
H	-2.66903100	1.04019100	-0.81183000
H	-1.50549900	-1.11153100	1.02044900
H	-1.48201500	-0.93620300	-0.75046900
H	2.19961200	-3.52714700	-0.96152200
H	2.79267300	-2.12245200	-0.03686300
H	2.29664000	-3.60859500	0.81334600
H	-1.31577200	-3.05621600	0.10204700
H	-0.16401000	-4.16283600	0.87300900
H	-0.23976600	-4.04740900	-0.90031900
O	1.18923700	2.04605900	-1.92403400
O	1.51612100	2.42261300	1.71031500
Np	1.34173900	2.22046500	-0.11025100
O	0.41565200	5.80757300	-0.36974500
H	-0.16659500	5.01805600	-0.25150200
H	0.70653300	5.74426800	-1.29500300
O	2.59675100	5.12799400	1.18422700
H	2.23152500	4.34194900	1.64037000
H	1.83655600	5.41485900	0.61266000
O	3.76922900	3.30326300	-0.45108800
H	3.48227100	4.08834400	0.09616100
H	3.72099200	3.61438900	-1.37120700

[NpO_2(DMOGA)(H_2O)$_2$]

GAS: H = -1408.08851 Hartree

G = -1408.165633 Hartree

S = 162.32 Cal/Mol-Kelvin

O	1.85337300	3.84559500	0.12115700
C	1.25452000	2.78341500	0.06366000
C	-0.28708600	2.84376800	0.11318700
O	-0.84888700	1.53450200	-0.07421200
C	-2.24467500	1.46571400	0.05241600
C	-2.64211800	-0.01274500	-0.01798600
N	-3.95366600	-0.32904700	-0.02728300
O	1.75161900	1.59096100	-0.02746200
O	-1.75544700	-0.88319600	-0.05803700
C	-4.36687000	-1.72781300	-0.13344100
C	-5.03861300	0.64526900	0.01194600
H	-0.59661200	3.23950900	1.08982800
H	-0.64963200	3.51860700	-0.67193300
H	-2.56977800	1.89110600	1.01595400
H	-2.73408500	2.03669100	-0.75108500
H	-4.98718200	-1.86421900	-1.02685900
H	-3.48162200	-2.35628900	-0.20497800
H	-4.95037900	-2.01293700	0.74942700
H	-4.67752400	1.63989200	0.26984000
H	-5.76771200	0.34381200	0.77201600
H	-5.55042000	0.69524300	-0.95749400

O	0.79659800	-0.66753100	-1.79244900
O	0.67917900	-0.52762700	1.78502400
Np	0.72429400	-0.54678200	-0.00737400
O	3.43974700	-0.37519500	-0.43187200
H	3.27978200	0.56788000	-0.17998600
H	3.30723900	-0.37167600	-1.39639700
O	2.15191800	-2.68085100	0.47188300
H	2.11561700	-2.63307300	1.44309100
H	2.98284400	-2.21941000	0.23442000

SMD： H = -1408.192943 Hartree

G = -1408.269075 Hartree

S = 160.233 Cal/Mol-Kelvin

O	1.89007700	4.01061500	0.01661200
C	1.29766400	2.91440200	-0.00755300
C	-0.23220300	2.95987200	-0.00627500
O	-0.75731000	1.63882900	-0.09820900
C	-2.16925600	1.57182200	-0.02999100
C	-2.56288200	0.10206300	-0.10947500
N	-3.86437300	-0.20590600	-0.03211500
O	1.85502900	1.76055800	-0.02739700
O	-1.67213500	-0.77225700	-0.25109100
C	-4.30050000	-1.60260300	0.00674800
C	-4.91020100	0.78365200	0.23763300
H	-0.57545900	3.44150300	0.91933800

H	-0.57852400	3.56619700	-0.85350200
H	-2.52781700	2.01246200	0.91040100
H	-2.61766400	2.13177300	-0.86239600
H	-5.03265100	-1.78087700	-0.78674400
H	-3.44557700	-2.26034900	-0.13417400
H	-4.76904900	-1.81644900	0.97362300
H	-4.64418500	1.76260300	-0.16008600
H	-5.09856600	0.86668100	1.31417700
H	-5.82828000	0.45639300	-0.25603500
O	1.02341400	-0.58498200	-1.84294700
O	0.66532800	-0.44114800	1.80264700
Np	0.84135800	-0.49843900	-0.02022900
O	3.31029100	-1.46649400	0.37002000
H	3.62919700	-0.93720700	1.12178100
H	3.85105300	-1.16367100	-0.38008000
O	0.43664100	-3.18381700	0.01447300
H	-0.25026700	-3.26054500	0.69971700
H	-0.05430700	-3.28799500	-0.81930100

$[NpO_2(DMOGA)_2(H_2O)_2]^-_a$

GAS： H = -1998.298792 Hartree

G = -1998.417011 Hartree

S = 248.813 Cal/Mol-Kelvin

O	-2.82760900	2.75937700	0.00232800
C	-1.62782900	2.33874600	0.04406300

C	-1.46285000	0.83310500	-0.18377000
O	-0.25041900	0.33556500	0.34881200
C	0.01217700	-0.95573500	-0.10211300
C	1.24259700	-1.51692200	0.62611200
N	1.69080500	-2.75372300	0.18517900
O	-0.62605400	3.07791900	0.16788700
O	1.77578200	-0.92792400	1.55046200
C	2.91042900	-3.29397500	0.76097400
C	1.16352300	-3.46828700	-0.96229800
H	-2.32817200	0.31059200	0.25293400
H	-1.50337700	0.67359200	-1.27644500
H	-0.84452100	-1.63418400	0.08382600
H	0.18328500	-0.96420100	-1.19437900
H	3.72425900	-3.31285400	0.02079500
H	3.20068100	-2.65713000	1.59609700
H	2.74565100	-4.32024200	1.11675300
H	0.13475600	-3.17746200	-1.17607400
H	1.16366000	-4.54537200	-0.75067200
H	1.76720400	-3.30443200	-1.86918300
O	-1.04613200	7.78170000	0.11235500
C	0.14113000	7.35330600	0.27308100
C	1.17761300	8.44044100	0.57190700
O	2.50335500	8.01371400	0.32495400
C	3.42936400	8.91985700	0.83587200
C	4.84780400	8.50134400	0.42198000
N	5.87875700	9.25907100	0.95921100

O	0.45949500	6.14384900	0.27873000
O	5.05580700	7.58137300	-0.34993500
C	7.24788500	8.85180900	0.69290500
C	5.71190000	10.29968800	1.95663400
H	0.93414900	9.33370700	-0.02473200
H	1.04794600	8.71593400	1.63411500
H	3.24325900	9.94632600	0.46111400
H	3.35984200	8.97519500	1.93810900
H	7.73319200	8.46950500	1.60341700
H	7.22553900	8.06307400	-0.05851400
H	7.83577600	9.70218700	0.32141200
H	4.71340100	10.73568800	1.91612000
H	6.43110600	11.10592200	1.76312500
H	5.88924700	9.93024000	2.97935200
O	-1.84383700	5.27814500	-1.73993800
O	-2.15361900	5.30710900	1.86623200
Np	-1.92987600	5.26808000	0.06925900
O	-3.55466800	7.37083400	-0.75225700
H	-2.72990800	7.87145900	-0.57721700
H	-3.37693600	6.94299600	-1.60902800
O	-4.60963500	4.69862600	0.50593100
H	-4.34360500	4.95711400	1.40653200
H	-4.27218900	3.78136500	0.42664600

SMD： H = -1998.482396 Hartree

G = -1998.59266 Hartree

S = 232.07 Cal/Mol-Kelvin

O	-2.91747400	2.74967800	-0.33243300
C	-1.72816600	2.32386400	-0.19649300
C	-1.52187300	0.81924600	-0.30834400
O	-0.15374200	0.49593900	-0.14143600
C	0.06754600	-0.90036800	-0.17542300
C	1.56147100	-1.15056600	0.04489800
N	1.96581900	-2.44662900	0.05773600
O	-0.74342500	3.08593500	0.02534800
O	2.34035300	-0.19883600	0.21004500
C	3.39203400	-2.75500100	0.12554600
C	1.09280900	-3.57024200	-0.27903700
H	-2.14356800	0.32930100	0.45666800
H	-1.89510400	0.48836400	-1.28968500
H	-0.52159700	-1.40190400	0.60746500
H	-0.24415800	-1.32378200	-1.14275900
H	3.77495600	-3.05053000	-0.85970200
H	3.93647400	-1.87771700	0.47048500
H	3.55567700	-3.58168800	0.82373900
H	0.06488400	-3.38419100	0.03193200
H	1.44715600	-4.45683500	0.25360600
H	1.10659800	-3.78575800	-1.35516400
O	-1.10665000	7.78538400	0.42846800
C	0.09571100	7.37124900	0.46868700
C	1.16907900	8.43883900	0.63090100

O	2.45185200	7.84661900	0.72420800
C	3.46474400	8.82236800	0.87054000
C	4.80622900	8.10071000	1.00788400
N	5.90790400	8.88366600	1.13791100
O	0.41357000	6.15167900	0.38068100
O	4.85673600	6.86126400	0.98511700
C	7.20405500	8.26773000	1.41368800
C	5.85543700	10.33336600	1.32318300
H	1.10764100	9.12244200	-0.23027500
H	0.93679700	9.03020400	1.52968300
H	3.47964800	9.49615700	0.00037900
H	3.28175600	9.44239900	1.76159900
H	7.50265800	8.44481100	2.45451700
H	7.13986200	7.19550800	1.23687500
H	7.96579300	8.69942700	0.75653800
H	5.01211800	10.77430900	0.79175900
H	6.77125200	10.76972600	0.91496700
H	5.78942600	10.60146400	2.38543500
O	-1.91269700	5.46793600	-1.78256300
O	-2.28524900	5.16341000	1.87235500
Np	-2.07485700	5.30635400	0.04604000
O	-3.85816700	7.90066400	-0.42643100
H	-2.94147000	8.05779500	-0.12629300
H	-3.72273500	7.39051000	-1.24330000
O	-5.13730600	4.44127900	0.12603200
H	-4.84722500	4.83119300	0.96774700

