Electronic supplementary information (ESI)

Influence of denticity and combined soft-hard strategy on the interaction of picolinic-type ligands with NpO_2^+

Hongcai Ling[a,b], Miaoren Xia[b], Wenkai Chen[*a,c], Zhifang Chai[b,d], Dongqi Wang[*b]

([a] College of Chemistry, Fuzhou University, Fuzhou 350116, P.R.China;

[b] Multidisciplinary Initiative Center, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, P.R.China;

[c] Key Laboratory of Applied Nuclear Techniques in Geosciences Sichuan, Chengdu University of Technology, Chengdu 610059, P.R.China;

[d] School of Radiation Medicine and Interdisciplinary Sciences (RAD-X), Soochow University, Suzhou 215123, P.R.China).

Email: dwang@ihep.ac.cn (D.Wang), qc2008@fzu.edu.cn (W.Chen)

Ligand exchange reactions:

L = PA^-:

Scheme 1

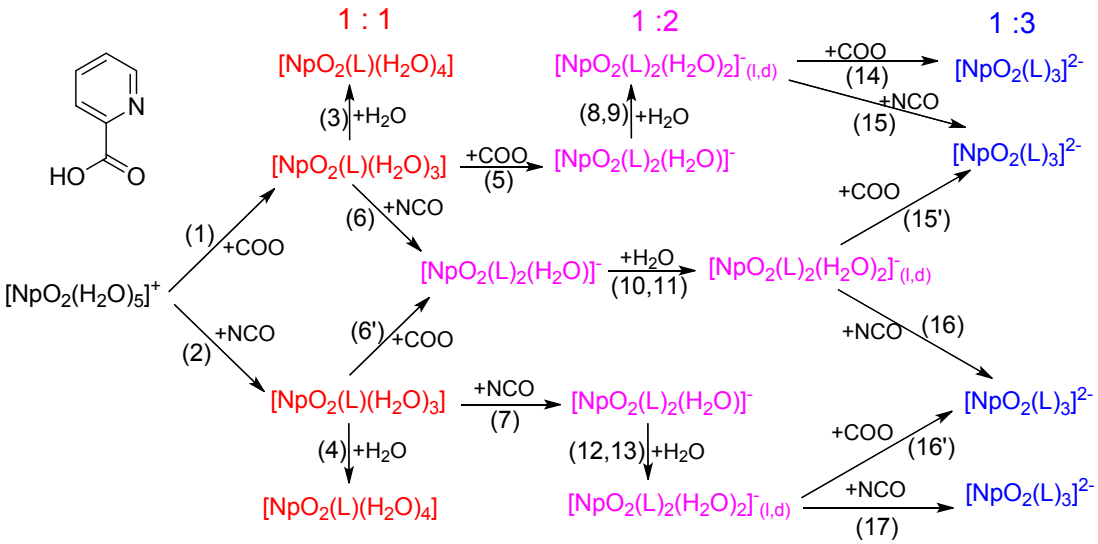


Table 1 **BS1**—6-31+G*, **BS2**—6-311++G**

Complexation reactions (kcal mol^{-1})	Gas					Aqueous (PCM)				
	ΔH	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**	**ΔH**	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**
(1) $[NpO_2(H_2O)_5]^+$+ PA^- → $[NpO_2(PA)(H_2O)_3]$_C + $2H_2O$	-95.24	-102.39	7.15	-94.73	-104.91	-7.54	-16.09	8.55	-9.00	-12.73
(2) $[NpO_2(H_2O)_5]^+$+ PA^- → $[NpO_2(PA)(H_2O)_3]$_N + $2H_2O$	-104.34	-110.90	6.55	-103.91	-108.14	-11.64	-20.75	9.12	-13.10	-17.79
(3) $[NpO_2(H_2O)_5]^+$+ PA^- → $[NpO_2(PA)(H_2O)_4]$_C + H_2O	-112.49	-108.67	-3.82	-114.12	-118.17	-7.37	-6.51	-0.86	-10.87	-14.14
(4) $[NpO_2(H_2O)_5]^+$+ PA^- → $[NpO_2(PA)(H_2O)_4]$_N + H_2O	-115.98	-112.16	-3.82	-117.47	-123.70	-26.37	-25.59	-0.78	-29.63	-33.85
(5) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)]^-$_ C_C + $4H_2O$	-122.94	-138.38	15.44	-121.29	-129.95	-12.16	-31.98	19.82	-12.19	-20.40
(6) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)]^-$_ C_N + $4H_2O$	-128.10	-142.43	14.33	-126.59	-135.94	-25.24	-41.24	16.00	-25.65	-34.06
(7) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)]^-$_N_N + $4H_2O$	-133.88	-147.24	13.36	-132.52	-134.38	-21.58	-36.78	15.20	-22.17	-31.35
(8) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ lC_C + $3H_2O$	-130.91	-135.81	4.90	-130.50	-138.97	-22.76	-30.92	8.17	-24.71	-32.48
(9) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ dC_C + $3H_2O$	-131.71	-138.07	6.30	-131.99	-140.37	-15.52	-23.43	7.90	-17.54	-25.27
(10) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ lC_N + $3H_2O$	-138.14	-142.50	4.36	-138.70	-147.45	-26.29	-33.34	7.06	-28.54	-36.80
(11) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ dC_N + $3H_2O$	-140.95	-144.93	3.98	-141.29	-150.45	-16.86	-23.58	6.73	-19.21	-27.62
(12) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ lN_N + $3H_2O$	-141.52	-145.62	4.10	-142.12	-151.78	-29.16	-34.62	5.46	-31.58	-40.43
(13) $[NpO_2(H_2O)_5]^+$+ $2PA^-$ → $[NpO_2(PA)_2(H_2O)_2]^-$_ dN_N + $3H_2O$	-143.43	-148.01	4.58	-143.86	-153.71	-24.10	-30.71	6.61	-26.44	-41.42
(14) $[NpO_2(H_2O)_5]^+$+ $3PA^-$ → $[NpO_2(PA)_3^{2-}$_C_C_C	-	-	-	-	-	-15.53	-32.40	16.87	-16.18	-28.55

(15) $[NpO_2(H_2O)_5]^{+}$+ 3PA^{-} → $[NpO_2(PA)_3^{2-}$_C_C_N	-64.94	-80.36	15.41	-63.15	-77.99	-16.90	-32.74	15.85	-17.78	-30.79
(16) $[NpO_2(H_2O)_5]^{+}$+ 3PA^{-} → $[NpO_2(PA)_3^{2-}$_C_N_N	-81.03	-94.31	13.28	-78.86	-94.30	-23.97	-41.03	17.07	-24.81	-38.51
(17) $[NpO_2(H_2O)_5]^{+}$+ 3PA^{-} → $[NpO_2(PA)_3^{2-}$_N_N_N	-82.92	-95.23	12.31	-81.80	-97.50	-17.12	-30.91	13.79	-17.46	-31.73
(18) $[NpO_2(H_2O)_5]^{+}$+ H_2O → $[NpO_2(H_2O)_6]^{+}$	-12.46	-2.04	-10.42	-14.54	-13.04	-4.48	4.47	-8.95	-9.20	-6.67

L = DPA^{2-}:

Scheme 2

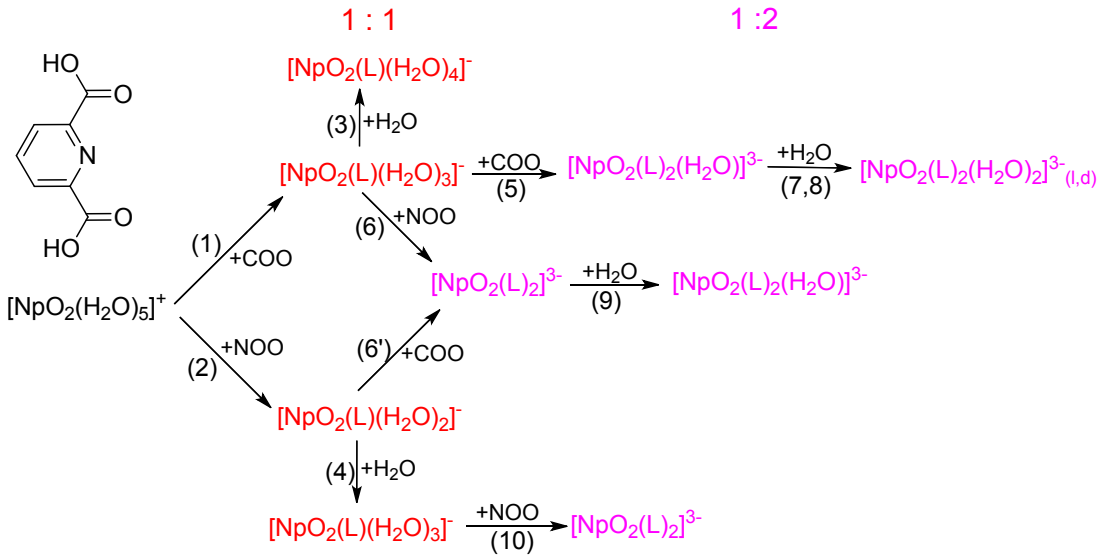


Table 2

Complexation reactions (kcal mol^{-1})	Gas					Aqueous (PCM)				
	ΔH	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**	**ΔH**	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**
(1) $[NpO_2(H_2O)_5]^+$+ DPA^{2-} → $[NpO_2(DPA)(H_2O)_3]^-$_C + $2H_2O$	-159.11	-168.22	9.11	-159.11	-164.68	-6.24	-15.75	9.51	-8.34	-20.22
(2) $[NpO_2(H_2O)_5]^+$+ DPA^{2-} → $[NpO_2(DPA)(H_2O)_2]^-$_N + $3H_2O$	-188.34	-202.30	13.96	-187.32	-193.96	-24.37	-40.71	16.34	-25.19	-31.18
(3) $[NpO_2(H_2O)_5]^+$+ DPA^{2-} → $[NpO_2(DPA)(H_2O)_4]^-$_C + H_2O	-195.00	-189.21	-5.80	-196.18	-201.31	-14.56	-16.15	1.59	-18.52	-23.97
(4) $[NpO_2(H_2O)_5]^+$+ DPA^{2-} → $[NpO_2(DPA)(H_2O)_3]^-$_N + $2H_2O$	-203.19	-206.57	3.39	-204.29	-217.75	-31.51	-39.02	7.51	-34.09	-39.84
(5) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2(H_2O)]^{3-}$_C_C + $4H_2O$	-128.38	-147.65	19.27	-127.64	-140.25	-8.62	-29.16	20.54	-10.04	-21.77
(6) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2]^{3-}$_C_N + $5H_2O$	-122.62	-147.91	25.29	-119.38	-133.04	-24.11	-51.41	27.30	-24.10	-36.18
(7) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2(H_2O)_2]^{3-}$_lC_C + $3H_2O$	-137.38	-148.51	11.13	-138.51	-149.08	-18.04	-28.56	10.52	-21.22	-32.59
(8) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2(H_2O)_2]^{3-}$_dC_C + $3H_2O$	-141.42	-149.02	7.61	-141.92	-154.35	-19.48	-30.13	10.65	-22.67	-34.03
(9) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2(H_2O)]^{3-}$_C_N + $3H_2O$	-139.34	-156.18	16.83	-138.62	-152.00	-29.67	-46.98	17.31	-31.48	-37.61
(10) $[NpO_2(H_2O)_5]^+$+ $2DPA^{2-}$ → $[NpO_2(DPA)_2]^{3-}$_N_N + $5H_2O$	-103.52	-129.55	26.03	-100.84	-58.34	-27.55	-53.32	25.78	-27.78	-40.43

L = $PADA^{2-}$:

Scheme 3

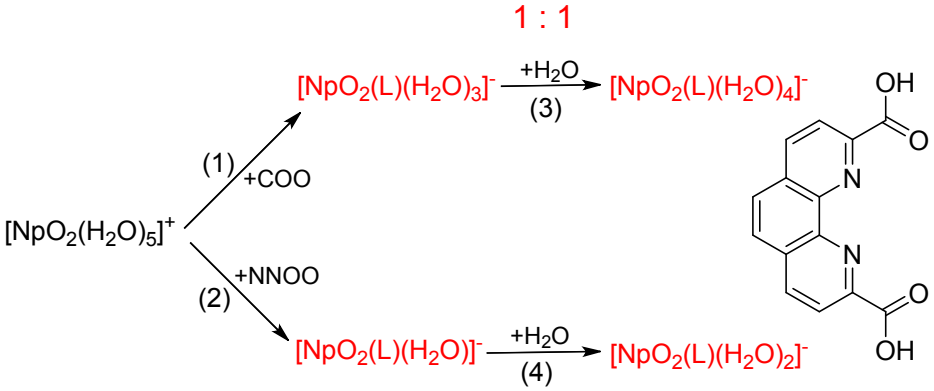


Table 3

Complexation reactions (kcal mol^{-1})	Gas					Aqueous (PCM)				
	ΔH	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**	**ΔH**	**ΔG**	**TΔS**	**ΔE(BS1)**	**ΔE(BS2)**
(1) $[NpO_2(H_2O)_5]^{+}$+ $PADA^{2-}$ → $[NpO_2(PADA)(H_2O)_3]^{-}$_C + $2H_2O$	-143.53	-148.30	4.77	-142.57	-151.94	-10.30	-16.49	6.19	-11.24	-20.70
(2) $[NpO_2(H_2O)_5]^{+}$+ $PADA^{2-}$ → $[NpO_2(PADA)(H_2O)]^{-}$_N + $4H_2O$	-179.03	-197.79	18.76	-175.35	-186.23	-32.11	-55.10	23.00	-29.96	-40.02
(3) $[NpO_2(H_2O)_5]^{+}$+ $PADA^{2-}$ → $[NpO_2(PADA)(H_2O)_4]^{-}$_C + H_2O	-150.42	-143.73	-6.69	-151.48	-160.48	-9.13	-4.98	-4.15	-11.92	-21.10
(4) $[NpO_2(H_2O)_5]^{+}$+ $PADA^{2-}$ → $[NpO_2(PADA)(H_2O)_2]^{-}$_N + $3H_2O$	-189.62	-198.45	8.82	-187.98	-198.55	-27.46	-39.27	11.80	-27.60	-44.83

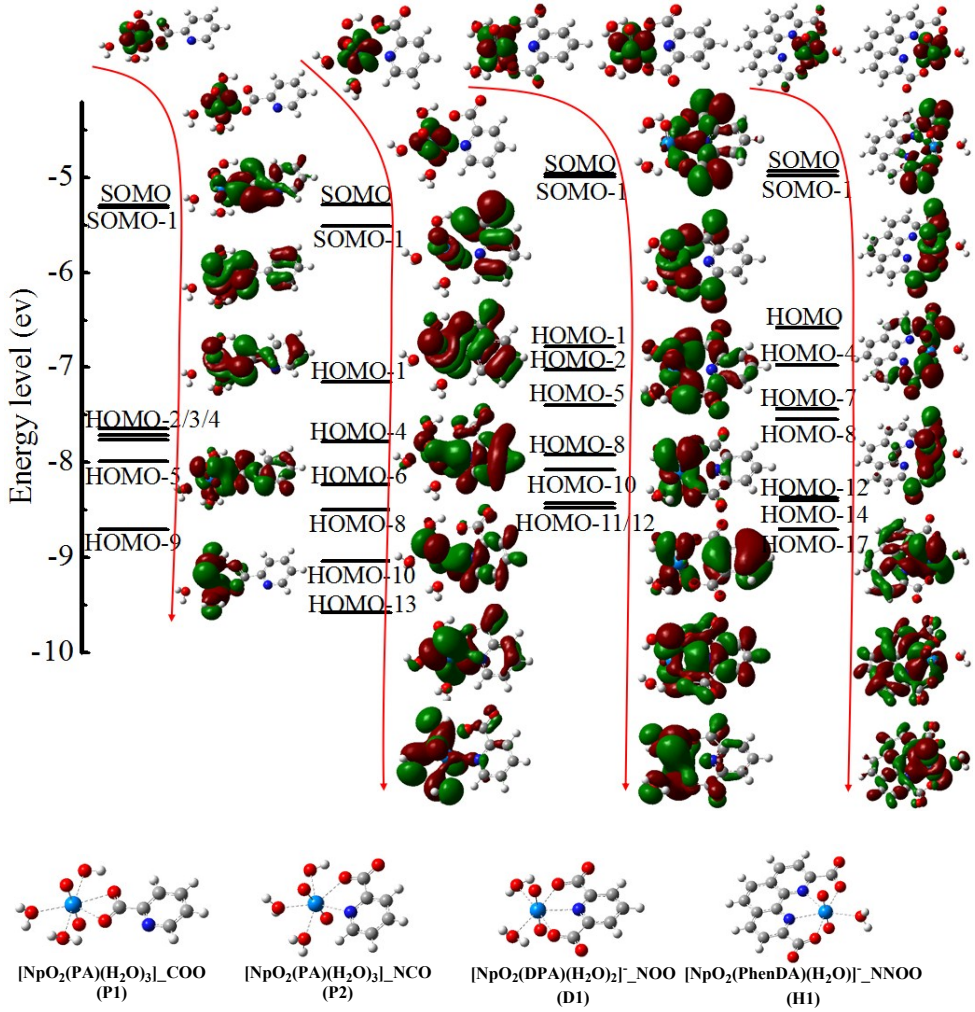
Table 4 Charge transfer (e^-) in the complexes from the ligands to NpO_2^+ by the CDA and ECDA methods calculated at the B3LYP level

Complexes	Charge Transfer	CDA	ECDA
(*N1*) $[NpO_2(H_2O)_5]^+$	$H_2O \rightarrow NpO_2^+$	0.5734	0.8157
(*P0*) $[NpO_2\ (PA)(H_2O)_3]$_C	$L+H_2O \rightarrow NpO_2^+$	0.5908	0.8713
(*P1*) $[NpO_2\ (PA)(H_2O)_3]$_N	$L+H_2O \rightarrow NpO_2^+$	0.5852	0.8780
(*P2*) $[NpO_2(PA)_2(H_2O)]^-$_C_N	$L+H_2O \rightarrow NpO_2^+$	0.6542	0.9885
(*P3*) $[NpO_2(PA)_2(H_2O)]^-$_N_N	$L+H_2O \rightarrow NpO_2^+$	0.6315	0.9681
(*P4*) $[NpO_2(PA)_3]^{2-}$_C_N_N	$L \rightarrow NpO_2^+$	0.7408	1.1201
(*P5*) $[NpO_2(PA)_3]^{2-}$_N_N_N	$L \rightarrow NpO_2^+$	0.6970	1.0751
(*D0*) $[NpO_2(DPA)(H_2O)_3]^-$_C	$L+H_2O \rightarrow NpO_2^+$	0.5942	0.8799
(*D1*) $[NpO_2(DPA)(H_2O)_2]^-$_N	$L+H_2O \rightarrow NpO_2^+$	0.6152	0.9411
(*D2*) $[NpO_2(DPA)_2]^{3-}$_C_N	$L \rightarrow NpO_2^+$	0.7429	1.1310
(*D3*) $[NpO_2(DPA)_2]^{3-}$_N_N	$L \rightarrow NpO_2^+$	0.7897	1.2131
(*H0*) $[NpO_2(PADA)(H_2O)_3]^-$_C	$L+H_2O \rightarrow NpO_2^+$	0.6097	0.8996
(*H1*) $[NpO_2(PADA)(H_2O)]^-$_N	$L+H_2O \rightarrow NpO_2^+$	0.6211	0.9770
(*H2*) $[NpO_2(PADA)(H_2O)_2]^-$_N	$L+H_2O \rightarrow NpO_2^+$	0.6483	0.9987

Table 5 Representative orbitals (α-spin MOs) with Np contributions (%) at the B3LYP level.

P0	HOMO-2	HOMO-3	HOMO-4	HOMO-5	HOMO-9		
Np	4.07	30.2	22.96	9.17	9.31		
5f/6d	5fy(3x2-y2):1.61	5fz3:24.42	5fz3:18.11	5fxz2:3.9	6dyz:8.79		
			5fxyz:1.33				
O15/O16	O15:6.99(2px),17.74(2py)	O15:13.87(2pz)	O15:22.27(2pz)	O15:29.33(2px),2.7(2py)	O15:1.77(2pz)		
	O16:30.12(2px),25.84(2py)	O16:19.67(2pz)	O16:25.69(2pz)	O16:11.94(2px)	O16:1.89(2pz)		
P1	HOMO-1	HOMO-4	HOMO-6	HOMO-8	HOMO-10	HOMO-13	
Np	6.45	39.92	11.02	21.43	13.87	3.93	
5f/6d	5fz3:4.54	5fz3:32.84	5fz3:1.02,5fxz2:2.91	5fxz2:15.61,	6dxz:11.31	6dyz:1.16	
			5fyz2:1.37	5fyz2:3.29	6dyz:2.18		
N9/O16	O16:32.17(2pz)	N9:2.35(2pz)	N9:26.39(2px),4.59(2pz)	N9:1.64(2s),16.16(2px)	N9:1.2(2pz)	N9:1.03(2px)	
		O16:9.63(2pz)	O16:1.44(2py)				
D1	HOMO-1	HOMO-2	HOMO-5	HOMO-8	HOMO-10	HOMO-11	HOMO-12
Np	2.08	18.84	5.48	23.88	4.42	5.81	10.78
5f/6d	5fx(x2-3y2):1.17	5fz3:14.55	5fyz2:1.26	5fxz2:21.18	6dxz:2.78	5fxz2:1.43,5fx(x2-3y2):1.25	6dyz:9.80
			6dxy:1.35			6dx2y2:1.55	
N9/O14/O17	N9:1.17(2s),2.39(2px)	O14:16.20(2pz)	O14:2.13(2px),29.08(2py)	N9:1.19(2px)	N9:20.48(2pz)	N9:3.5(2s),34.85(2px)	N9:0.92(2px)
	O14:1.95(2px),2.43(2py)	O17:16.21(2pz)	O17:2.13(2px),29.12(2py)	O14:2.54(2py)		O14:2.15(2py)	O14:1.83(2pz)
	O17:1.94(2px),2.42(2py)			O17:2.54(2py)		O17:2.15(2py)	O17:1.83(2pz)
H1	HOMO	HOMO-4	HOMO-7	HOMO-8	HOMO-12	HOMO-14	HOMO-17
Np	2.26	19.39	2.63	36.2	6.92	6.55	6.3
5f/6d	5fy(3x2-y2):1.40	5fz3:13.47	6dx2y2:1.04	5fz3:29.76	5fxz2:1.56	5fy(3x2-y2):1.99	6dz2:1.01
		5fz(x2-y2):2.51			6dxz:2.74	6dxy:2.28	
N22/N23/O25/O28	O25:6.69(2py)	O25:15.87(2pz)	O25:22.81(2px),13.43(2py)	O25:6.32(2pz)	N22:5.72(2px),4.76(2py)	N22:13.29(2px),6.05(2py),2.23(2pz)	N22:4.75(2px),4.41(2py)
	O28:6.26(2py)	O28:17.27(2pz)	O28:18.83(2px),19.07(2py)	O28:6.48(2pz)	N23:4.44(2px),2.46(2py)	N23:16.43(2px),4.13(2py),2.71(2pz)	N23:6.01(2px),3.20(2py)

Figure 1 The representative α-spin frontier orbitals of NpO_2^+ complexes. The isosurface value of MO is set as 0.02 a.u.



QTAIM analysis

Np-Om-n: yl—the oxygen of the neptunyl
water—the oxygen of the water
carb—the oxygen of the carboxyl of the ligand
n—the serial number of the atom

Np-N-n: n—the serial number of the atom

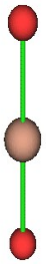
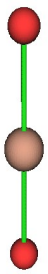
d—Å

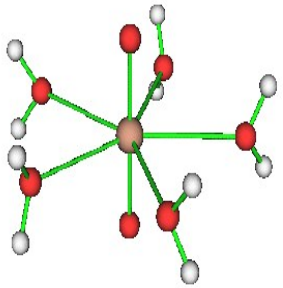
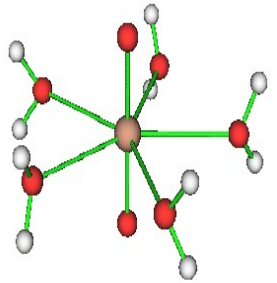
ρb—$e \cdot bohr^{-3}$

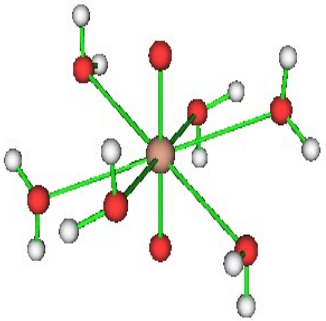
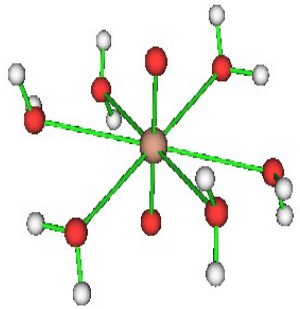
▽2ρb—$e \cdot bohr^{-5}$

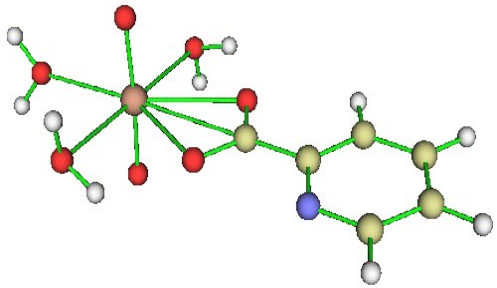
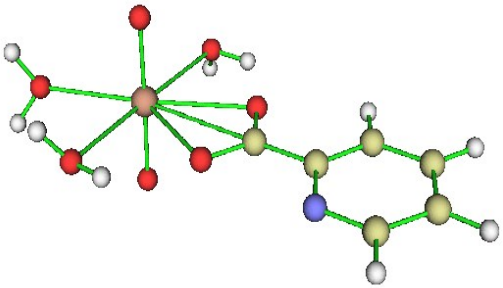
MBO, δ, Hb, ε—a.u.