H	-4.51333200	3.69697400	0.01253300

$[NpO_2(DMOGA)_2(H_2O)_2]^-_i$

GAS: H = -1998.304987 Hartree

G = -1998.421906 Hartree

S = 246.077 Cal/Mol-Kelvin

O	-2.32483100	2.79821600	-0.19593200
C	-1.10299800	2.55281800	-0.00544400
C	-0.74057200	1.06383500	-0.01540100
O	0.64699800	0.83374600	0.15133100
C	0.93322100	-0.52839400	0.12756600
C	2.44485800	-0.74439700	0.29042400
N	2.86811600	-2.06565500	0.29951000
O	-0.21773300	3.42652700	0.18676800
O	3.22495000	0.18426300	0.41584700
C	4.29367600	-2.33627700	0.36926600
C	2.02402200	-3.21660700	0.03995000
H	-1.31752300	0.57169800	0.78600700
H	-1.09559400	0.63978700	-0.96950700
H	0.39875900	-1.06400000	0.93651400
H	0.60019200	-0.99221300	-0.82106600
H	4.66310500	-2.76569300	-0.57416500
H	4.80793400	-1.39502900	0.56071700
H	4.50922100	-3.04833900	1.17752800
H	0.96969700	-2.97972700	0.17888500

H	2.27737900	-4.02532700	0.73840900
H	2.16016600	-3.60310600	-0.98272200
O	-1.82945600	7.91496900	-0.08306900
C	-3.05468100	8.15858700	-0.25268100
C	-3.42947300	9.64212900	-0.16873300
O	-4.80794500	9.87586000	-0.39546100
C	-5.11419600	11.22695600	-0.25941600
C	-6.61135400	11.44910500	-0.51844100
N	-7.05340700	12.75991800	-0.41016200
O	-3.93652300	7.28559800	-0.46354100
O	-7.36321000	10.53650800	-0.81597000
C	-8.47438000	13.02517600	-0.55562000
C	-6.25208800	13.87336500	0.06249400
H	-3.13170200	10.00191400	0.83079500
H	-2.81344400	10.19047400	-0.90093900
H	-4.86025200	11.59534100	0.75320200
H	-4.52837200	11.84520600	-0.96782300
H	-8.63937900	13.83946400	-1.27406900
H	-8.95389700	12.11465200	-0.91355800
H	-8.92559000	13.31751600	0.40465800
H	-5.18634700	13.67649900	-0.05171000
H	-6.45063800	14.10509700	1.12119000
H	-6.48786900	14.77018900	-0.52524200
O	-1.61227900	5.40948700	-1.89417200
O	-2.54046300	5.30336800	1.60287300
Np	-2.07634700	5.35643000	-0.14585000

O	0.53370900	5.99186800	0.03097500
H	0.68490600	5.02332700	0.06126200
H	0.48200500	6.19462200	-0.91886000
O	-4.68572400	4.71903700	-0.32576500
H	-4.63388300	4.51176900	0.62305500
H	-4.83781600	5.68760400	-0.35152800

SMD： H = -1998.484 Hartree

G = -1998.594102 Hartree

S = 231.729 Cal/Mol-Kelvin

O	-2.36005400	2.75156200	-0.41805300
C	-1.14333400	2.44385000	-0.22237700
C	-0.82316300	0.95360500	-0.19154900
O	0.56901600	0.74259300	-0.03407500
C	0.87806200	-0.63529900	0.04681600
C	2.39575000	-0.77872000	0.17511400
N	2.88453300	-2.04030500	0.28228900
O	-0.22949700	3.29708900	-0.04166600
O	3.11955600	0.22913300	0.19096100
C	4.32897900	-2.25835800	0.30700700
C	2.08041700	-3.25083200	0.12769000
H	-1.38853200	0.50105500	0.63803900
H	-1.19173000	0.49418800	-1.12115900
H	0.37782300	-1.09220500	0.91441600
H	0.52611400	-1.16529200	-0.85128200

H	4.66298800	-2.72696300	-0.62710300
H	4.83793100	-1.30455000	0.43181000
H	4.58844200	-2.92212700	1.13839500
H	1.03157600	-3.07022600	0.35915100
H	2.45081600	-4.01167500	0.82144600
H	2.15617900	-3.64635200	-0.89328600
O	-1.80923700	7.95000900	0.27341100
C	-3.02642600	8.25528200	0.07752800
C	-3.34777700	9.74476800	0.02848900
O	-4.74471100	9.95283400	-0.08597100
C	-5.05514900	11.32670300	-0.21575700
C	-6.57874900	11.47247200	-0.23039700
N	-7.07635900	12.72653200	-0.37132000
O	-3.93987100	7.39965500	-0.09435400
O	-7.30110100	10.46979500	-0.11383600
C	-8.51937700	12.94804900	-0.33705300
C	-6.27050800	13.94151200	-0.46082200
H	-2.94835800	10.22408700	0.93473600
H	-2.81079800	10.17852200	-0.82975600
H	-4.63448500	11.90152000	0.62335900
H	-4.62067700	11.73152400	-1.14229500
H	-8.83900000	13.47060400	-1.24553000
H	-9.03226500	11.99042000	-0.27077200
H	-8.79002800	13.56367800	0.52922800
H	-5.22295200	13.72015900	-0.65676500
H	-6.33929900	14.52144000	0.46789400

H	-6.64507900	14.56205800	-1.28175000
O	-1.65203300	5.64457400	-1.83354500
O	-2.51844800	5.05473000	1.69255700
Np	-2.08514400	5.34961900	-0.07045900
O	0.60033100	5.95465900	0.59988500
H	0.70735400	5.00203800	0.40793300
H	0.77304500	6.37928500	-0.25803000
O	-4.77091000	4.74434800	-0.74224500
H	-4.94276100	4.32012800	0.11604700
H	-4.87815300	5.69699000	-0.55061600

$[NpO_2(DMOGA)_2(H_2O)]^-$

GAS: H = -1921.908068 Hartree

G = -1922.014885 Hartree

S = 224.815 Cal/Mol-Kelvin

O	-2.89633800	-0.04636900	0.06683300
C	-2.43746200	1.06612700	-0.19566000
C	-0.96133700	1.30595000	0.19597000
O	-0.43464500	2.45480500	-0.46722300
C	0.65383100	3.05302300	0.17808600
C	0.80986800	4.45099600	-0.43151000
N	1.74159300	5.29444100	0.08372200
O	-3.03688300	2.07448200	-0.71591600
O	0.07597300	4.79824500	-1.36178000
C	1.72850300	6.69130900	-0.35040500

C	2.66814600	4.94390600	1.14471300
H	-0.93094100	1.45876200	1.28529400
H	-0.36504500	0.41615400	-0.04631400
H	0.46191800	3.15196100	1.25679800
H	1.57830800	2.46291900	0.04221800
H	2.48566300	6.87356500	-1.12527300
H	0.73725100	6.93656200	-0.73654700
H	1.94967400	7.32831100	0.51337200
H	2.69119900	3.86604500	1.30705600
H	2.39346200	5.43235200	2.09006700
H	3.68297000	5.26443300	0.87501100
O	-1.73307000	7.03262600	-0.81589800
C	-2.92399300	7.40981800	-0.59926200
C	-3.10137500	8.93034800	-0.50407100
O	-4.45528700	9.32500200	-0.37883200
C	-4.56333600	10.70522200	-0.24215400
C	-6.04282700	11.10457600	-0.13937200
N	-6.29066400	12.46088500	0.02547900
O	-3.89856400	6.63474300	-0.45045100
O	-6.94509100	10.28886000	-0.21428400
C	-7.66299200	12.89398500	0.22437100
C	-5.27464100	13.47348200	0.24018700
H	-2.51308700	9.27901600	0.36314000
H	-2.64419800	9.38164900	-1.40061900
H	-4.02435500	11.06244300	0.65679100
H	-4.10727800	11.23270000	-1.10359000

H	-7.91180100	13.70938900	-0.46836600
H	-8.31654100	12.04183200	0.04012200
H	-7.82179000	13.25539300	1.25171000
H	-4.30286800	13.15003900	-0.13249000
H	-5.16854400	13.73489600	1.30546100
H	-5.54866400	14.38829300	-0.30168500
O	-2.93233800	4.53521600	-2.49029200
O	-1.94663700	4.51400300	0.99435400
Np	-2.45495600	4.53150100	-0.74968700
O	-4.99488400	3.76372400	-0.45762200
H	-5.21669000	4.06969100	-1.35241800
H	-4.62238200	2.85597300	-0.58322400

SMD： H = -1922.091643 Hartree

G = -1922.190377 Hartree

S = 207.805 Cal/Mol-Kelvin

O	-2.90198500	0.04049200	-0.15599700
C	-2.43074800	1.18960300	-0.26431200
C	-0.93416800	1.35358100	0.00059400
O	-0.53067700	2.69039600	-0.27587300
C	0.79123800	2.96826100	0.14198100
C	1.04334300	4.45594100	-0.07460600
N	2.28218800	4.91812000	0.16586900
O	-3.08711700	2.24557800	-0.56761000
O	0.11013000	5.19987100	-0.45409700