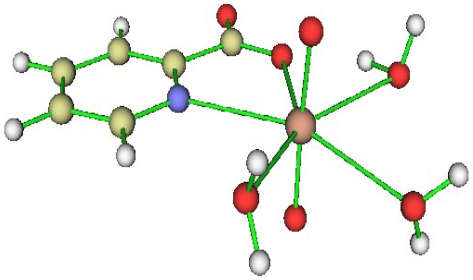
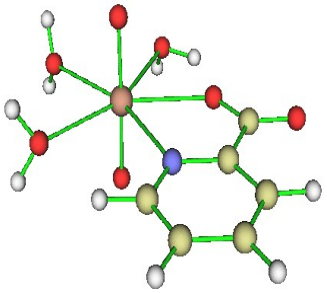
Table 6

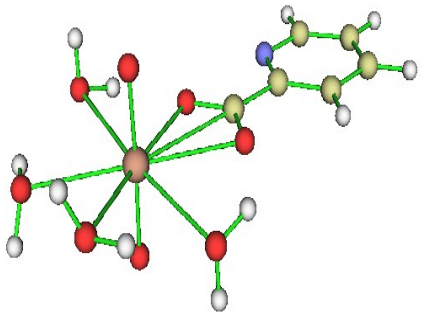
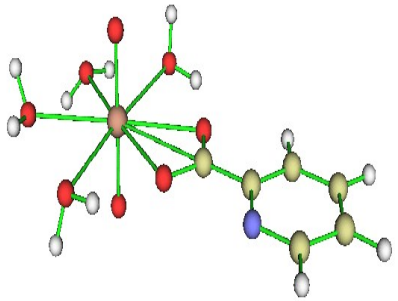
	NpO_2^+													
	Gas							Aqueous(PCM)						
														
∠O-Np-O	180							180						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-1	1.737	1.6	2.97	0.335	0.12	-0.347	0.001904	1.781	1.29	2.86	0.294	0.179	-0.269	0
Np-Oyl-2	1.737	1.6	2.97	0.335	0.12	-0.347	0.001904	1.781	1.29	2.86	0.294	0.179	-0.269	0
	$[NpO_2(H_2O)_5]^+$													

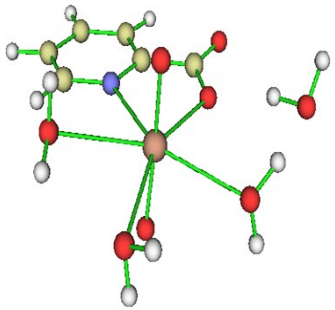
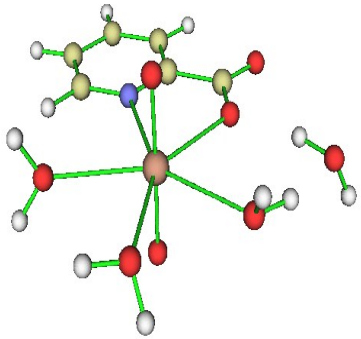
	Gas							Aqueous(PCM)						
														
∠O-Np-O	179.986							179.945						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-1	1.78	1.257	2.856	0.295	0.187	-0.271	0.000109	1.794	1.146	2.823	0.283	0.215	-0.249	0.00011
Np-Oyl-2	1.78	1.257	2.856	0.295	0.187	-0.271	0.000102	1.794	1.145	2.823	0.283	0.215	-0.249	0.000111
Np-Owater-4	2.574	0.221	0.84	0.0384	0.158	1.51E-03	0.224	2.555	0.228	0.862	0.0408	0.164	1.23E-03	0.22
Np-Owater-7	2.573	0.222	0.844	0.0385	0.158	1.51E-03	0.224	2.555	0.228	0.864	0.0408	0.164	1.24E-03	0.22
Np-Owater-10	2.573	0.221	0.841	0.0385	0.158	1.52E-03	0.224	2.554	0.228	0.867	0.0408	0.164	1.24E-03	0.22
Np-Owater-13	2.573	0.221	0.838	0.0385	0.158	1.51E-03	0.224	2.556	0.228	0.864	0.0407	0.164	1.24E-03	0.22
Np-Owater-16	2.573	0.221	0.839	0.0385	0.158	1.51E-03	0.224	2.556	0.228	0.861	0.0407	0.164	1.22E-03	0.22
	$[NpO_2(H_2O)_6]^+$													
	Gas							Aqueous(PCM)						

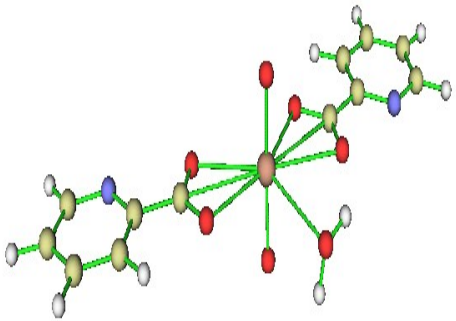
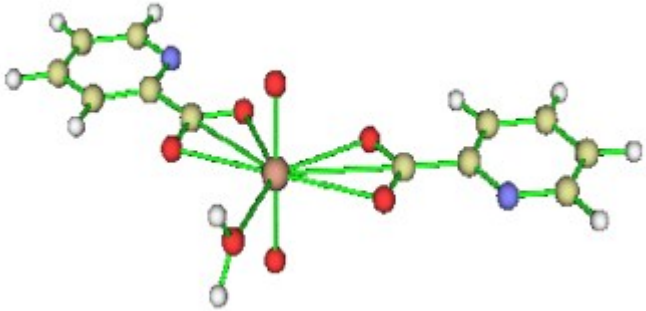
														
∠O-Np-O	179.996							179.865						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-1	1.798	1.044	2.821	0.285	0.226	-0.251	0.00369	1.8	0.928	2.82	0.282	0.232	-0.245	0.000867
Np-Oyl-2	1.798	1.044	2.821	0.285	0.226	-0.251	0.00369	1.8	0.927	2.82	0.282	0.232	-0.245	0.000684
Np-Owater-4	2.672	0.101	0.726	0.0326	0.124	2.67E-04	0.163	2.653	0.13	0.767	0.034	0.125	2.78E-04	0.206
Np-Owater-7	2.67	0.103	0.728	0.0327	0.124	3.31E-04	0.138	2.786	0.0987	0.624	0.0244	0.0909	4.93E-04	0.101
Np-Owater-10	2.672	0.107	0.728	0.0323	0.121	4.49E-04	0.207	2.682	0.115	0.713	0.032	0.118	2.77E-04	0.155
Np-Owater-13	2.672	0.102	0.726	0.0326	0.124	2.67E-04	0.163	2.652	0.132	0.768	0.0341	0.125	2.66E-04	0.204
Np-Owater-16	2.67	0.103	0.728	0.0327	0.124	3.31E-04	0.138	2.791	0.0982	0.619	0.0242	0.0897	4.66E-04	0.0969
Np-Owater-19	2.672	0.107	0.728	0.0323	0.121	4.49E-04	0.207	2.674	0.118	0.72	0.0325	0.12	2.97E-04	0.159
	$[NpO_2(PA)(H_2O)_3]$_C													
	Gas							Aqueous(PCM)						

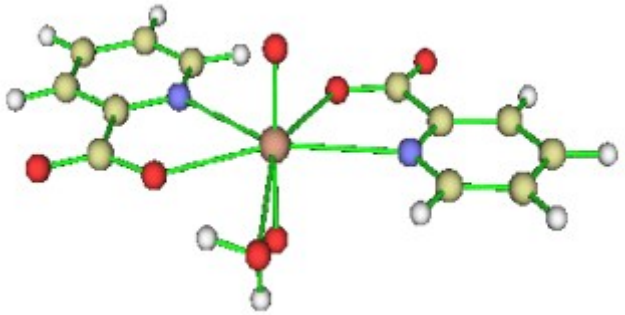
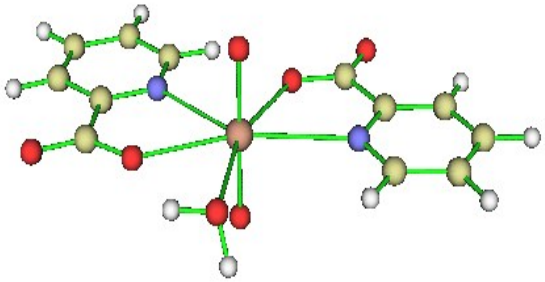
														
∠O-Np-O	175.289							178.623						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-14	1.791	0.589	2.833	0.289	0.223	-0.258	0.00464	1.802	0.608	2.81	0.278	0.223	-0.239	0.00108
Np-Oyl-15	1.792	0.585	2.832	0.288	0.224	-0.257	0.00494	1.802	0.61	2.81	0.278	0.223	-0.239	0.00171
Np-Owater-17	2.607	0.16	0.792	0.0376	0.151	4.06E-04	0.0729	2.604	0.132	0.809	0.0373	0.142	7.29E-04	0.377
Np-Owater-20	2.602	0.15	0.796	0.038	0.153	4.02E-04	0.0707	2.637	0.131	0.789	0.0346	0.13	7.11E-04	0.365
Np-Owater-23	2.562	0.0642	0.854	0.0399	0.17	1.55E-03	0.217	2.551	0.174	0.883	0.0398	0.167	1.81E-03	0.174
Np-Ocarb-12	2.55	0.269	0.917	0.0446	0.167	-9.49E-04	0.0166	2.565	0.266	0.906	0.0434	0.154	-8.14E-04	0.356
Np-Ocarb-13	2.501	0.275	0.969	0.05	0.188	-1.51E-03	0.0311	2.545	0.221	0.931	0.0455	0.162	-9.99E-04	0.357
	$[NpO_2(PA)(H_2O)_3]$_N													
	Gas							Aqueous(PCM)						

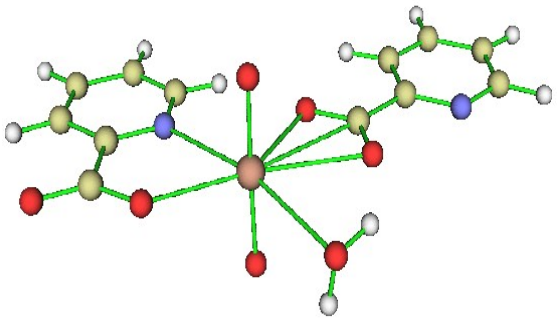
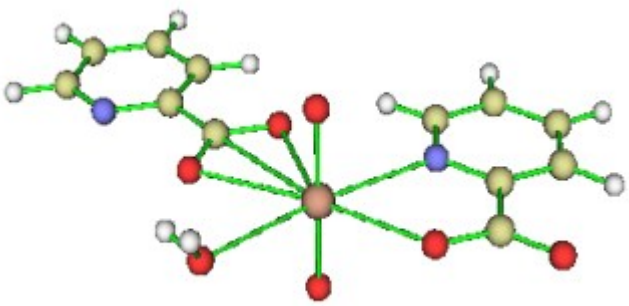
														
∠O-Np-O	172.91							177.794						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-14	1.802	0.746	2.825	0.281	0.238	-0.244	0.00546	1.804	0.714	2.808	0.276	0.228	-0.236	0.00181
Np-Oyl-15	1.806	0.756	2.821	0.279	0.243	-0.24	0.00096	1.804	0.727	2.807	0.276	0.229	-0.236	0.00179
Np-Owater-17	2.624	0.109	0.788	0.0364	0.143	7.35E-04	0.24	2.552	0.169	0.88	0.0403	0.167	1.58E-03	0.185
Np-Owater-20	2.656	0.128	0.751	0.0337	0.132	6.75E-04	0.161	2.555	0.202	0.873	0.04	0.166	1.64E-03	0.184
Np-Owater-23	2.645	0.134	0.748	0.0351	0.133	1.76E-05	0.164	2.614	0.104	0.792	0.037	0.138	4.77E-04	0.377
Np-N-6	2.627	0.231	0.875	0.0426	0.143	-9.89E-04	0.127	2.644	0.217	0.869	0.0415	0.131	-7.63E-04	0.392
Np-Ocarb-13	2.397	0.364	1.131	0.0604	0.245	-1.86E-03	0.0738	2.444	0.272	1.073	0.0544	0.214	-6.02E-04	0.363
	$[NpO_2(PA)(H_2O)_4]$_C													
	Gas							Aqueous(PCM)						

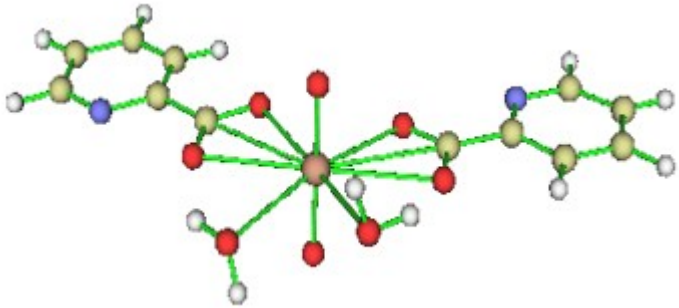
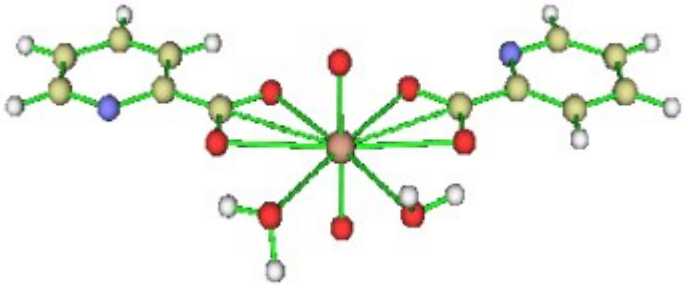
														
∠O-Np-O	176.761							179.203						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-14	1.804	0.433	2.821	0.28	0.239	-0.242	0.00539	1.81	0.427	2.807	0.275	0.246	-0.232	0.00293
Np-Oyl-15	1.804	0.426	2.823	0.281	0.237	-0.243	0.00545	1.81	0.428	2.807	0.275	0.246	-0.232	0.00292
Np-Owater-17	2.743	0.0946	0.633	0.0282	0.106	7.45E-05	0.00926	2.685	0.129	0.71	0.0315	0.119	4.26E-04	0.153
Np-Owater-20	2.651	0.135	0.745	0.0341	0.13	4.38E-04	0.0612	2.651	0.159	0.763	0.034	0.127	5.03E-04	0.273
Np-Owater-23	2.659	0.135	0.739	0.0336	0.127	4.39E-04	0.0635	2.649	0.165	0.764	0.0341	0.128	5.08E-04	0.274
Np-Owater-26	2.728	0.102	0.642	0.0293	0.11	6.79E-05	0.0506	2.687	0.129	0.708	0.0314	0.119	4.20E-04	0.157
Np-Ocarb-12	2.591	0.267	0.867	0.0407	0.15	-7.39E-04	0.019	2.591	0.27	0.877	0.0412	0.146	-8.69E-04	0.211
Np-Ocarb-13	2.523	0.292	0.938	0.0475	0.177	-1.21E-03	0.0256	2.591	0.249	0.875	0.0413	0.146	-9.01E-04	0.213
	$[NpO_2(PA)(H_2O)_4]$_N													
	Gas							Aqueous(PCM)						