C	2.61935400	6.31211300	-0.12651700
C	3.41238400	4.04255200	0.48393100
H	-0.73748000	1.10506900	1.05318600
H	-0.37300600	0.64471900	-0.62270000
H	0.92047300	2.71844100	1.20561500
H	1.50958300	2.36960100	-0.43443500
H	3.21735500	6.37550400	-1.04319600
H	1.70662300	6.89132100	-0.25114100
H	3.20180300	6.72453900	0.70196100
H	3.09109800	3.17188100	1.05524800
H	4.11990100	4.60360000	1.09873100
H	3.92442600	3.71021200	-0.42681300
O	-2.01311700	7.26611100	0.11351100
C	-3.21317200	7.67726800	0.02075600
C	-3.38810900	9.19125900	0.02901200
O	-4.75610000	9.55391700	-0.05038000
C	-4.89717700	10.95867700	-0.14481200
C	-6.38631200	11.30441600	-0.15941400
N	-6.70073400	12.61967100	-0.28348300
O	-4.20530700	6.90741800	-0.08889800
O	-7.24239300	10.41085100	-0.06761300
C	-8.09299700	13.04358300	-0.16825000
C	-5.71422900	13.69714900	-0.24191100
H	-2.92569500	9.59147800	0.94411700
H	-2.82281300	9.60049900	-0.82242700
H	-4.41294300	11.45637000	0.70972500

H	-4.40742600	11.33080300	-1.05757700
H	-8.31183400	13.79092100	-0.93713100
H	-8.74781400	12.18448400	-0.30309900
H	-8.28362100	13.48979600	0.81625400
H	-4.75240200	13.37581000	-0.64047200
H	-5.56990000	14.07043000	0.78023200
H	-6.07276100	14.52339500	-0.86225900
O	-2.60849300	4.89877900	-2.06035000
O	-2.35365400	4.54315600	1.59861700
Np	-2.47998100	4.72217300	-0.23060700
O	-5.25433500	3.86307500	-0.24170300
H	-5.38109000	4.22488700	-1.13510400
H	-4.78345100	3.01551600	-0.40074500

$[NpO_2(DMOGA)_2]^-$

GAS： H = -1845.511106 Hartree

G = -1845.605922 Hartree

S = 199.557 Cal/Mol-Kelvin

O	-4.02407700	1.19898900	-0.42299100
C	-3.22228600	2.13648600	-0.48688700
C	-1.72485800	1.75814900	-0.36961800
O	-0.89886900	2.82172000	-0.84632600
C	0.40524900	2.84063800	-0.33304700
C	0.94859200	4.25222300	-0.59486100
N	2.15303700	4.60920100	-0.09039300

O	-3.47127400	3.38613600	-0.59738500
O	0.26244600	5.05433400	-1.23975100
C	2.53340000	6.02530000	-0.15546400
C	3.03659400	3.71107900	0.62999000
H	-1.50970800	1.56871100	0.69257300
H	-1.52854100	0.83793100	-0.93572200
H	0.39908100	2.65135500	0.75000600
H	1.04183400	2.07887900	-0.81827600
H	3.17584000	6.24772900	0.70245600
H	3.08622900	6.24419800	-1.07831900
H	1.63515000	6.64751700	-0.10702000
H	2.71352600	2.67469100	0.52494800
H	3.06727600	3.95872400	1.69992200
H	4.05633300	3.78732600	0.23027700
O	-0.10211200	9.50051800	0.18612100
C	-0.90394200	8.56308600	0.25057500
C	-2.40133100	8.94145700	0.13305900
O	-3.22743500	7.87813600	0.61015200
C	-4.53154700	7.85916300	0.09685900
C	-5.07491600	6.44761700	0.35884100
N	-6.27950400	6.09078100	-0.14543500
O	-0.65497700	7.31349100	0.36183700
O	-4.38873600	5.64551200	1.00364400
C	-6.65990700	4.67466900	-0.08075000
C	-7.16260700	6.98892400	-0.86638200
H	-2.59761000	9.86192100	0.69877200

H	-2.61639700	9.13045700	-0.92922300
H	-5.16811900	8.62101000	0.58196200
H	-4.52538700	8.04826200	-0.98622600
H	-5.76160200	4.05246600	-0.12829700
H	-7.21369400	4.45577900	0.84152800
H	-7.30143800	4.45218800	-0.93934100
H	-6.84079700	8.02551700	-0.75940600
H	-8.18291400	6.91112300	-0.46848500
H	-7.19122700	6.74261200	-1.93669200
O	-2.74163700	6.08252200	-1.63176200
O	-1.38454100	4.61710900	1.39585800
Np	-2.06313900	5.34982800	-0.11792200

SMD： H = -1845.689658 Hartree

G = -1845.785727 Hartree

S = 202.194 Cal/Mol-Kelvin

O	-3.39238600	0.76937800	-0.22684600
C	-2.69850000	1.81037300	-0.23160000
C	-1.18286500	1.60133300	-0.14157000
O	-0.50749900	2.84706800	-0.21145200
C	0.89087800	2.75205700	-0.05655700
C	1.44344100	4.17513000	0.00297900
N	2.77331400	4.32654300	0.14387100
O	-3.14506600	3.00396400	-0.30000300
O	0.66435100	5.15074100	-0.06158100

C	3.36771900	5.66029700	0.22093000
C	3.73537600	3.22625900	0.15082900
H	-0.95304600	1.09212900	0.80590400
H	-0.86641100	0.93992400	-0.96047200
H	1.14169400	2.21775200	0.87171200
H	1.33841600	2.19938100	-0.89490800
H	3.94606800	5.74955400	1.14656000
H	4.04136800	5.82128300	-0.62823900
H	2.58358800	6.41430900	0.20767800
H	3.24783200	2.26036300	0.26699000
H	4.42684700	3.36214300	0.98829800
H	4.31355300	3.22211100	-0.78056200
O	-0.73387400	9.93039200	-0.00914300
C	-1.42773900	8.88938000	-0.00452000
C	-2.94337400	9.09841800	-0.09456900
O	-3.61875700	7.85268800	-0.02468200
C	-5.01711900	7.94770700	-0.17970700
C	-5.56969100	6.52464700	-0.23940100
N	-6.89955500	6.37327900	-0.38044500
O	-0.98114300	7.69579300	0.06369400
O	-4.79063200	5.54901300	-0.17480900
C	-7.49400600	5.03954300	-0.45745200
C	-7.86157000	7.47360900	-0.38708200
H	-3.25985400	9.75984900	0.72430100
H	-3.17316000	9.60759400	-1.04206700
H	-5.46474700	8.50033800	0.65862800

H	-5.26783000	8.48207200	-1.10797000
H	-6.70989100	4.28551100	-0.44429800
H	-8.16756800	4.87855600	0.39178700
H	-8.07245500	4.95031900	-1.38301900
H	-7.37407400	8.43942900	-0.50409800
H	-8.43905700	7.47821200	0.54473700
H	-8.55367200	7.33738000	-1.22396800
O	-1.94966400	5.50639600	-1.94766700
O	-2.17663200	5.19336700	1.71134700
Np	-2.06315000	5.34988000	-0.11816000

$[NpO_2(DMOGA)_3]^{2-}$

GAS: H = -2435.59254 Hartree

G = -2435.73231 Hartree

S = 294.171 Cal/Mol-Kelvin

O	-3.28017600	-1.64366000	-0.57393700
C	-3.88592300	-0.60090000	-0.19017400
C	-5.38996500	-0.84423600	0.04707400
O	-6.12986100	0.33192500	0.37392100
C	-7.46415300	0.02052000	0.57788900
C	-8.27203600	1.28363800	0.90224200
N	-9.63699800	1.08816800	1.11168900
O	-3.37629200	0.52195200	0.00895800
O	-7.77504000	2.39463000	0.96296300
C	-10.44173100	2.22419200	1.51835400

C	-10.29267400	-0.20211700	1.18697400
H	-5.80539000	-1.30848800	-0.86237400
H	-5.48599200	-1.58528900	0.85891700
H	-7.90896100	-0.46488200	-0.31566500
H	-7.59146400	-0.70534200	1.40729500
H	-10.77720800	2.12543600	2.56296700
H	-9.82945800	3.12080300	1.42302100
H	-11.33336500	2.31276600	0.88130200
H	-9.70577000	-0.97666500	0.69478500
H	-11.26692600	-0.15128200	0.68092400
H	-10.47416400	-0.51477400	2.22867800
O	0.13375600	-2.56026600	-1.29174900
C	1.13706200	-3.30453900	-0.96612900
C	2.19840700	-2.49520600	-0.19948000
O	3.39596100	-3.23125200	0.10605100
C	4.32784800	-2.34954100	0.63847100
C	5.61450600	-3.06995300	1.04471300
N	6.62530600	-2.24682900	1.53552600
O	1.29342700	-4.50203500	-1.21077800
O	5.77114200	-4.28026800	0.95610100
C	7.83174200	-2.86492400	2.04272100
C	6.50353300	-0.81792100	1.77371400
H	2.45189000	-1.60594400	-0.79084400
H	1.74021000	-2.12635100	0.73121200
H	4.57518800	-1.54609400	-0.08136000
H	3.93058100	-1.82579600	1.53125600

H	7.92229800	-2.73486700	3.13396400
H	7.78770400	-3.92940300	1.81061400
H	8.72333500	-2.41855600	1.57698200
H	5.68527000	-0.36967400	1.21430200
H	7.42308300	-0.31071200	1.45324800
H	6.35458800	-0.59724600	2.84348700
O	-0.18089900	1.95645500	-0.16677500
C	1.03169400	1.69645500	-0.39349500
C	1.97053800	2.91101600	-0.24806500
O	3.34291300	2.54651700	-0.09632500
C	4.15935900	3.66380400	-0.14889000
C	5.61690200	3.27482300	0.13066800
N	6.54720200	4.30303400	0.02042500
O	1.49815900	0.59520100	-0.76583300
O	5.95242800	2.14645800	0.45233100
C	7.95584300	3.98222500	0.15933000
C	6.24973600	5.64035600	-0.45532300
H	1.84840000	3.53606100	-1.15055500
H	1.64227300	3.51227700	0.61370400
H	4.09778300	4.16215800	-1.13677300
H	3.85747300	4.43044200	0.59563600
H	8.43554300	4.65751200	0.88176800
H	8.03429200	2.95322600	0.50903700
H	8.48443900	4.07750300	-0.80184000
H	5.20206400	5.89538400	-0.29710500
H	6.47957900	5.76364000	-1.52621500

H	6.85530700	6.36756200	0.10197400
O	-0.66322300	-0.89386600	1.06649700
O	-1.24756800	-0.07888500	-2.41750100
Np	-0.95788300	-0.50605800	-0.67957800

SMD： H = -2435.961025 Hartree

G = -2436.092344 Hartree

S = 276.385 Cal/Mol-Kelvin

O	-2.00400000	0.90959700	1.10678900
C	-0.79985400	0.83940100	0.70770400
C	-0.22380000	-0.56405000	0.55424200
O	1.15161400	-0.50858700	0.21498600
C	1.70609700	-1.80407800	0.09640600
C	3.19815400	-1.66461300	-0.21054200
N	3.90830800	-2.81846800	-0.31702800
O	-0.08930100	1.85083600	0.44207000
O	3.71461600	-0.54311300	-0.32890600
C	5.30468300	-2.75780700	-0.74595500
C	3.28710100	-4.13909600	-0.40224100
H	-0.37542700	-1.10661600	1.49941200
H	-0.80136100	-1.09372800	-0.21943300
H	1.56503500	-2.36968500	1.02996900
H	1.20807700	-2.36938300	-0.70659700
H	5.39500800	-2.95067500	-1.82288200
H	5.71082600	-1.77175700	-0.52635000

H	5.88115600	-3.51567000	-0.20757900
H	2.37949900	-4.19482600	0.19877700
H	3.98928700	-4.88088100	-0.01241500
H	3.04527600	-4.40208900	-1.44017400
O	-4.35674400	3.62465500	2.00213900
C	-5.46480000	4.12406800	1.57260100
C	-5.34175700	5.54200000	1.00894100
O	-6.61203800	6.05791700	0.63778100
C	-6.48346600	7.33819100	0.05094700
C	-7.88080000	7.87230000	-0.26196300
N	-7.95058400	9.11729500	-0.80080200
O	-6.56757000	3.54932200	1.59877100
O	-8.88758300	7.19276700	-0.00779200
C	-9.24959500	9.64157700	-1.21364400
C	-6.78483900	9.84499700	-1.30146000
H	-4.86908500	6.18751100	1.76310200
H	-4.66836300	5.51216400	0.13953400
H	-5.95900800	8.02711300	0.73106300
H	-5.88703100	7.28309400	-0.87332100
H	-9.41606300	9.48467400	-2.28754900
H	-10.03907300	9.13856400	-0.65709200
H	-9.28787400	10.71501200	-1.00817500
H	-5.90259600	9.66563900	-0.68650800
H	-7.00164700	10.91591500	-1.26406300
H	-6.55924700	9.57550700	-2.34154400
O	-0.24812700	5.49603400	0.25536000

C	-1.02526700	6.43372900	0.60579400
C	-0.62966900	7.85116500	0.20237000
O	-1.71080800	8.73800200	0.43309400
C	-1.38501300	10.07330200	0.10774500
C	-2.63452400	10.93088100	0.31921200
N	-2.51514300	12.25896000	0.06332400
O	-2.08998600	6.25372300	1.26611000
O	-3.69923600	10.41020300	0.68994500
C	-3.62621400	13.14942700	0.39543900
C	-1.22836900	12.92076900	-0.15359000
H	0.25765800	8.14522800	0.78562400
H	-0.33629300	7.85016500	-0.85750400
H	-0.56422000	10.43859500	0.74372400
H	-1.04921300	10.15092400	-0.93790800
H	-3.68090900	13.95005900	-0.34745300
H	-4.55882000	12.58742800	0.39042800
H	-3.48473000	13.59985900	1.38657800
H	-0.53603500	12.27977100	-0.69943600
H	-0.76566200	13.22305500	0.79462100
H	-1.39652700	13.81670200	-0.75671400
O	-2.68118200	3.59091700	-0.58107800
O	-1.40302600	3.62142500	2.87820900
Np	-2.04401300	3.61006400	1.14935700

$[NpO_2(ODA)(H_2O)_4]^-$

GAS： H = -1501.719296 Hartree

G = -1501.796536 Hartree

S = 162.566 Cal/Mol-Kelvin

O	-3.44604400	3.68385700	1.04466800
C	-2.22544200	3.39841700	1.13908200
C	-1.75592900	2.01900100	0.67081000
O	-0.37001700	2.05440700	0.40206500
C	0.09215600	0.98387700	-0.38419900
C	1.49736300	1.21957400	-0.95594200
O	2.05832800	0.27060600	-1.47725200
O	-1.34188700	4.21580200	1.55300700
O	2.03014200	2.42433600	-0.91684000
H	-1.99900400	1.26385400	1.43870700
H	-2.32743800	1.76251600	-0.23330600
H	0.12426100	0.04026600	0.18222900
H	-0.57198800	0.81769600	-1.24937300
O	-2.06358800	5.18127700	-1.22985400
O	-2.20987100	7.27692800	1.73373200
Np	-2.11552600	6.18678700	0.29985800
O	1.23204800	4.50377900	0.43831600
H	0.44867800	4.21078200	0.94801000
H	1.53651200	3.16762600	-0.42362300
O	-0.07034800	6.92604400	-0.21230200
H	0.27078500	7.49377100	0.49689500
H	0.90900200	5.34078400	0.01784700
O	-4.51157700	6.83496900	-0.61527900
H	-4.46574200	7.34911700	-1.43652400

H	-4.74547500	5.90359900	-0.91732800
O	-4.65984400	4.26870600	-1.38504500
H	-4.50713300	3.84779500	-0.50937700
H	-3.72311400	4.41980900	-1.65394000

SMD： H = -1501.887282 Hartree

G = -1501.962953 Hartree

S = 159.263 Cal/Mol-Kelvin

O	0.42150600	-1.79657800	0.34856400
C	1.36467000	-0.94822500	0.28304600
C	2.78648100	-1.48458200	0.25203800
O	3.71507300	-0.42659400	0.15083600
C	5.05552100	-0.89137800	0.03832300
C	6.04254500	0.28502600	-0.07675200
O	7.25517600	-0.05848800	-0.18990300
O	1.14296500	0.30118600	0.22711800
O	5.58226900	1.45785400	-0.05194000
H	2.95072900	-2.08633300	1.16010100
H	2.86405700	-2.17273700	-0.60503000
H	5.32727000	-1.50128000	0.91419200
H	5.16454300	-1.53642400	-0.84773900
O	-1.29347300	-0.17281500	-1.80460600
O	-1.58380700	0.13680400	1.82198000
Np	-1.42650700	-0.02602000	0.00952800
O	0.30248500	2.79273900	-0.81603100

H	0.69662700	1.95601600	-0.49347400
H	-0.01878700	2.56050600	-1.70394400
O	-2.11033800	3.01535400	0.55380800
H	-1.97983400	2.47413700	1.35203800
H	-1.23687100	2.94519100	0.09368700
O	-4.55981500	-0.02784200	-0.03307500
H	-5.04283400	-0.07097400	0.80982600
H	-5.25596600	0.07342100	-0.70466800
O	-3.32597900	-2.48167700	-0.48711400
H	-3.84530800	-1.66014400	-0.31293100
H	-2.82228300	-2.24607900	-1.28515400

$[NpO_2(ODA)(H_2O)_3]^-_c$

GAS: H = -1425.259876 Hartree

G = -1425.337754 Hartree

S = 163.909 Cal/Mol-Kelvin

O	-0.13774000	-1.86541600	-0.13145600
C	-1.05212600	-1.00586200	-0.35916500
C	-2.50728500	-1.43573900	-0.40492600
O	-3.32578700	-0.34642500	-0.15184600
C	-4.72253200	-0.67362000	-0.19345700
C	-5.65646400	0.54160400	0.15445100
O	-6.86674100	0.21415100	0.07840200
O	-0.74244100	0.21247300	-0.55191600
O	-5.10661900	1.62092500	0.45292800

H	-2.68336200	-1.88326500	-1.40698000
H	-2.63698800	-2.26050200	0.32074100
H	-4.97877700	-1.04937800	-1.19922000
H	-4.92707100	-1.49304700	0.51754600
O	1.27722500	0.24805700	1.78376800
O	2.06782800	-0.22124400	-1.69747100
Np	1.58647900	0.00151700	0.02158500
O	0.31143100	2.53042800	0.17329100
H	-0.46292600	2.09743300	-0.24931200
H	0.16356100	2.36707600	1.12170000
O	2.98889400	2.19731400	-0.33669200
H	3.11011800	2.08542900	-1.29502600
H	2.17065200	2.73325400	-0.24309900
O	2.36402500	-2.37714500	0.77135800
H	1.51479700	-2.70410200	0.39924500
H	2.17729200	-2.29720500	1.72267200