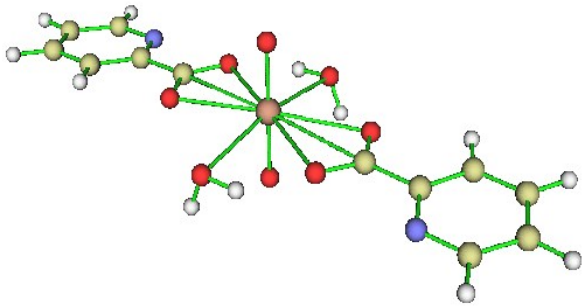
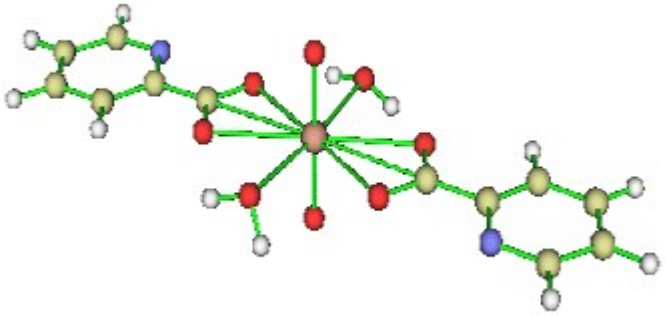
														
∠O-Np-O	173.119							178.299						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-14	1.809	0.876	2.814	0.274	0.229	-0.232	0.00503	1.811	0.79	2.807	0.273	0.248	-0.23	0.00241
Np-Oyl-15	1.807	0.9	2.819	0.275	0.226	-0.235	0.00466	1.811	0.788	2.806	0.274	0.249	-0.231	0.00115
Np-Owater-17	2.679	0.0841	0.724	0.0329	0.12	2.05E-04	0.235	2.564	0.138	0.859	0.0387	0.165	1.75E-03	0.278
Np-Owater-20	2.724	0.0641	0.677	0.029	0.107	5.49E-04	0.2	2.634	0.146	0.783	0.035	0.134	7.41E-04	0.3
Np-Owater-23	3.968		0.0377					2.57	0.107	0.877	0.0409	0.157	3.54E-04	0.286
Np-Owater-26	2.576	0.127	0.879	0.0409	0.155	2.25E-04	0.232	4.181		0.0198				
Np-N-6	2.635	0.234	0.871	0.0422	0.135	-8.42E-04	0.415	2.66	0.213	0.853	0.0403	0.129	-7.53E-04	0.348
Np-Ocarb-13	2.386	0.301	1.169	0.062	0.248	-1.96E-03	0.383	2.459	0.219	1.07	0.0525	0.21	-4.14E-04	0.34
	$[NpO_2(PA)_2(H_2O)]^-$_ C_C													
	Gas							Aqueous(PCM)						

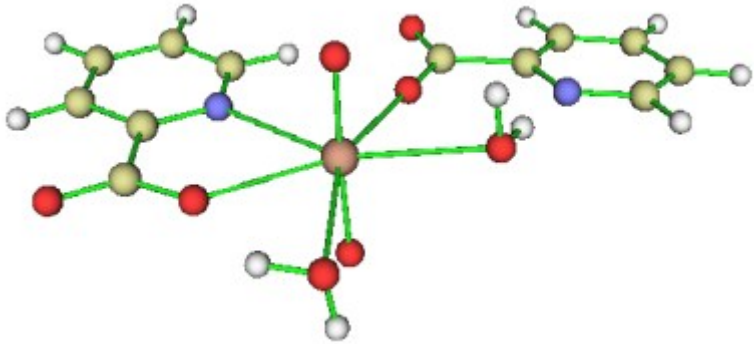
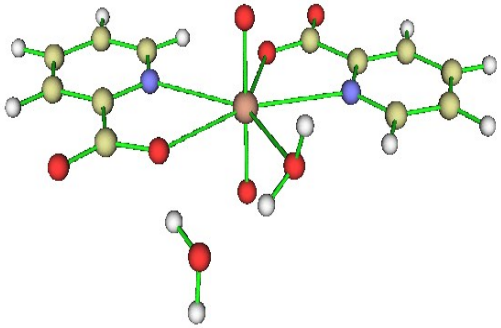
														
∠O-Np-O	177.126							178.22						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.799	0.646	2.838	0.283	0.227	-0.247	0.0057	1.811	0.409	2.795	0.271	0.237	-0.227	0.00271
Np-Oyl-28	1.81	0.626	2.8	0.274	0.247	-0.232	0.00792	1.811	0.417	2.795	0.271	0.238	-0.227	0.00281
Np-Owater-30	2.682	0.199	0.7	0.0327	0.122	5.26E-05	0.104	2.552	0.197	0.894	0.0392	0.168	2.03E-03	0.151
Np-Ocarb-12	2.573	0.254	0.922	0.0429	0.155	-8.61E-04	0.333	2.562	0.263	0.949	0.0437	0.155	-7.24E-04	0.33
Np-Ocarb-13	2.539	0.288	0.955	0.0462	0.169	-1.11E-03	0.194	2.531	0.283	0.972	0.0467	0.168	-9.29E-04	0.371
Np-Ocarb-25	2.549	0.284	0.944	0.0449	0.165	-8.43E-04	0.244	2.532	0.309	0.974	0.0466	0.168	-9.05E-04	0.373
Np-Ocarb-26	2.679	0.157	0.766	0.0343	0.119	-6.81E-04	0.232	2.566	0.227	0.945	0.0433	0.154	-7.29E-04	0.327
	$[NpO_2(PA)_2(H_2O)]^-$_N_N													
	Gas							Aqueous(PCM)						

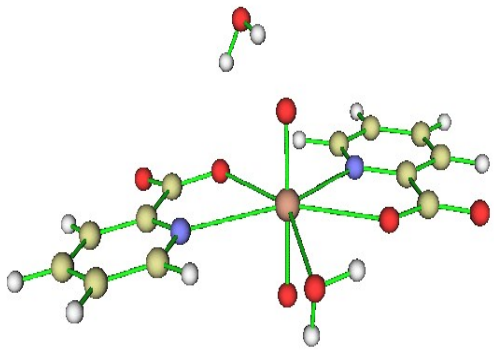
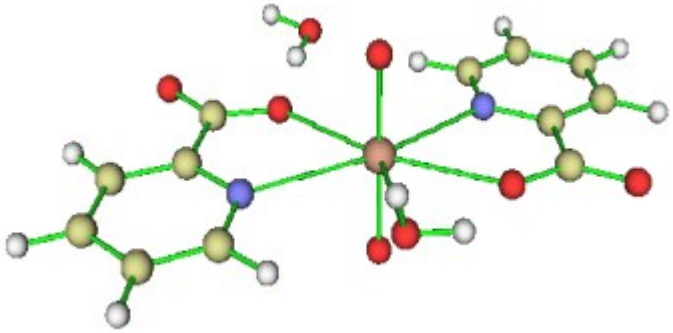
														
∠O-Np-O	175.878							178.843						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.805	0.527	2.829	0.279	0.238	-0.239	0.00577	1.813	0.366	2.794	0.27	0.241	-0.225	0.00417
Np-Oyl-28	1.816	0.527	2.789	0.27	0.256	-0.225	0.00713	1.814	0.375	2.794	0.269	0.242	-0.224	0.0042
Np-Owater-30	2.71	0.123	0.669	0.0311	0.114	-8.50E-05	0.059	2.686	0.0598	0.732	0.0317	0.115	3.79E-04	0.337
Np-N-6	2.621	0.188	0.86	0.0431	0.144	-9.06E-04	0.414	2.657	0.194	0.853	0.0402	0.128	-5.58E-04	0.406
Np-N-19	2.673	0.109	0.82	0.0385	0.129	-2.56E-04	0.371	2.676	0.148	0.839	0.0386	0.123	-3.16E-04	0.378
Np-Ocarb-13	2.498	0.23	0.997	0.0487	0.192	-2.77E-04	0.282	2.489	0.231	1.014	0.0491	0.191	-5.33E-04	0.345
Np-Ocarb-26	2.436	0.317	1.111	0.0555	0.224	-8.64E-04	0.275	2.427	0.312	1.126	0.0561	0.224	-6.78E-04	0.344
	$[NpO_2(PA)_2(H_2O)]^-$_ C_N													
	Gas							Aqueous(PCM)						

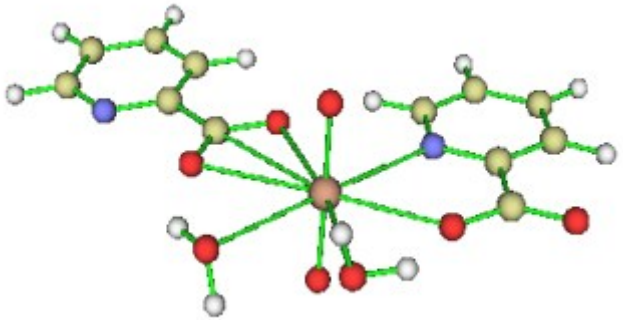
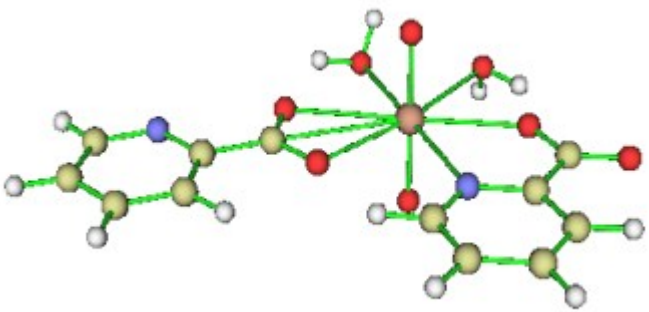
														
∠O-Np-O	177.038							179.4						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.801	0.565	2.835	0.28	0.218	-0.242	0.00722	1.82	0.449	2.792	0.266	0.246	-0.218	0.00357
Np-Oyl-28	1.814	0.579	2.794	0.27	0.239	-0.225	0.00682	1.821	0.465	2.791	0.265	0.247	-0.217	0.00419
Np-Owater-30	2.692	0.188	0.691	0.0325	0.116	-1.22E-04	0.164	2.686	0.106	0.741	0.0313	0.115	5.63E-04	0.327
Np-N-19	2.643	0.214	0.846	0.0406	0.135	-3.22E-04	0.423	2.662	0.232	0.851	0.0399	0.126	-5.36E-04	0.39
Np-Ocarb-12	2.582	0.268	0.912	0.0413	0.148	-4.35E-04	0.361	2.555	0.291	0.953	0.0444	0.157	-8.19E-04	0.354
Np-Ocarb-13	2.683	0.157	0.765	0.0335	0.116	-4.37E-04	0.287	2.635	0.195	0.833	0.0374	0.129	-5.83E-04	0.317
Np-Ocarb-26	2.41	0.344	1.162	0.0586	0.233	-1.25E-03	0.318	2.437	0.299	1.134	0.0549	0.217	-5.81E-04	0.326
	$[NpO_2(PA)_2(H_2O)_2]^-$_ lC_C													
	Gas							Aqueous(PCM)						

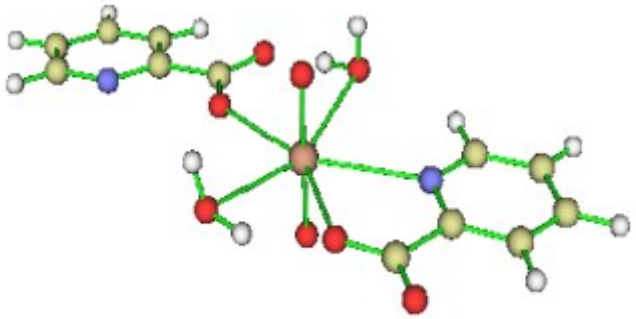
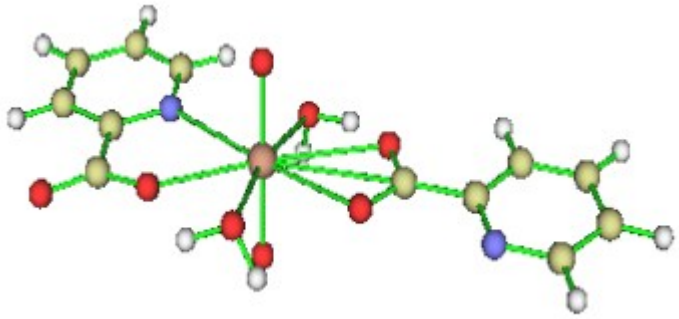
														
∠O-Np-O	175.383							178.759						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.806	0.385	2.819	0.278	0.239	-0.238	0.00103	1.819	0.218	2.79	0.266	0.246	-0.218	0.000737
Np-Oyl-28	1.807	0.399	2.815	0.277	0.241	-0.236	0.00121	1.819	0.23	2.79	0.266	0.246	-0.218	0.000864
Np-Owater-30	2.736	0.191	0.652	0.0293	0.104	-7.36E-05	0.297	2.669	0.125	0.743	0.0325	0.12	5.73E-04	0.354
Np-Owater-33	2.744	0.199	0.638	0.0288	0.103	-9.77E-05	0.276	2.658	0.131	0.75	0.0333	0.123	5.80E-04	0.349
Np-Ocarb-12	2.554	0.368	0.937	0.0443	0.161	-7.76E-04	0.329	2.571	0.344	0.932	0.0426	0.15	-6.35E-04	0.362
Np-Ocarb-13	2.705	0.174	0.744	0.032	0.112	-5.62E-04	0.106	2.632	0.215	0.838	0.0375	0.13	-5.93E-04	0.323
Np-Ocarb-25	2.739	0.176	0.712	0.0296	0.103	-4.77E-04	0.0902	2.631	0.234	0.84	0.0375	0.13	-5.71E-04	0.325
Np-Ocarb-26	2.559	0.34	0.928	0.0439	0.159	-7.77E-04	0.31	2.579	0.313	0.923	0.042	0.147	-6.22E-04	0.362
	$[NpO_2(PA)_2(H_2O)_2]^-$_ dC_C													
	Gas							Aqueous(PCM)						