SMD： H = -1425.468229 Hartree

G = -1425.54678 Hartree

S = 165.324 Cal/Mol-Kelvin

O	0.42936400	-1.81598900	-0.06279700
C	1.31776300	-0.91618200	-0.16689700
C	2.76810000	-1.38319400	-0.13845500
O	3.65207000	-0.28149900	-0.11257300
C	5.01278300	-0.68455400	-0.01851700

C	5.95197500	0.53235400	0.07424200
O	7.17880500	0.23758600	0.17400400
O	1.04076000	0.31663900	-0.28371200
O	5.44607100	1.68631000	0.04700900
H	2.90097700	-2.02337400	0.74764700
H	2.94292500	-2.02012500	-1.02106000
H	5.16512400	-1.31723000	0.87017500
H	5.29780600	-1.29016100	-0.89355200
O	-1.71147600	0.11770700	-1.80453700
O	-1.39141400	-0.04583300	1.85112500
Np	-1.53916200	0.03243600	0.02299300
O	-1.15733300	2.74536800	-0.00698000
H	-0.45186800	2.82495700	0.65896500
H	-0.68151200	2.80367900	-0.85405700
O	-4.16899600	1.08745800	0.11787400
H	-3.90496500	1.98751500	0.37703900
H	-4.25030400	1.14661100	-0.84967100
O	-2.93444500	-2.18156400	0.07000600
H	-2.77532000	-2.56650000	0.94943900
H	-2.47181600	-2.78196600	-0.54082600

$[NpO_2(ODA)(H_2O)_3]^-_e$

GAS: H = -1425.346835 Hartree

G = -1425.418 Hartree

S = 149.778 Cal/Mol-Kelvin

O	-3.17909800	3.79246700	0.41941200
C	-2.13799700	3.14423900	0.36257200
C	-2.26051400	1.60747300	0.32312700
O	-1.02333900	1.01084400	-0.04981600
C	-0.98865200	-0.41163800	0.02349600
C	0.44073600	-0.94051700	-0.21810500
O	0.57759900	-2.15259600	-0.35614900
O	-0.92822300	3.60613200	0.34938000
O	1.36089100	-0.03423600	-0.22994300
H	-2.56308400	1.25120200	1.32027100
H	-3.04768900	1.32945900	-0.39031300
H	-1.31951900	-0.74187500	1.02007400
H	-1.66790400	-0.84643300	-0.72218000
O	1.38119300	2.82648200	-1.43709300
O	1.05802500	1.95442300	2.08253500
Np	1.15249700	2.32925600	0.31558100
O	0.35388900	5.50931400	-1.13199500
H	-0.40303100	5.07173800	-0.67307900
H	0.73147100	4.74023600	-1.61040700
O	1.83745600	4.74637600	0.95360200
H	1.29816700	4.88933300	1.74833900
H	1.35653800	5.22752000	0.21328000
O	3.60274600	1.30736500	-0.13041300
H	3.09253000	0.46091800	-0.18054800
H	3.58868200	1.62812000	-1.04849100

SMD： H = -1425.492932 Hartree

G = -1425.566139 Hartree

S = 154.077 Cal/Mol-Kelvin

O	-3.38259700	3.68993700	0.33965000
C	-2.29945800	3.07570300	0.33538700
C	-2.36789300	1.54792200	0.24588900
O	-1.10366500	1.00328100	-0.11614400
C	-1.01109600	-0.40985300	0.02031900
C	0.42808500	-0.87825500	-0.20846200
O	0.62936200	-2.10632000	-0.21734600
O	-1.13716400	3.61437300	0.43783800
O	1.32356100	0.02917600	-0.36719300
H	-2.68136200	1.16127700	1.22717500
H	-3.13161300	1.26250600	-0.48800100
H	-1.32275200	-0.71631000	1.02938800
H	-1.67074200	-0.90977700	-0.70114300
O	1.22830700	2.93269900	-1.49922600
O	1.09315500	2.00767700	2.07414900
Np	1.14268000	2.46329200	0.29097000
O	0.10730000	5.59873300	-0.98636000
H	-0.52816600	5.07657400	-0.43930900
H	0.50092900	4.88246600	-1.52555800
O	2.12894800	4.93329700	0.74146200
H	1.84463200	5.13337000	1.64970800
H	1.42568700	5.33782100	0.16574000

O	3.93561100	0.86683500	-0.02255000
H	3.11491800	0.34952100	-0.18071700
H	4.04670200	1.35966000	-0.85252700

$[NpO_2(ODA)(H_2O)_2]^-$

GAS: H = -1348.920893 Hartree

G = -1348.98789 Hartree

S = 141.008 Cal/Mol-Kelvin

O	3.54294700	2.16849500	-0.05959100
C	2.43497400	1.64062300	-0.09415600
C	1.20466300	2.57077300	-0.03181400
O	0.00171700	1.85962000	-0.31871700
C	-1.20059200	2.56908300	-0.02355100
C	-2.43267000	1.64165400	-0.09541400
O	-3.53911700	2.17191000	-0.05027500
O	2.16210300	0.37973400	-0.15370100
O	-2.16356200	0.38088000	-0.17537800
H	1.14925300	2.99724900	0.98121600
H	1.33516400	3.39682000	-0.74342300
H	-1.14376100	2.98542300	0.99367300
H	-1.33084600	3.40241500	-0.72671900
O	0.00825800	-1.17369500	-1.66948400
O	-0.01057200	-0.34119200	1.83863500
Np	-0.00091200	-0.68099400	0.07710300
O	2.16792600	-2.25446700	0.02167600

H	2.63945700	-1.38678800	0.06755300
H	2.01905000	-2.36280200	-0.93462200
O	-2.16555800	-2.25173900	0.01096700
H	-2.63793200	-1.38406200	0.05295800
H	-2.01691900	-2.36496600	-0.94470100

SMD： H = -1349.082541 Hartree

G = -1349.151662 Hartree

S = 145.478 Cal/Mol-Kelvin

O	2.25668500	3.58610300	-0.03664000
C	1.74516100	2.44777400	0.02366500
C	2.71241000	1.26086900	-0.00629000
O	2.02117500	0.04250700	0.24141200
C	2.76824800	-1.12691300	-0.06990600
C	1.87717500	-2.37267700	-0.01313900
O	2.45582400	-3.47425900	-0.12003200
O	0.49392500	2.19536200	0.08882400
O	0.61545000	-2.20304300	0.11833500
H	3.18943900	1.23176100	-0.99667200
H	3.50228000	1.41560500	0.74053600
H	3.18903300	-1.04771400	-1.08322500
H	3.60503600	-1.24854600	0.63063200
O	-0.89475700	0.06566300	1.84932000
O	-0.54340400	-0.15224900	-1.81637300
Np	-0.70263400	-0.04204000	0.01767400

O	-2.58992600	1.75593300	-0.34695400
H	-2.16727000	2.40124300	-0.94008500
H	-2.65884300	2.22630000	0.50210300
O	-2.87205700	-1.56925000	-0.00628400
H	-2.68114600	-2.22569900	-0.69933300
H	-2.79487200	-2.07165500	0.82356900

$[NpO_2(ODA)_2(H_2O)_2]^{3-}{}_a$

GAS: H = -1879.669555 Hartree

G = -1879.771081 Hartree

S = 213.679 Cal/Mol-Kelvin

O	-2.01210000	2.97667700	-0.17655200
C	-1.19289200	1.98449200	-0.14797000
C	-1.85389800	0.61452500	-0.31397900
O	-0.97772100	-0.46866400	-0.40083600
C	-1.71152700	-1.68767300	-0.55398500
C	-0.86529300	-3.00169000	-0.70924500
O	-1.62170700	-4.00672400	-0.82493400
O	0.04262900	2.14328000	0.01836300
O	0.37907500	-2.92147000	-0.70660100
H	-2.55247900	0.50924700	0.54104400
H	-2.50087200	0.69140500	-1.20916600
H	-2.38522500	-1.82028900	0.31316800
H	-2.36965800	-1.60840400	-1.43960800
O	-0.58648300	7.13518600	0.32820000

C	0.65553900	7.39551700	0.54193100
C	0.97306600	8.88456300	0.69358200
O	2.30897600	9.18880300	0.95997100
C	2.47862500	10.60398500	1.08797200
C	3.93145100	11.11112800	1.40271000
O	3.95229500	12.37066700	1.49609500
O	1.52345000	6.48995500	0.61651700
O	4.84967000	10.27566100	1.51961500
H	0.61975300	9.36920200	-0.23865000
H	0.30023400	9.26155100	1.48891100
H	2.14439500	11.09761400	0.15622800
H	1.81193800	10.98066700	1.88626500
O	0.00611600	4.84799400	-1.59471600
O	-0.41338300	4.48565100	1.98717700
Np	-0.20632600	4.66941500	0.19629000
O	-1.97492100	6.94302900	-2.15339500
H	-1.62226200	7.30131800	-1.31658700
H	-1.35645400	6.20233000	-2.29357800
O	-3.32498800	4.09112600	2.10140200
H	-2.41021900	4.28029300	2.38122900
H	-3.15272200	3.56702100	1.29593200

SMD： H = -1880.218841 Hartree

G = -1880.309851 Hartree

S = 191.545 Cal/Mol-Kelvin

O	2.46709500	-1.62073000	-0.37935200
C	2.99609900	-0.46816300	-0.27531600
C	4.51771800	-0.40769800	-0.25273500
O	4.95931100	0.93018500	-0.15422200
C	6.37311500	1.02964000	-0.03893300
C	6.82858900	2.49961100	0.03981400
O	8.07778800	2.64996500	0.17603400
O	2.31715100	0.59518000	-0.17779500
O	5.95651900	3.40618000	-0.03641500
H	4.86596900	-1.00950000	0.60220000
H	4.90084700	-0.89519800	-1.16323500
H	6.72352600	0.50032900	0.86119200
H	6.86573000	0.55349500	-0.90159200
O	-2.46826300	-1.61279200	0.38522200
C	-2.99746000	-0.46413200	0.24756100
C	-4.51896600	-0.40474500	0.23587500
O	-4.96315000	0.93198700	0.13628900
C	-6.37830500	1.02841400	0.03464600
C	-6.83786900	2.49769700	-0.03251500
O	-8.08813300	2.64583400	-0.16112000
O	-2.31786900	0.59457100	0.10798500
O	-5.96754100	3.40583700	0.04534800
H	-4.87168900	-1.00968500	-0.61529200
H	-4.89557700	-0.89029300	1.14990400
H	-6.73580300	0.50192000	-0.86430900
H	-6.86139300	0.54717200	0.89990700

O	-0.18031500	-0.65695300	-1.85059100
O	0.17439000	-0.48816700	1.82762800
Np	-0.00326900	-0.57942300	-0.01232000
O	-1.20630900	-3.34597200	-1.44787700
H	-1.76778200	-2.85364700	-0.81383900
H	-0.77569000	-2.60513100	-1.91538900
O	1.27519200	-3.14975600	1.67314900
H	0.83653300	-2.34988800	2.02629500
H	1.83489900	-2.74988700	0.97532700

$[NpO_2(ODA)_2(H_2O)_2]^{3-}{}_i$

GAS: H = -1879.673525 Hartree

G = -1879.774079 Hartree

S = 211.635 Cal/Mol-Kelvin

O	-2.03218000	1.48241300	0.06637200
C	-2.91900200	0.57629300	0.11273500
C	-4.36774200	1.08289600	0.14751300
O	-5.34718100	0.10755200	-0.07724300
C	-6.65245000	0.67928000	0.01620200
C	-7.86198200	-0.27961500	-0.27462800
O	-8.96085600	0.32468900	-0.11914900
O	-2.64151400	-0.65384100	0.18022500
O	-7.63082400	-1.45690600	-0.61714700
H	-4.50031200	1.56443200	1.13826000
H	-4.43612200	1.90487500	-0.58940800

H	-6.79566400	1.10683200	1.02658900
H	-6.73154900	1.53249500	-0.68470100
O	2.06053000	-1.54250300	0.15904400
C	2.92092100	-0.61103200	0.14407000
C	4.38456600	-1.07139500	0.16229500
O	5.33153800	-0.06715200	-0.07134500
C	6.65407000	-0.60152500	0.00297300
C	7.83236600	0.39462900	-0.29077400
O	8.94932700	-0.18160800	-0.15991700
O	2.60360000	0.61257000	0.15815200
O	7.56406000	1.57038900	-0.61038100
H	4.54242600	-1.55169600	1.14963700
H	4.46856100	-1.88971800	-0.57755200
H	6.82036500	-1.03338900	1.00803100
H	6.74988000	-1.44594700	-0.70625400
O	0.04585100	0.01370800	-1.65796300
O	-0.01745400	-0.07301800	1.97321700
Np	0.01306100	-0.02705400	0.17238300
O	-0.90471500	-2.51658500	-0.60319400
H	-1.77698500	-2.09424700	-0.43003500
H	-0.63673100	-2.13676400	-1.45913500
O	0.83832600	2.52885400	-0.42056000
H	1.72982500	2.12501400	-0.33300100
H	0.53912200	2.22845500	-1.29724100

SMD： H = -1880.218412 Hartree

G = -1880.312188 Hartree

S = 197.369 Cal/Mol-Kelvin

O	-2.02708900	1.79592200	0.20791800
C	-2.94617000	0.92321100	0.17812700
C	-4.37957600	1.43409200	0.07224600
O	-5.28032400	0.35731800	-0.08939900
C	-6.63272200	0.78374100	-0.18823800
C	-7.58212800	-0.41734100	-0.36034900
O	-8.80257900	-0.10564500	-0.48491700
O	-2.72448100	-0.32253700	0.24684900
O	-7.08936800	-1.57723100	-0.36156400
H	-4.60474800	2.01253500	0.98340900
H	-4.43505500	2.13682400	-0.77365400
H	-6.92791400	1.34264100	0.71429100
H	-6.76197600	1.46633300	-1.04289000
O	2.03568500	-1.82305400	0.15323200
C	2.94679600	-0.94203400	0.15027200
C	4.38029100	-1.43336300	-0.02341400
O	5.27636700	-0.34235800	-0.08518600
C	6.62842400	-0.75347900	-0.23862400
C	7.57246400	0.46067700	-0.32832000
O	8.79618300	0.16270900	-0.45430700
O	2.71680300	0.29709200	0.28801200
O	7.07238700	1.61628600	-0.27595000
H	4.61893200	-2.10390700	0.81804100
H	4.42699400	-2.04268000	-0.93997600

H	6.93893500	-1.38587200	0.60817300
H	6.74579000	-1.36025200	-1.15064300
O	0.07023400	0.18040200	-1.60854700
O	-0.07042500	-0.19763600	2.04169800
Np	0.00026700	-0.00911300	0.21917500
O	-1.51639200	-2.73002800	-0.58709100
H	-2.09708400	-1.97573700	-0.35955700
H	-0.96386400	-2.35902800	-1.29565200
O	1.54471600	2.74365100	-0.49770600
H	2.11485200	1.98297700	-0.26584600
H	0.98226800	2.36152600	-1.19351200

$[NpO_2(ODA)_2(H_2O)]^{3-}$

GAS： H = -1803.274137 Hartree

G = -1803.363182 Hartree

S = 187.411 Cal/Mol-Kelvin

O	-2.71723600	-0.01539900	-0.00703100
C	-2.33918300	1.16797300	-0.09045200
C	-0.82267000	1.39915200	0.12719100
O	-0.45174700	2.70452700	-0.27067600
C	0.86013900	3.09447800	0.08582100
C	1.07153900	4.60922100	-0.16234100
O	2.25171500	4.99886500	-0.11556000
O	-3.02694400	2.21369600	-0.30530400
O	0.01251600	5.28416500	-0.35976600

H	-0.59625300	1.25235600	1.19798900
H	-0.25201000	0.64337700	-0.43764500
H	1.03709300	2.88859400	1.15609900
H	1.60613500	2.52117500	-0.48904100
O	-3.04289600	6.99889200	-0.14421600
C	-4.07437300	7.74993100	-0.17602400
C	-3.73390400	9.25018400	-0.05727900
O	-4.83952000	10.11837200	-0.11405100
C	-4.42555700	11.47459600	0.01138300
C	-5.55683100	12.56444300	-0.03651900
O	-5.07419700	13.72710400	0.09007400
O	-5.26301300	7.37272900	-0.28553300
O	-6.74399800	12.20547700	-0.18604400
H	-3.17562900	9.37571800	0.89042100
H	-3.00508300	9.47693100	-0.85873800
H	-3.87519800	11.61107700	0.96270700
H	-3.69802500	11.71908800	-0.78713600
O	-2.49870100	4.65647900	-2.06629300
O	-2.29438100	4.54802500	1.55025700
Np	-2.37045100	4.62105200	-0.25406300
O	-4.99373800	4.73704500	-0.57132500
H	-5.16304600	5.72367300	-0.42109800
H	-4.76377400	4.68742500	-1.51563800

SMD： H = -1803.835922 Hartree

G = -1803.922793 Hartree

S = 182.837 Cal/Mol-Kelvin

O	-2.69464700	-0.04170700	0.30920400
C	-2.33453700	1.13669400	0.10856800
C	-0.84405800	1.43812800	0.28952100
O	-0.56389500	2.78367600	-0.07822700
C	0.76642700	3.20391600	0.19684300
C	0.90916100	4.70187800	-0.07789400
O	2.05193200	5.19103200	0.02970100
O	-3.09965800	2.10832600	-0.22083800
O	-0.15346100	5.34635700	-0.38634700
H	-0.57384500	1.26818300	1.34167500
H	-0.25562200	0.74330600	-0.32452500
H	1.01680200	3.01268000	1.25014000
H	1.48168600	2.64905400	-0.42485200
O	-2.80370800	7.07115600	-0.79382900
C	-3.79614900	7.79901300	-0.46452300
C	-3.46474800	9.27906100	-0.28191300
O	-4.62902000	10.04021100	-0.02434200
C	-4.32570300	11.41828800	0.15314600
C	-5.59470600	12.26770600	0.35359800
O	-5.36623500	13.49771100	0.54870800
O	-4.97734300	7.40614500	-0.27960400
O	-6.71975200	11.70218100	0.30506700
H	-2.74257800	9.36381200	0.54664400
H	-2.95100500	9.63458400	-1.18880800

H	-3.66458000	11.55776800	1.02310100
H	-3.78264600	11.80692800	-0.72328300
O	-2.33466900	4.33273000	-2.30494800
O	-2.68558100	4.75428800	1.34071800
Np	-2.50006600	4.54481900	-0.48119600
O	-5.09732300	4.80604000	-0.87362700
H	-5.10436500	5.78954700	-0.66310600
H	-5.12532900	4.76691000	-1.84460400

$[NpO_2(ODA)_2]^{3-}$

GAS: H = -1726.839302 Hartree

G = -1726.920664 Hartree

S = 171.241 Cal/Mol-Kelvin

O	-3.66285900	0.94909100	-0.83178200
C	-2.96270500	1.97582100	-0.68804100
C	-1.54562000	1.75347900	-0.10068400
O	-0.70615400	2.81312600	-0.50454600
C	0.56357600	2.84939300	0.10939800
C	1.27064100	4.17742100	-0.26383000
O	2.52052700	4.16454400	-0.21350300
O	-3.25226300	3.18375400	-0.93517400
O	0.49075500	5.13126400	-0.55780300
H	-1.61456500	1.72721200	1.00151900
H	-1.14819700	0.78018800	-0.44084300
H	0.45298700	2.79842100	1.20741400