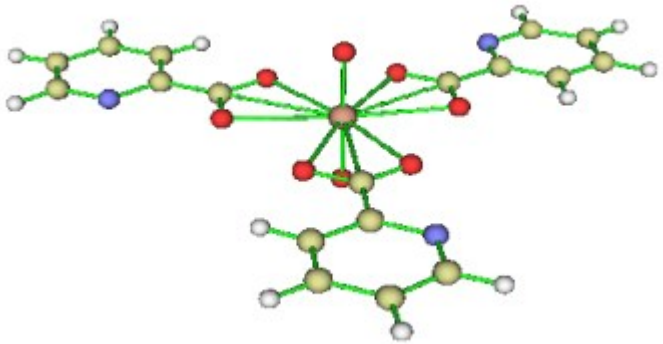
														
∠O-Np-O	179.732							179.788						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.798	0.407	2.84	0.285	0.229	-0.249	0.00476	1.813	0.0924	2.79	0.269	0.24	-0.224	0.00247
Np-Oyl-28	1.816	0.339	2.792	0.271	0.26	-0.226	0.00764	1.814	0.131	2.787	0.269	0.243	-0.223	0.00354
Np-Owater-30	2.688	0.225	0.696	0.032	0.121	7.72E-05	0.0549	2.621	0.112	0.791	0.0358	0.136	8.34E-04	0.4
Np-Owater-33	2.691	0.191	0.699	0.0316	0.12	1.64E-04	0.053	2.624	0.119	0.788	0.0356	0.135	8.11E-04	0.395
Np-Ocarb-12	2.6	0.299	0.884	0.0396	0.145	-3.89E-04	0.0325	2.565	0.302	0.926	0.0433	0.154	-6.80E-04	0.35
Np-Ocarb-13	2.672	0.18	0.776	0.0339	0.122	-4.23E-04	0.0436	2.571	0.27	0.918	0.0428	0.152	-6.76E-04	0.347
Np-Ocarb-25	2.598	0.3	0.884	0.0398	0.145	-4.24E-04	0.0447	2.609	0.243	0.863	0.0393	0.138	-5.42E-04	0.34
Np-Ocarb-26	2.703	0.161	0.746	0.0317	0.113	-3.92E-04	0.0418	2.615	0.216	0.854	0.0389	0.136	-5.62E-04	0.337
	$[NpO_2(PA)_2(H_2O)_2]^-$_ lN_N													
	Gas							Aqueous(PCM)						

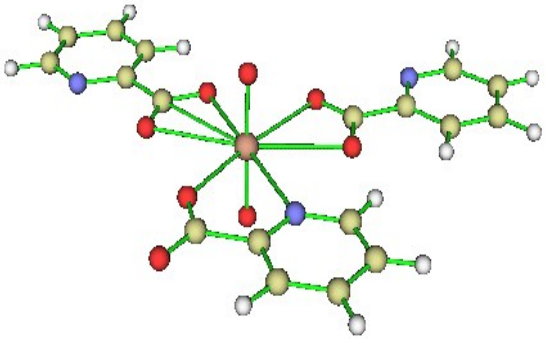
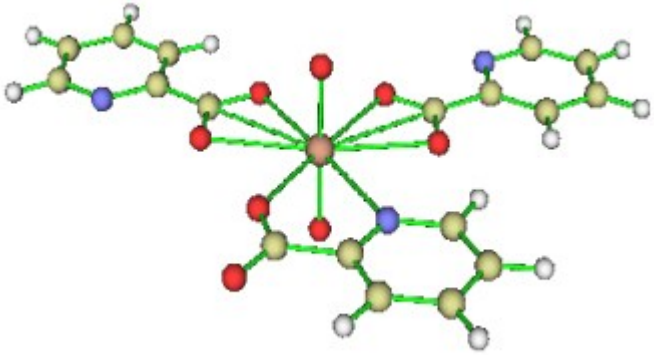
														
∠O-Np-O	175.633							178.737						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.811	0.703	2.804	0.274	0.247	-0.231	0.0029	1.815	0.438	2.791	0.268	0.245	-0.222	0.00229
Np-Oyl-28	1.811	0.725	2.807	0.274	0.246	-0.231	0.00406	1.814	0.447	2.792	0.269	0.244	-0.223	0.00397
Np-Owater-30	2.637	0.108	0.783	0.0366	0.135	-6.06E-05	0.244	2.587	0.0564	0.865	0.0396	0.15	4.46E-04	0.277
Np-Owater-33	2.7	0.136	0.689	0.0318	0.115	-7.45E-05	0.214	4.119		0.0266				
Np-N-6	4.342		0.017					2.674	0.171	0.84	0.0388	0.123	-3.65E-04	0.38
Np-N-19	2.656	0.227	0.841	0.0397	0.133	-3.97E-04	0.263	2.656	0.186	0.852	0.0403	0.129	-5.61E-04	0.41
Np-Ocarb-13	2.407	0.368	1.127	0.0521	0.257	2.67E-03	0.292	2.422	0.302	1.129	0.0568	0.227	-7.62E-04	0.341
Np-Ocarb-26	2.487	0.249	1.006	0.0494	0.197	-1.91E-04	0.321	2.486	0.19	1.035	0.0491	0.193	1.60E-04	0.344
	$[NpO_2(PA)_2(H_2O)_2]^-$_ dN_N													
	Gas							Aqueous(PCM)						

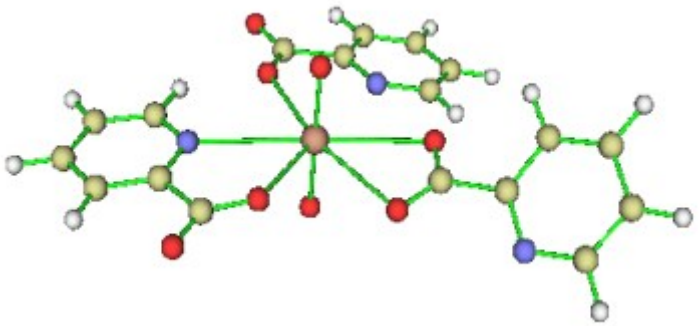
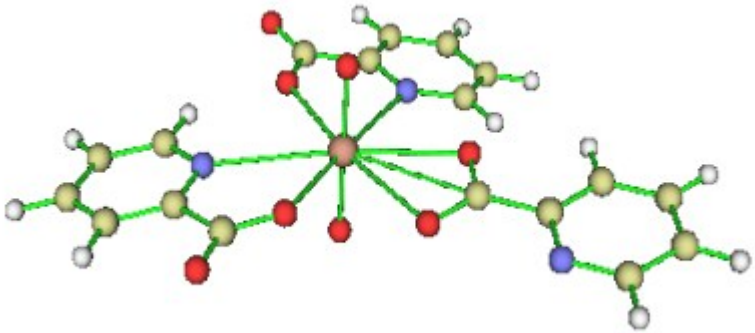
														
∠O-Np-O	177.418							179.226						
	d	MBO	δ	ρb	▽2ρb	Hb	ε	d	MBO	δ	ρb	▽2ρb	Hb	ε
Np-Oyl-27	1.811	0.532	2.8	0.272	0.236	-0.229	0.00759	1.81	0.437	2.801	0.272	0.237	-0.228	0.00651
Np-Oyl-28	1.817	0.659	2.778	0.268	0.243	-0.222	0.0123	1.811	0.443	2.799	0.271	0.238	-0.227	0.00396
Np-Owater-30	2.697	0.12	0.686	0.0324	0.115	-2.45E-04	0.204	2.648	0.067	0.757	0.0346	0.127	3.13E-04	0.32
Np-Owater-33	3.977		0.0479					4.518		0.0148				
Np-N-6	2.616	0.173	0.874	0.0436	0.143	-8.73E-04	0.414	2.685	0.175	0.832	0.038	0.12	-3.16E-04	0.382
Np-N-19	2.662	0.116	0.831	0.0393	0.129	-2.45E-04	0.363	2.689	0.165	0.835	0.0375	0.118	-2.43E-04	0.383
Np-Ocarb-13	2.481	0.254	1.023	0.0505	0.195	-3.34E-04	0.345	2.46	0.221	1.079	0.0519	0.206	-6.89E-04	0.331
Np-Ocarb-26	2.443	0.298	1.108	0.0544	0.215	-6.53E-04	0.33	2.498	0.244	1.001	0.048	0.186	1.08E-04	0.345
	$[NpO_2(PA)_2(H_2O)_2]^-$_ lC_N													
	Gas							Aqueous(PCM)						

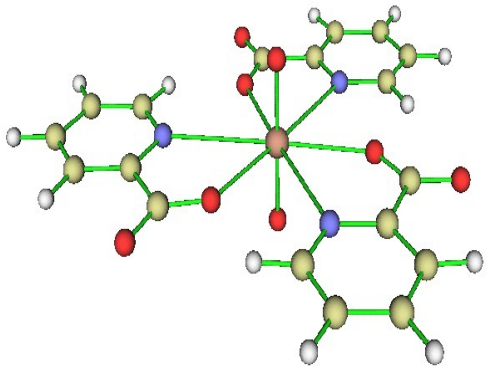
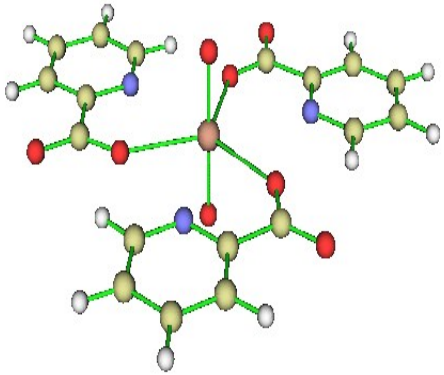
														
∠O-Np-O	177.375							179.139						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.806	0.281	2.82	0.278	0.245	-0.238	0.0027	1.819	0.158	2.794	0.266	0.245	-0.219	0.00194
Np-Oyl-28	1.805	0.255	2.825	0.279	0.242	-0.24	0.00103	1.818	0.153	2.795	0.267	0.244	-0.219	0.0017
Np-Owater-30	2.726	0.199	0.661	0.0294	0.11	1.22E-04	0.0574	2.676	0.147	0.735	0.0321	0.117	5.30E-04	0.349
Np-Owater-33	2.765	0.178	0.629	0.0271	0.0966	1.95E-05	0.0793	2.75	0.136	0.662	0.0276	0.0969	2.51E-04	0.339
Np-N-19	2.735	0.236	0.783	0.0328	0.114	4.30E-04	0.115	2.746	0.247	0.8	0.0332	0.103	6.02E-05	0.389
Np-Ocarb-12	2.621	0.293	0.867	0.0378	0.139	-3.89E-04	0.158	2.574	0.328	0.93	0.0425	0.149	-6.97E-04	0.36
Np-Ocarb-13	2.744	0.161	0.707	0.0291	0.101	-3.48E-04	0.118	2.689	0.194	0.781	0.0332	0.112	-5.03E-04	0.294
Np-Ocarb-26	2.509	0.267	0.978	0.0461	0.185	3.52E-04	0.0719	2.5	0.267	1.002	0.0474	0.184	2.18E-04	0.338
	$[NpO_2(PA)_2(H_2O)_2]^-$_ dC_N													
	Gas							Aqueous(PCM)						

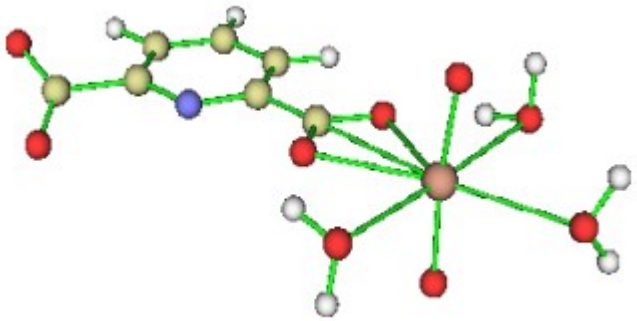
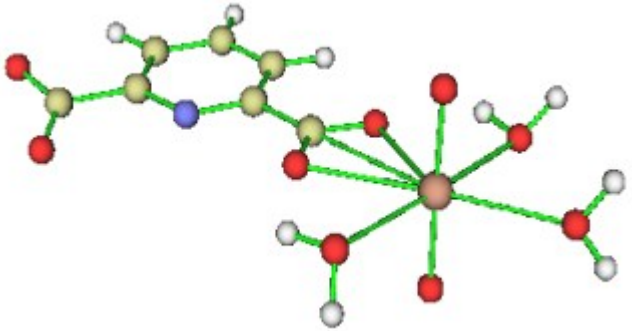
														