H	1.18360100	1.99255100	-0.21039800
O	-0.46364900	9.75199600	0.59341300
C	-1.16315300	8.72464600	0.45098400
C	-2.58049300	8.94547300	-0.13609400
O	-3.41920800	7.88510500	0.26795600
C	-4.68955800	7.84973100	-0.34507200
C	-5.39747400	6.52228300	0.02824700
O	-6.64737200	6.53615600	-0.02214300
O	-0.87267200	7.51715300	0.69925000
O	-4.61833200	5.56788500	0.32228600
H	-2.97891700	9.91835700	0.20398100
H	-2.51175000	8.97156500	-1.23828600
H	-5.30851900	8.70706500	-0.02461100
H	-4.57964400	7.90088100	-1.44312600
O	-2.23782500	6.01199700	-1.80266500
O	-1.88854900	4.68970100	1.56613800
Np	-2.06318300	5.35082000	-0.11824000

SMD： H = -1727.434717 Hartree

G = -1727.513836 Hartree

S = 166.521 Cal/Mol-Kelvin

O	-3.71001700	0.86289000	-0.14332600
C	-2.95363800	1.85936500	-0.10326600
C	-1.45070200	1.58217200	-0.17515700
O	-0.73761500	2.80678900	-0.21363100

C	0.66803100	2.67476200	-0.08195800
C	1.29453600	4.04438900	0.18704700
O	2.54385900	4.08914600	0.24799500
O	-3.32478500	3.07470700	0.00936400
O	0.50250900	5.03080900	0.35138300
H	-1.15874000	0.99607900	0.70921600
H	-1.23377800	0.97183100	-1.06314000
H	0.91444700	2.00811100	0.75776500
H	1.10912600	2.24089800	-0.99042400
O	-0.43531800	9.83206400	0.11590800
C	-1.20621200	8.84445600	0.10014600
C	-2.69798700	9.14719400	-0.07257400
O	-3.44986400	7.95672500	0.07159700
C	-4.80324900	8.04947100	-0.33247100
C	-5.40385000	6.64541700	-0.44527300
O	-6.63628600	6.57779500	-0.66251100
O	-0.85383100	7.62304600	0.19687300
O	-4.61099600	5.65465800	-0.33242400
H	-3.00286000	9.90309100	0.66537800
H	-2.85051000	9.58229600	-1.07248200
H	-5.39316200	8.64330200	0.38039400
H	-4.88219100	8.54093400	-1.31456600
O	-1.84396900	5.39506600	-1.79719000
O	-2.24163000	5.24038600	1.87337300
Np	-2.04168900	5.30882800	0.03760200

$[NpO_2(ODA)_3]^{5-}$

GAS: H = -2257.396871 Hartree

G = -2257.517798 Hartree

S = 254.514 Cal/Mol-Kelvin

O	-0.75443400	3.37849100	0.03960700
C	0.30450900	2.64022300	-0.01278900
C	-0.05176700	1.12508500	-0.02549400
O	1.06812400	0.25608000	-0.06388500
C	0.66442500	-1.10367300	-0.06792100
C	1.80303800	-2.18883500	-0.10459100
O	1.32455200	-3.36320300	-0.09873400
O	1.47920300	3.01101900	-0.04864800
O	3.00125200	-1.83052900	-0.13528800
H	-0.67237100	0.92184400	0.86716900
H	-0.71409100	0.94639000	-0.89330400
H	0.04204900	-1.31853500	0.82392600
H	0.00169000	-1.30139100	-0.93433500
O	-4.55182700	5.11002800	-0.07113400
C	-5.71169800	4.56881200	-0.24690500
C	-6.82931100	5.64097000	-0.40211300
O	-8.13770600	5.11308600	-0.54376900
C	-9.09500900	6.14677600	-0.70765800
C	-10.59936000	5.71173000	-0.85835000
O	-11.35726700	6.71422800	-1.02757900
O	-5.98059000	3.36729500	-0.29874600

O	-10.90391200	4.49987900	-0.79693200
H	-6.77251400	6.31380500	0.47374900
H	-6.56554400	6.26813100	-1.27464800
H	-9.04725100	6.84895400	0.14914900
H	-8.84401700	6.76068200	-1.59569700
O	-1.12602400	7.53110000	0.22646100
C	-1.02086800	8.79803400	0.45820100
C	0.46583700	9.23356500	0.60657000
O	0.65690300	10.62606300	0.79348600
C	2.03259200	10.94273700	0.93226800
C	2.40189800	12.45924200	1.12973600
O	3.65331900	12.61873500	1.25797500
O	-1.93159700	9.62180100	0.56141900
O	1.49633100	13.32232500	1.13951900
H	0.89341600	8.66407300	1.45341900
H	1.00869400	8.88204600	-0.29032600
H	2.46617700	10.38933500	1.78921500
H	2.59612500	10.58666800	0.04631500
O	-2.05361200	5.44407900	-1.73910200
O	-2.24979600	5.25272100	1.87046700
Np	-2.15126300	5.34901000	0.06577800

SMD： H = -2258.559906 Hartree

G = -2258.671357 Hartree

S = 234.569 Cal/Mol-Kelvin

O	-2.03794000	2.75166200	-0.03695200
C	-0.83664400	2.32362700	0.09188400
C	-0.68343800	0.81288200	-0.08957200
O	0.67220800	0.42142500	0.02078800
C	0.82592300	-0.98549400	-0.11425900
C	2.30630600	-1.40970400	-0.08768100
O	2.48798900	-2.65783200	-0.19849100
O	0.16008800	3.03670000	0.34856000
O	3.19108400	-0.52010500	0.03203800
H	-1.30523100	0.31038700	0.66888400
H	-1.09670000	0.53559400	-1.07223100
H	0.29302900	-1.51027000	0.69502000
H	0.38223200	-1.33173500	-1.06153700
O	-4.47165900	6.49022300	0.25062000
C	-5.45310500	5.73542100	-0.08337600
C	-6.79104500	6.46251900	-0.21952100
O	-7.81960000	5.56876800	-0.60098300
C	-9.07797600	6.22349500	-0.69881400
C	-10.20866200	5.24875600	-1.07936700
O	-11.34947600	5.79049600	-1.16632000
O	-5.37683800	4.50243700	-0.29006400
O	-9.92893700	4.03437400	-1.26896300
H	-7.02259500	6.94393100	0.74418400
H	-6.67336700	7.27240300	-0.95735600
H	-9.33675000	6.70229300	0.25915500
H	-9.03722200	7.02594600	-1.45284800

O	-0.13676000	6.61290300	0.41905900
C	-0.30627100	7.87872500	0.53473400
C	0.99716800	8.67122500	0.64623800
O	0.75136700	10.06302700	0.72459100
C	1.96459600	10.80314200	0.78052400
C	1.71620500	12.32207800	0.81824900
O	2.77443200	13.01585000	0.85792700
O	-1.41286800	8.46286500	0.56301100
O	0.52921400	12.74564200	0.80753700
H	1.54374100	8.31557400	1.53462900
H	1.62279600	8.42923400	-0.22756800
H	2.54744900	10.52014900	1.67191200
H	2.59397400	10.57295300	-0.09397000
O	-2.15866100	5.41670300	-1.57656200
O	-2.34799600	5.09475300	2.09430100
Np	-2.25175900	5.25585500	0.25906800

$[NpO_2(MIDA)(H_2O)_2]^-$

GAS： H = -1368.326467 Hartree

G = -1368.394807 Hartree

S = 143.834 Cal/Mol-Kelvin

O	3.58646500	1.99883000	-0.23688400
C	2.46976600	1.50129500	-0.13026900
C	1.22774300	2.37827100	-0.42045800
N	-0.00147700	1.88171800	0.23012600

C	-1.23441800	2.37728600	-0.41462200
C	-2.47405100	1.49614300	-0.12588400
O	-3.59156300	1.99279200	-0.22830900
O	2.18937200	0.26883300	0.16558500
O	-2.19158900	0.26251800	0.16319400
H	1.44608400	3.42192500	-0.14681500
H	1.07204300	2.33937800	-1.50398900
H	-1.45491100	3.41915700	-0.13567100
H	-1.08180000	2.34487800	-1.49882100
C	0.00177600	2.21387800	1.66488900
H	-0.00347500	3.30770100	1.81758100
H	0.89222500	1.79084300	2.13521600
H	-0.88037100	1.78052500	2.14145100
O	0.00016300	-0.39940900	-1.84663700
O	0.00037500	-1.19263300	1.67950900
Np	0.00094500	-0.74237200	-0.08178800
O	2.14375900	-2.36560800	0.02431500
H	1.97005400	-2.45503200	0.97830700
H	2.62254700	-1.50107300	-0.02453300
O	-2.13856400	-2.36766500	0.01205000
H	-1.97349800	-2.45852800	0.96736200
H	-2.61870100	-1.50375700	-0.03920800

SMD： H = -1368.481032 Hartree

G = -1368.553778 Hartree

S = 153.106 Cal/Mol-Kelvin

O	3.34457200	-2.57681700	-0.25266000
C	2.44931500	-1.71580400	-0.14370600
C	2.79432600	-0.25750000	-0.48233100
N	1.87819900	0.70159800	0.15380800
C	1.83555400	1.99928200	-0.53714300
C	0.55544700	2.79174500	-0.23888700
O	0.53776300	4.00907400	-0.49576000
O	1.23033100	-1.96125600	0.18875400
O	-0.44192000	2.11923600	0.22557800
H	3.84486400	-0.06260800	-0.22211600
H	2.70708300	-0.16191700	-1.57080100
H	2.70899800	2.62520200	-0.30152800
H	1.84676200	1.82386100	-1.61887100
C	2.24488600	0.89133900	1.57019600
H	3.25448200	1.32276300	1.66403500
H	2.22613500	-0.06801700	2.09329700
H	1.53228500	1.56454300	2.05269100
O	-0.46607200	-0.27167900	-1.83899000
O	-0.85218500	-0.46881600	1.83379400
Np	-0.63964100	-0.36034100	-0.00122300
O	-2.77436600	-2.37708000	-0.28269600
H	-2.34070000	-2.97378600	0.35137400
H	-2.41879300	-2.66360200	-1.14143800
O	-3.17266300	1.72276700	0.07801800
H	-3.28721700	1.30092100	0.94578300

H	-2.25548500	2.07536600	0.12759300

$[NpO_2(MIDA)_2]^{3-}_{trans}$

GAS: H = -1765.641985 Hartree

G = -1765.728212 Hartree

S = 181.481 Cal/Mol-Kelvin

O	3.13311900	3.56615600	0.16465800
C	2.56436500	2.45606600	0.07871900
C	3.33173400	1.22732200	0.65031000
N	2.95456300	-0.00044800	-0.03676800
C	3.32751800	-1.22866700	0.65231100
C	2.56224700	-2.45747700	0.07870600
O	3.13227900	-3.56694400	0.16441400
O	1.42403300	2.18072100	-0.40659400
O	1.42181300	-2.18361800	-0.40756800
H	4.42334200	1.42391200	0.60801900
H	3.04894300	1.11937600	1.70468000
H	4.41918300	-1.42648100	0.61605500
H	3.03842100	-1.11947300	1.70487900
C	3.41390400	-0.00110700	-1.41925700
H	4.52634900	0.00380800	-1.48890200
H	3.02162800	0.88375900	-1.92607800
H	3.03015500	-0.89099500	-1.92387000
O	-3.13156100	3.56770400	-0.16127500
C	-2.56127200	2.45823400	-0.07721800

C	-3.32805000	1.22953200	-0.64890500
N	-2.95347700	0.00109900	0.03906200
C	-3.33376500	-1.22621000	-0.64724600
C	-2.56590700	-2.45595800	-0.07857700
O	-3.13577200	-3.56552100	-0.16412600
O	-1.41949400	2.18432300	0.40579400
O	-1.42416800	-2.18195300	0.40409800
H	-4.41960800	1.42731300	-0.60981800
H	-3.04172400	1.12041500	-1.70224700
H	-4.42541700	-1.42173500	-0.60168800
H	-3.05420100	-1.11816600	-1.70247600
C	-3.40928800	0.00179500	1.42279800
H	-4.52154500	-0.00233600	1.49516400
H	-3.02360600	0.89126900	1.92663700
H	-3.01635600	-0.88347600	1.92839200
O	0.36183900	-0.00501100	1.78293900
O	-0.36272900	0.00417000	-1.78484500
Np	-0.00018200	-0.00035600	-0.00101700

SMD： H = -1766.228853 Hartree

G = -1766.314294 Hartree

S = 179.827 Cal/Mol-Kelvin

O	3.21904600	-3.45543000	-0.50130100
C	2.67394500	-2.34742300	-0.28633500
C	3.52008100	-1.08511200	-0.49689900

N	2.97484800	0.07261700	0.20842200
C	3.46651900	1.34527000	-0.31806000
C	2.50830000	2.50693700	-0.02631400
O	2.97897000	3.66763400	-0.01424600
O	1.45466200	-2.17904500	0.05608700
O	1.27514200	2.20980100	0.13480600
H	4.56459000	-1.30008300	-0.21765600
H	3.51349800	-0.87577200	-1.57350800
H	4.47047600	1.59825800	0.05806700
H	3.54270500	1.27157000	-1.40984000
C	3.24451500	-0.02291700	1.64930500
H	4.32819500	-0.01871100	1.86089800
H	2.81772600	-0.94587600	2.05023200
H	2.78856300	0.82274600	2.17184800
O	-3.00872400	-3.60393000	0.54404200
C	-2.51281900	-2.47295300	0.32863200
C	-3.36695600	-1.24352300	0.66083900
N	-2.94307400	-0.05621700	-0.08019100
C	-3.42991900	1.18082100	0.53084700
C	-2.68640900	2.42750500	0.02768300
O	-3.24899400	3.53719600	0.20498000
O	-1.33257400	-2.25595100	-0.11002400
O	-1.54078300	2.25260000	-0.50137500
H	-4.42939500	-1.48643700	0.49612000
H	-3.24411300	-1.05214000	1.73395600
H	-4.51242000	1.32479200	0.37745200

H	-3.26726700	1.12369200	1.61400600
C	-3.37975900	-0.14526900	-1.48067500
H	-4.48047500	-0.18272700	-1.56094000
H	-2.96891300	-1.04554700	-1.94560200
H	-3.02102200	0.72335100	-2.03748500
O	0.23248600	-0.07764600	-1.87504500
O	-0.22960600	0.04232400	1.78794200
Np	0.01132700	-0.02185300	-0.04146500

$[NpO_2(MIDA)_2]^{3-}_{cis}$

GAS: H = -1765.628945 Hartree

G = -1765.714901 Hartree

S = 180.911 Cal/Mol-Kelvin

O	-3.03637500	3.56773500	-0.45162300
C	-2.50144200	2.44955200	-0.29076300
C	-3.17485200	1.23640500	-0.99530500
N	-2.95150000	0.00350800	-0.25470900
C	-3.18189000	-1.21972300	-1.00866700
C	-2.51148700	-2.44384200	-0.31996100
O	-3.04531600	-3.55931100	-0.50255400
O	-1.45665200	2.15523200	0.36805400
O	-1.47118200	-2.15998300	0.35011700
H	-4.25139200	1.45437400	-1.15637400
H	-2.70167800	1.12278200	-1.97853600
H	-4.26003900	-1.43115300	-1.16779000

H	-2.71351400	-1.09717800	-1.99300900
C	-3.66437500	-0.00247400	1.01359200
H	-4.77070600	-0.00543100	0.87320300
H	-3.38362300	0.88371600	1.58844200
H	-3.37722500	-0.89072600	1.58206100
O	3.04192600	-3.56650500	-0.45679600
C	2.50624100	-2.44929500	-0.29167600
C	3.17718900	-1.23376600	-0.99408900
N	2.94591200	-0.00130300	-0.25504800
C	3.17708700	1.22167600	-1.00958700
C	2.50861100	2.44670200	-0.32049400
O	3.04322600	3.56164500	-0.50454800
O	1.46308200	-2.15733000	0.37063400
O	1.46930000	2.16380000	0.35140800
H	4.25537300	-1.44722000	-1.14981400
H	2.70914800	-1.12251400	-1.97994100
H	4.25525100	1.43175500	-1.17013600
H	2.70723400	1.09938600	-1.99331700
C	3.65438600	0.00699300	1.01598700
H	4.76106600	0.00584400	0.87916100
H	3.36715600	-0.87613300	1.59207900
H	3.36796500	0.89812600	1.58012400
O	0.00493100	-0.00174800	2.09353000
O	-0.00323500	-0.00254900	-1.53272000
Np	0.00064100	-0.00131500	0.28584800

SMD： H = -1766.217971 Hartree

G = -1766.301099 Hartree

S = 174.958 Cal/Mol-Kelvin

O	-2.90068500	3.58169100	-0.56498700
C	-2.47567600	2.43367300	-0.29925000
C	-3.28521300	1.23271100	-0.80561100
N	-2.95829800	0.00802800	-0.07809800
C	-3.29853200	-1.20771400	-0.81474200
C	-2.50293600	-2.42068100	-0.31497000
O	-2.95642600	-3.56231200	-0.56028800
O	-1.39269300	2.17512000	0.32995400
O	-1.40170200	-2.17832000	0.28846700
H	-4.35912800	1.47746100	-0.76784700
H	-3.02643100	1.09628600	-1.86243500
H	-4.37529000	-1.43957200	-0.77979000
H	-3.03621600	-1.06689500	-1.87019000
C	-3.59280100	0.00564400	1.24620600
H	-4.69407800	0.00801800	1.16921600
H	-3.28490800	0.89021100	1.81041400
H	-3.28865300	-0.88338800	1.80569000
O	3.00690900	-3.57557300	-0.50676300
C	2.51882000	-2.43503300	-0.32879100
C	3.32547700	-1.22278900	-0.81044300
N	2.96194100	-0.00480000	-0.08925200
C	3.32674000	1.21392300	-0.80852100

C	2.52390500	2.42775000	-0.32434000
O	3.01100000	3.56719400	-0.51241300
O	1.37625400	-2.19457500	0.19051800
O	1.38634800	2.19067600	0.20730300
H	4.40139600	-1.45173100	-0.74272200
H	3.09325900	-1.08614300	-1.87371200
H	4.40330300	1.44041200	-0.74196100
H	3.09314300	1.07940500	-1.87173800
C	3.55385600	-0.00651600	1.25543900
H	4.65713600	-0.00528200	1.21355200
H	3.23168000	-0.89445300	1.80640100
H	3.22978900	0.87879000	1.80947700
O	0.06301400	-0.03072900	2.04763700
O	-0.10469600	0.02678500	-1.62493100
Np	-0.01431100	-0.00205600	0.21227200