∠O-Np-O	178.079							179.132						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.801	0.731	2.837	0.282	0.229	-0.245	0.00745	1.81	0.126	2.8	0.274	0.253	-0.232	0.00582
Np-Oyl-28	1.816	0.696	2.789	0.27	0.256	-0.225	0.0081	1.811	0.156	2.794	0.274	0.257	-0.23	0.00253
Np-Owater-30	2.671	0.19	0.723	0.0335	0.124	1.35E-05	0.162	2.651	0.128	0.75	0.0337	0.131	4.75E-04	0.111
Np-Owater-33	2.614	0.133	0.819	0.0384	0.143	-1.27E-04	0.227	2.671	0.114	0.731	0.0328	0.125	2.62E-04	0.0699
Np-N-19	2.687	0.166	0.813	0.0372	0.124	-6.11E-05	0.351	2.76	0.207	0.782	0.0318	0.105	2.29E-04	0.0691
Np-Ocarb-12	3.872		0.0562					2.727	0.166	0.733	0.0305	0.105	-4.92E-04	0.0762
Np-Ocarb-13	2.482	0.174	1.0394	0.0484	0.2	7.46E-04	0.317	2.589	0.251	0.898	0.0408	0.149	-5.94E-04	0.104
Np-Ocarb-26	2.501	0.237	0.987	0.0477	0.19	-1.59E-06	0.221	2.481	0.263	1.021	0.0489	0.198	2.36E-04	0.0866
	$[NpO_2(PA)_3^{2-}$_C_C_C													
	Gas							Aqueous(PCM)						

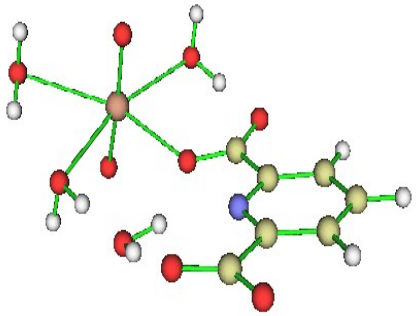
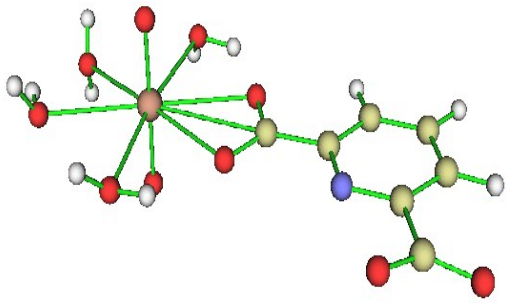
														
∠O-Np-O								179.933						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-14								1.822		2.779	0.263	0.251	-0.214	0.000408
Np-Oyl-15								1.822		2.778	0.263	0.251	-0.214	0.00031
Np-Ocarb-12								2.593	0.282	0.909	0.0405	0.143	-4.29E-04	0.349
Np-Ocarb-13								2.618	0.243	0.884	0.0383	0.134	-3.69E-04	0.338
Np-Ocarb-28								2.599	0.28	0.9	0.0399	0.141	-4.05E-04	0.348
Np-Ocarb-29								2.615	0.245	0.887	0.0386	0.135	-3.85E-04	0.341
Np-Ocarb-41								2.603	0.277	0.899	0.0396	0.14	-4.00E-04	0.345
Np-Ocarb-42								2.608	0.248	0.892	0.0392	0.138	-3.88E-04	0.344
	$[NpO_2(PA)_3^{2-}$_C_C_N													
	Gas							Aqueous(PCM)						

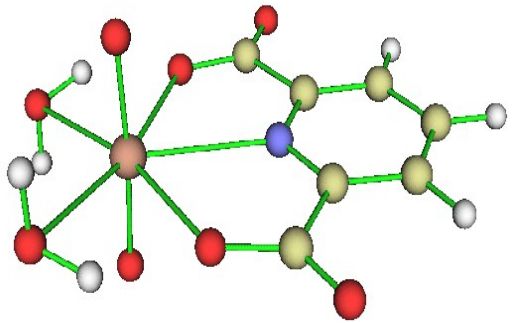
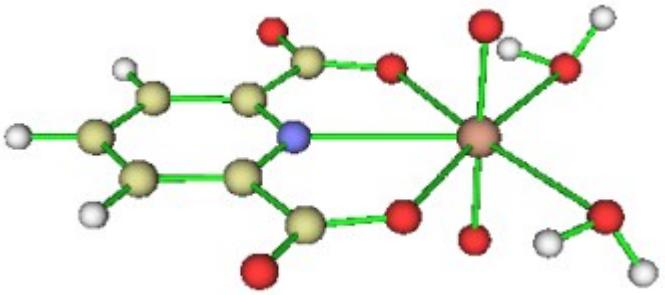
														
∠O-Np-O	178.137							179.43						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-14	1.801	0.281	2.823	0.278	0.224	-0.24	0.00172	1.821		2.782	0.264	0.25	-0.215	0.00115
Np-Oyl-15	1.801	0.28	2.823	0.278	0.224	-0.24	0.00171	1.821		2.782	0.264	0.25	-0.215	0.00113
Np-N-35	2.88	0.148	0.682	0.0237	0.0781	8.83E-04	0.334	2.828	0.189	0.741	0.0276	0.0857	4.14E-04	0.349
Np-Ocarb-12	2.605	0.303	0.884	0.039	0.138	-2.25E-04	0.361	2.62	0.285	0.881	0.0381	0.132	-4.21E-04	0.346
Np-Ocarb-13	2.741	0.196	0.759	0.0289	0.0985	-1.00E-04	0.289	2.655	0.225	0.846	0.0355	0.121	-3.89E-04	0.34
Np-Ocarb-28	2.713	0.191	0.796	0.0305	0.106	-2.69E-05	0.325	2.602	0.267	0.903	0.0398	0.14	-4.70E-04	0.339
Np-Ocarb-29	2.8	0.196	0.706	0.0251	0.0855	7.74E-05	0.277	2.66	0.255	0.84	0.0349	0.121	-2.68E-04	0.32
Np-Ocarb-42	2.503	0.324	1.024	0.0456	0.184	9.65E-04	0.316	2.466	0.327	1.081	0.0504	0.202	4.03E-04	0.327
	$[NpO_2(PA)_3^{2-}$_C_N_N													
	Gas							Aqueous(PCM)						

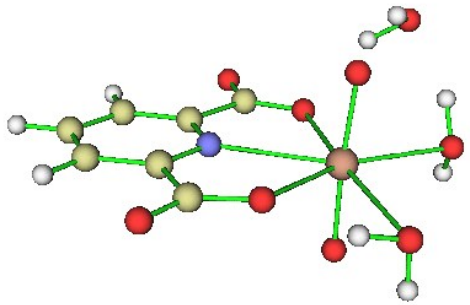
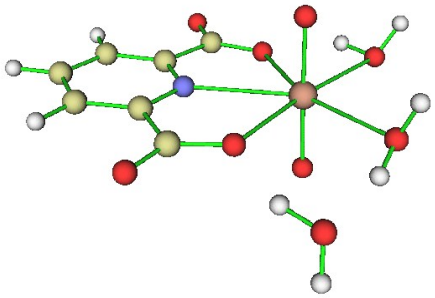
														
∠O-Np-O	178.275							179.297						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-40	1.809	0.556	2.822	0.273	0.232	-0.231	0.00197	1.827	0.232	2.78	0.261	0.256	-0.209	0.00173
Np-Oyl-41	1.81	0.515	2.824	0.273	0.232	-0.231	0.00252	1.827	0.21	2.784	0.26	0.255	-0.209	0.000184
Np-N-6	2.88	0.15	0.684	0.024	0.0771	7.15E-04	0.314	2.91	0.166	0.684	0.0233	0.0706	4.02E-04	0.263
Np-N-19	3.029	0.12	0.589	0.0172	0.0559	8.26E-04	0.203	2.923	0.169	0.682	0.0226	0.0689	4.68E-04	0.267
Np-Ocarb-13	2.501	0.342	1.0424	0.0462	0.183	7.37E-04	0.319	2.488	0.322	1.063	0.0477	0.19	6.35E-04	0.312
Np-Ocarb-26	2.563	0.257	0.957	0.0393	0.158	1.31E-03	0.295	2.478	0.32	1.067	0.0488	0.196	5.97E-04	0.294
Np-Ocarb-38	2.715	0.19	0.792	0.0307	0.104	-1.91E-04	0.296	2.612	0.263	0.899	0.0391	0.134	-5.80E-04	0.323
Np-Ocarb-39	2.798	0.214	0.712	0.0254	0.085	-3.84E-05	0.289	2.732	0.205	0.777	0.03	0.1	-3.28E-04	0.286
	$[NpO_2(PA)_3^{2-}$_N_N_N													
	Gas							Aqueous(PCM)						

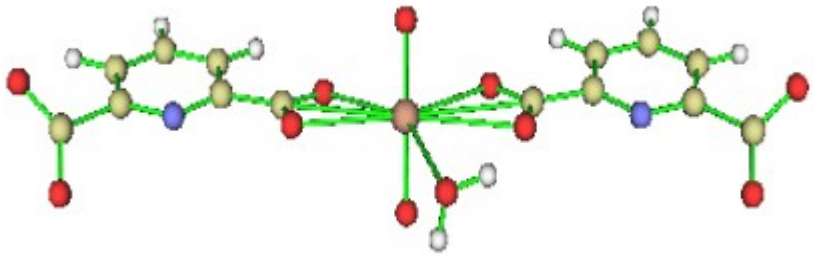
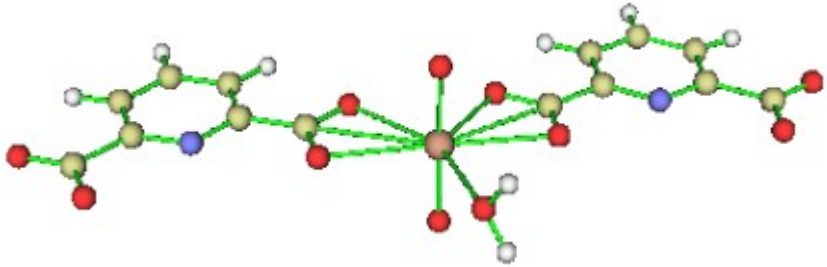
														
∠O-Np-O	179.992							179.942						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-40	1.801	0.477	2.825	0.278	0.223	-0.24	0.000317	1.821	0.294	2.784	0.264	0.249	-0.215	0.000219
Np-Oyl-41	1.801	0.477	2.825	0.278	0.223	-0.24	0.000287	1.821	0.295	2.784	0.264	0.249	-0.215	0.000224
Np-N-6	2.998	0.128	0.609	0.0185	0.0598	8.01E-04	0.253	3.002	0.147	0.627	0.0191	0.0585	5.33E-04	0.199
Np-N-19	2.997	0.128	0.608	0.0185	0.0599	8.16E-04	0.255	3.008	0.147	0.623	0.0189	0.0577	5.23E-04	0.187
Np-N-32	2.997	0.128	0.608	0.0185	0.0599	8.03E-04	0.254	3.009	0.148	0.623	0.0188	0.0577	5.29E-04	0.19
Np-Ocarb-13	2.52	0.31	0.998	0.0433	0.177	1.25E-03	0.303	2.456	0.345	1.082	0.0506	0.208	6.60E-04	0.293
Np-Ocarb-26	2.521	0.308	0.997	0.0433	0.177	1.25E-03	0.304	2.453	0.347	1.088	0.0509	0.21	6.67E-04	0.291
Np-Ocarb-39	2.521	0.309	0.996	0.0433	0.177	1.26E-03	0.304	2.455	0.348	1.083	0.0507	0.209	6.78E-04	0.292
	$[NpO_2(DPA)(H_2O)_3]^-$_C													
	Gas							Aqueous(PCM)						

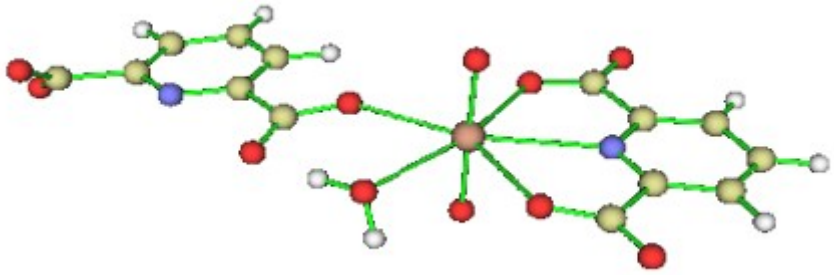
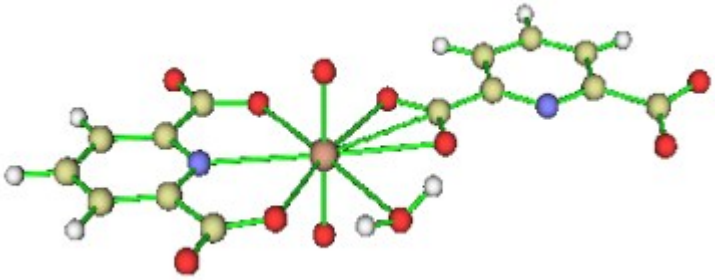
														
∠O-Np-O	172.546							178.605						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-1	1.808	0.688	2.813	0.277	0.245	-0.237	0.00776	1.803	0.663	2.809	0.28	0.243	-0.241	0.00244
Np-Oyl-2	1.804	0.674	2.825	0.28	0.24	-0.241	0.00777	1.802	0.663	2.81	0.28	0.242	-0.241	0.00261
Np-Owater-4	2.675	0.129	0.709	0.0329	0.126	9.80E-05	0.0376	2.609	0.115	0.8	0.0364	0.147	7.71E-04	0.0998
Np-Owater-7	2.618	0.157	0.785	0.0371	0.145	1.17E-04	0.101	2.629	0.113	0.788	0.0348	0.14	7.43E-04	0.0859
Np-Owater-10	2.634	0.0665	0.78	0.0348	0.14	9.94E-04	0.0741	2.54	0.16	0.882	0.041	0.177	1.69E-03	0.0117
Np-Ocarb-23	2.464	0.378	1.022	0.055	0.204	-2.47E-03	0.0669	2.568	0.255	0.902	0.0429	0.158	-8.05E-04	0.0228
Np-Ocarb-24	2.498	0.293	0.988	0.0508	0.188	-1.95E-03	0.0557	2.54	0.243	0.935	0.0456	0.169	-9.77E-04	0.0183
	$[NpO_2(DPA)(H_2O)_4]^-$_C													
	Gas							Aqueous(PCM)						

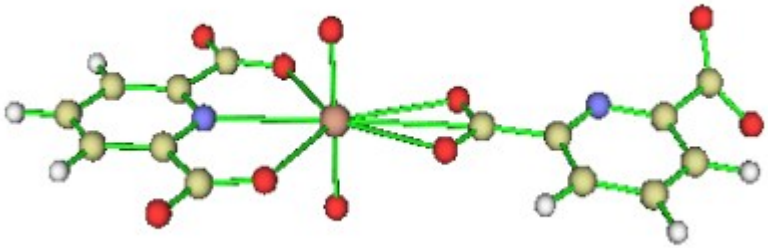
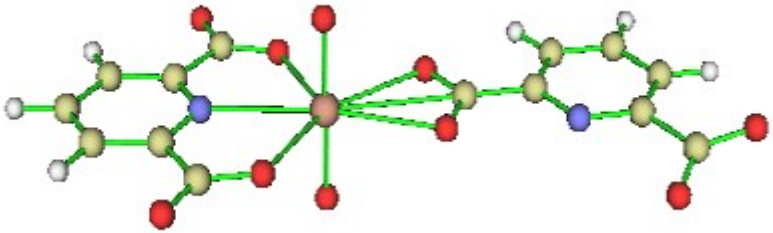
														
∠O-Np-O	174.057							179.163						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-1	1.798	0.984	2.839	0.284	0.224	-0.25	0.00379	1.81	0.571	2.807	0.275	0.246	-0.233	0.000817
Np-Oyl-2	1.805	0.953	2.815	0.279	0.237	-0.24	0.00483	1.81	0.588	2.81	0.275	0.246	-0.232	0.002
Np-Owater-4	2.556	0.119	0.898	0.0434	0.166	-2.45E-04	0.0866	2.652	0.153	0.76	0.0337	0.128	5.56E-04	0.171
Np-Owater-7	4.019		0.0359					2.645	0.15	0.767	0.0339	0.129	6.74E-04	0.307
Np-Owater-10	2.689	0.0756	0.699	0.0326	0.119	-9.74E-05	0.0777	2.782	0.135	0.624	0.243	0.0928	7.26E-04	0.169
Np-Owater-28	2.582	0.107	0.851	0.0419	0.152	-6.49E-04	0.278	2.654	0.187	0.759	0.0339	0.126	4.13E-04	0.226
Np-Ocarb-23	2.354	0.339	1.205	0.065	0.275	-2.11E-03	0.181	2.593	0.252	0.879	0.041	0.146	-8.88E-04	0.179
Np-Ocarb-24	3.782		0.0671					2.6	0.252	0.868	0.0405	0.142	-8.77E-04	0.26
	$[NpO_2(DPA)(H_2O)_2]^-$_N													
	Gas							Aqueous(PCM)						

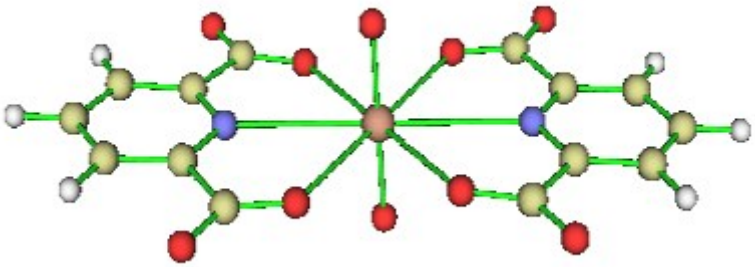
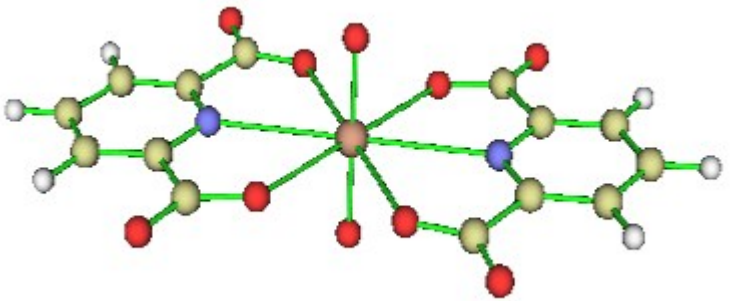
														
∠O-Np-O	175.049							179.065						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-16	1.802	0.431	2.811	0.278	0.223	-0.239	0.00274	1.812	0.455	2.795	0.271	0.237	-0.227	0.00242
Np-Oyl-17	1.803	0.431	2.811	0.278	0.223	-0.239	0.00275	1.812	0.455	2.795	0.271	0.237	-0.227	0.00242
Np-Owater-19	2.688	0.111	0.698	0.0328	0.117	-1.07E-04	0.21	2.658	0.0947	0.751	0.0335	0.123	5.23E-04	0.345
Np-Owater-22	2.688	0.111	0.699	0.0328	0.117	-1.03E-04	0.21	2.658	0.0947	0.751	0.0335	0.123	5.23E-04	0.345
Np-N-6	2.55	0.219	0.916	0.05	0.167	-1.90E-03	0.431	2.593	0.199	0.891	0.0458	0.149	-1.16E-03	0.375
Np-Ocarb-11	2.467	0.246	1.037	0.0517	0.203	-4.20E-04	0.359	2.487	0.236	1.019	0.0493	0.192	-4.24E-05	0.343
Np-Ocarb-14	2.467	0.246	1.037	0.0517	0.203	-4.20E-04	0.359	2.487	0.236	1.019	0.0493	0.192	-4.23E-05	0.343
	$[NpO_2(DPA)(H_2O)_3]^-$_N													
	Gas							Aqueous(PCM)						

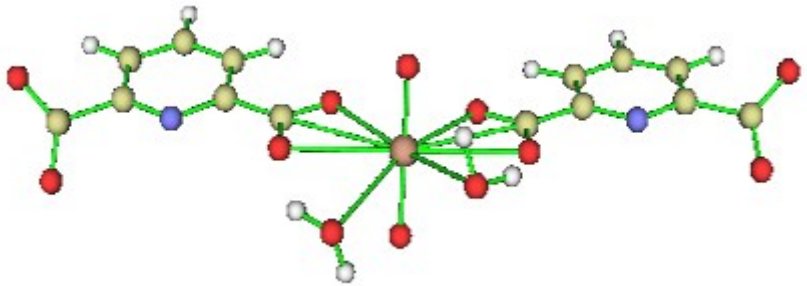
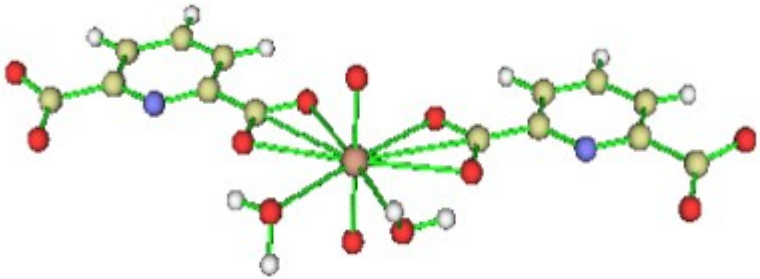
														
∠O-Np-O	175.619							178.896						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-16	1.805	0.497	2.812	0.278	0.239	-0.239	0.00315	1.812	0.549	2.795	0.271	0.238	-0.227	0.00216
Np-Oyl-17	1.814	0.593	2.764	0.271	0.255	-0.226	0.00624	1.81	0.544	2.796	0.272	0.236	-0.228	0.00101
Np-Owater-19	3.616		0.074					4.182		0.0244				
Np-Owater-22	2.678	0.112	0.711	0.0331	0.123	5.32E-05	0.0903	2.647	0.0734	0.765	0.0343	0.127	5.11E-04	0.344
Np-Owater-25	2.586	0.136	0.844	0.0406	0.156	1.23E-04	0.254	2.618	0.105	0.842	0.0367	0.137	5.86E-04	0.286
Np-N-6	2.559	0.218	0.902	0.0493	0.166	-1.89E-03	0.352	2.595	0.207	0.886	0.0456	0.149	-1.13E-03	0.376
Np-Ocarb-11	2.469	0.251	1.06	0.0515	0.206	-4.39E-04	0.225	2.488	0.204	1.036	0.0488	0.192	1.66E-04	0.339
Np-Ocarb-14	2.477	0.255	1.02	0.0508	0.203	-4.32E-04	0.311	2.49	0.229	1.017	0.0489	0.19	-6.05E-06	0.345
	$[NpO_2(DPA)_2(H_2O)]^{3-}$_C_C													
	Gas							Aqueous(PCM)						

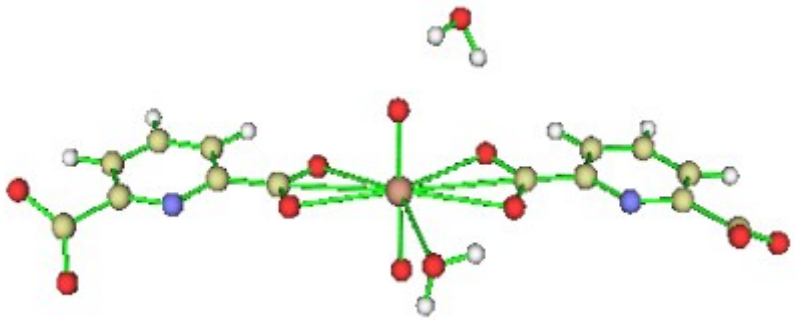
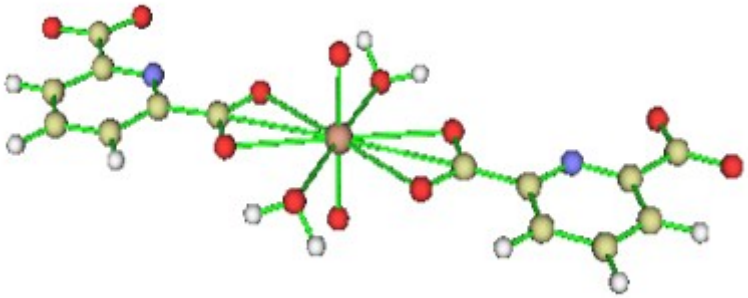
														
∠O-Np-O	176.473							178.51						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.804	0.726	2.83	0.278	0.221	-0.238	0.00842	1.813	0.571	2.793	0.27	0.239	-0.225	0.00374
Np-Oyl-32	1.816	0.703	2.785	0.268	0.242	-0.223	0.00804	1.813	0.568	2.793	0.27	0.239	-0.225	0.00346
Np-Owater-34	2.715	0.206	0.667	0.0311	0.11	-1.98E-04	0.168	2.58	0.219	0.861	0.0378	0.155	1.57E-03	0.189
Np-Ocarb-14	2.588	0.255	0.921	0.0417	0.144	-9.07E-04	0.316	2.569	0.239	0.944	0.0431	0.153	-7.25E-04	0.329
Np-Ocarb-15	2.514	0.345	1.005	0.0487	0.174	-1.32E-03	0.364	2.532	0.297	0.978	0.0467	0.168	-9.38E-04	0.372
Np-Ocarb-26	2.72	0.181	0.736	0.0314	0.105	-6.99E-04	0.252	2.556	0.259	0.951	0.0444	0.158	-8.10E-04	0.338
Np-Ocarb-27	2.534	0.318	0.982	0.464	0.165	-9.87E-04	0.353	2.521	0.298	0.99	0.0478	0.173	-1.06E-03	0.369
	$[NpO_2(DPA)_2(H_2O)]^{3-}$_C_N													
	Gas							Aqueous(PCM)						

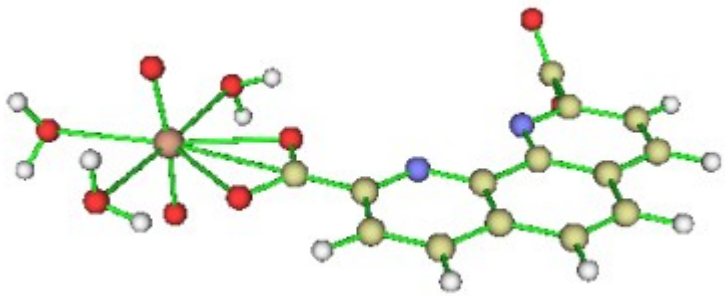
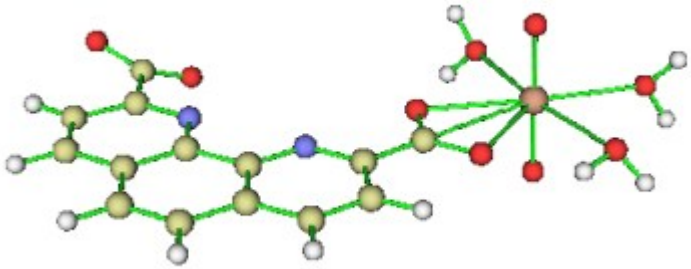
														
∠O-Np-O	178.487							179.472						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.814	0.787	2.81	0.272	0.252	-0.227	0.0012	1.832	0.0881	2.776	0.26	0.28	-0.206	0.00427
Np-Oyl-32	1.817	0.779	2.797	0.269	0.259	-0.222	0.00365	1.832	0.114	2.775	0.26	0.281	-0.206	0.00436
Np-Owater-34	2.636	0.183	0.801	0.0364	0.134	4.02E-05	0.149	2.709	0.11	0.698	0.0297	0.113	4.67E-04	0.0571
Np-N-21	2.665	0.139	0.807	0.0383	0.133	1.68E-04	0.207	2.673	0.191	0.824	0.0379	0.131	-3.78E-05	0.0429
Np-Ocarb-14	3.976		0.0478					2.643	0.242	0.846	0.0361	0.13	-4.52E-04	0.0322
Np-Ocarb-15	2.513	0.273	1.0276	0.0447	0.183	1.01E-03	0.188	2.61	0.285	0.891	0.0394	0.139	-6.18E-04	0.0421
Np-Ocarb-26	2.548	0.253	0.99	0.0425	0.167	4.95E-04	0.329	2.521	0.313	1.021	0.0446	0.18	3.82E-04	0.0284
Np-Ocarb-29	2.577	0.225	0.951	0.0396	0.154	5.54E-04	0.228	2.571	0.221	0.927	0.0402	0.156	5.07E-04	0.0875
	$[NpO_2(DPA)_2]^{3-}$_C_N													
	Gas							Aqueous(PCM)						

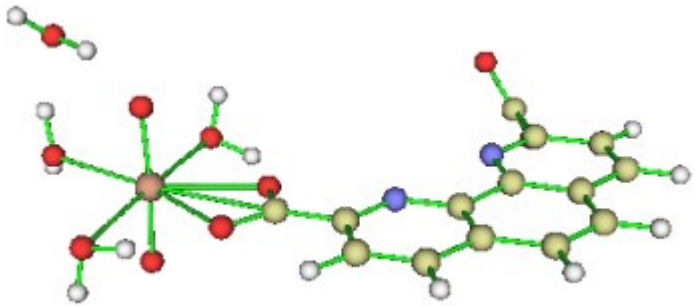
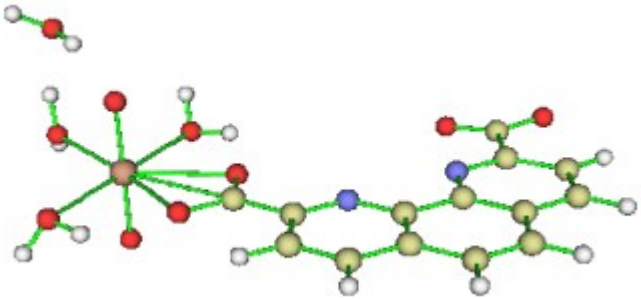
														
∠O-Np-O	178.322							179.645						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.812	0.615	2.813	0.271	0.238	-0.227	0.00374	1.823	0.45	2.777	0.265	0.273	-0.215	0.00541
Np-Oyl-32	1.814	0.607	2.81	0.27	0.24	-0.225	0.00175	1.823	0.451	2.777	0.265	0.273	-0.215	0.00536
Np-N-21	2.666	0.152	0.808	0.038	0.13	2.89E-04	0.354	2.594	0.166	0.875	0.0454	0.158	-1.09E-03	0.132
Np-Ocarb-14	2.671	0.202	0.848	0.0345	0.117	-5.32E-04	0.304	2.579	0.223	0.931	0.042	0.153	-7.12E-04	0.0487
Np-Ocarb-15	2.577	0.278	0.939	0.0423	0.148	-6.76E-04	0.355	2.585	0.232	0.914	0.0421	0.152	-8.32E-04	0.171
Np-Ocarb-26	2.566	0.236	0.976	0.0404	0.156	7.14E-04	0.313	2.46	0.273	1.082	0.0515	0.214	-2.23E-04	0.0369
Np-Ocarb-29	2.559	0.239	0.981	0.0412	0.159	6.70E-04	0.303	2.473	0.263	1.084	0.0507	0.201	-5.97E-05	0.0208
	$[NpO_2(DPA)_2]^{3-}$_N_N													
	Gas							Aqueous(PCM)						

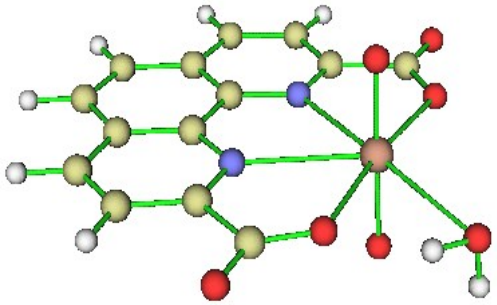
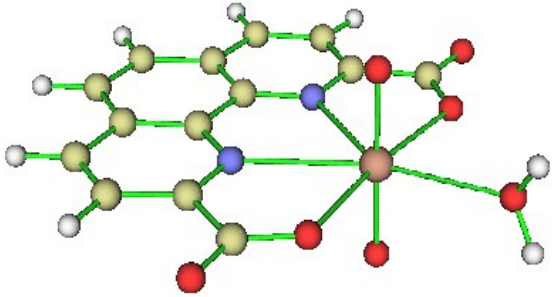
														
∠O-Np-O	179.999							179.999						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.812	0.489	2.819	0.273	0.25	-0.229	0.00327	1.824	0.0985	2.779	0.262	0.253	-0.212	0.000682
Np-Oyl-32	1.812	0.489	2.819	0.273	0.25	-0.229	0.00327	1.824	0.0984	2.779	0.262	0.253	-0.212	0.0007
Np-N-6	2.857	0.131	0.685	0.025	0.0842	8.18E-04	0.119	2.786	0.15	0.747	0.0299	0.0961	4.66E-04	0.299
Np-N-21	2.857	0.131	0.685	0.025	0.0841	8.17E-04	0.119	2.786	0.15	0.747	0.0299	0.0961	4.66E-04	0.298
Np-Ocarb-11	2.683	0.274	0.852	0.0311	0.114	5.73E-04	0.317	2.581	0.305	0.952	0.039	0.148	7.49E-04	0.331
Np-Ocarb-14	2.683	0.274	0.853	0.0311	0.114	5.74E-04	0.317	2.581	0.305	0.952	0.039	0.148	7.49E-04	0.331
Np-Ocarb-26	2.683	0.274	0.852	0.031	0.114	5.74E-04	0.317	2.582	0.305	0.952	0.039	0.148	7.48E-04	0.331
Np-Ocarb-29	2.683	0.274	0.852	0.031	0.114	5.73E-04	0.317	2.581	0.305	0.952	0.039	0.148	7.48E-04	0.331
	$[NpO_2(DPA)_2(H_2O)_2]^{3-}$_lC_C													
	Gas							Aqueous(PCM)						

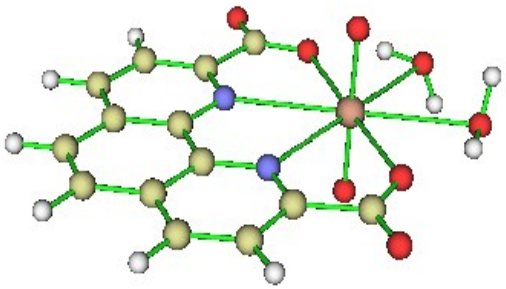
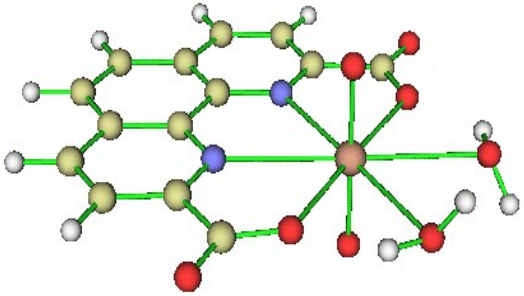
														
∠O-Np-O	174.671							178.603						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.814	0.502	2.797	0.272	0.25	-0.228	0.00351	1.825	0.261	2.786	0.265	0.271	-0.215	0.00419
Np-Oyl-32	1.813	0.49	2.797	0.272	0.249	-0.228	0.00315	1.825	0.256	2.786	0.265	0.271	-0.215	0.00427
Np-Owater-34	2.814	0.238	0.577	0.0251	0.0865	-2.27E-04	0.189	2.666	0.104	0.739	0.0323	0.126	6.18E-04	0.0721
Np-Owater-37	2.807	0.231	0.582	0.0256	0.0875	-2.62E-04	0.214	2.667	0.103	0.739	0.0323	0.126	6.19E-04	0.0711
Np-Ocarb-14	2.701	0.189	0.759	0.0327	0.111	-8.03E-04	0.14	2.605	0.234	0.863	0.0396	0.141	-6.35E-04	0.0564
Np-Ocarb-15	2.542	0.379	0.967	0.0459	0.164	-1.13E-03	0.311	2.576	0.326	0.921	0.0418	0.156	-6.09E-04	0.128
Np-Ocarb-26	2.715	0.181	0.744	0.0317	0.108	-7.81E-04	0.103	2.605	0.234	0.863	0.0396	0.141	-6.35E-04	0.0566
Np-Ocarb-27	2.54	0.379	0.968	0.0462	0.165	-1.15E-03	0.331	2.576	0.326	0.921	0.0418	0.156	-6.10E-04	0.128
	$[NpO_2(DPA)_2(H_2O)_2]^{3-}$_dC_C													
	Gas							Aqueous(PCM)						

														
∠O-Np-O	177.902							179.877						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-31	1.817	0.757	2.774	0.269	0.257	-0.223	0.0114	1.823	0.308	2.784	0.265	0.265	-0.215	0.0031
Np-Oyl-32	1.81	0.665	2.804	0.275	0.245	-0.232	0.0104	1.823	0.308	2.784	0.265	0.265	-0.215	0.00347
Np-Owater-34	2.689	0.2	0.695	0.0322	0.119	1.13E-05	0.106	2.624	0.121	0.79	0.0355	0.139	7.89E-04	0.207
Np-Owater-37	4.008		0.0468					2.626	0.128	0.785	0.0354	0.138	7.87E-04	0.21
Np-Ocarb-14	2.567	0.27	0.941	0.0442	0.155	-1.24E-03	0.32	2.595	0.27	0.895	0.0407	0.146	-6.94E-04	0.176
Np-Ocarb-15	2.498	0.343	1.021	0.051	0.185	-1.80E-03	0.202	2.588	0.25	0.889	0.0413	0.148	-7.45E-04	0.224
Np-Ocarb-26	2.686	0.186	0.763	0.0341	0.116	-8.36E-04	0.248	2.62	0.229	0.854	0.0386	0.137	-6.83E-04	0.202
Np-Ocarb-27	2.562	0.292	0.94	0.0439	0.158	-9.41E-04	0.211	2.574	0.277	0.913	0.0425	0.154	-7.50E-04	0.192
	$[NpO_2(PADA)(H_2O)_3]^-$_C													
	Gas							Aqueous(PCM)						

														
∠O-Np-O	172.998							178.837						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.802	0.712	2.832	0.281	0.231	-0.244	0.00713	1.811	0.762	2.807	0.274	0.246	-0.231	0.00141
Np-Oyl-28	1.807	0.706	2.813	0.277	0.24	-0.237	0.00474	1.81	0.769	2.807	0.274	0.247	-0.231	0.00161
Np-Owater-30	2.6	0.181	0.811	0.0385	0.15	3.29E-04	0.11	2.57	0.229	0.865	0.0394	0.161	1.18E-03	0.142
Np-Owater-33	2.622	0.0592	0.795	0.0354	0.143	1.17E-03	0.109	2.62	0.157	0.819	0.0348	0.141	1.32E-03	0.0999
Np-Owater-36	2.668	0.136	0.717	0.0334	0.127	1.83E-04	0.0497	2.616	0.106	0.796	0.0365	0.141	6.30E-04	0.194
Np-Ocarb-22	2.454	0.387	1.0311	0.0565	0.209	-2.67E-03	0.286	2.533	0.317	0.966	0.0468	0.17	-1.18E-03	0.203
Np-Ocarb-23	2.543	0.264	0.933	0.0463	0.167	-1.52E-03	0.246	2.556	0.247	0.922	0.0445	0.16	-1.08E-03	0.27
	$[NpO_2(PADA)(H_2O)_4]^-$_C													
	Gas							Aqueous(PCM)						

														
∠O-Np-O	175.322							178.575						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.79	0.58	2.842	0.288	0.199	-0.257	0.00434	1.799	0.581	2.82	0.28	0.216	-0.243	0.000777
Np-Oyl-28	1.821	0.692	2.722	0.263	0.258	-0.214	0.00734	1.82	0.634	2.733	0.264	0.254	-0.215	0.00499
Np-Owater-30	2.596	0.154	0.815	0.0388	0.146	4.29E-04	0.287	2.589	0.0974	0.824	0.0386	0.147	7.46E-04	0.371
Np-Owater-33	3.833		0.042					3.886		0.0369				
Np-Owater-36	2.614	0.122	0.777	0.0376	0.141	2.48E-04	0.24	2.623	0.111	0.797	0.0358	0.135	7.18E-04	0.361
Np-Owater-39	2.55	0.134	0.894	0.0418	0.167	9.42E-04	0.165	2.525	0.198	0.927	0.0436	0.177	1.10E-03	0.157
Np-Ocarb-22	2.425	0.382	1.0697	0.0605	0.217	-3.29E-03	0.401	2.529	0.269	0.956	0.0473	0.168	-1.18E-03	0.358
Np-Ocarb-23	2.573	0.261	0.895	0.0432	0.151	-1.16E-03	0.34	2.559	0.274	0.918	0.0442	0.156	-9.08E-04	0.354
	$[NpO_2(PADA)(H_2O)]^-$_N													
	Gas							Aqueous(PCM)						

														
∠O-Np-O	178.507							178.904						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.803	0.567	2.83	0.28	0.236	-0.241	0.00679	1.822	0.546	2.789	0.266	0.264	-0.216	0.00313
Np-Oyl-28	1.813	0.534	2.802	0.273	0.252	-0.229	0.00871	1.823	0.544	2.788	0.265	0.264	-0.216	0.00393
Np-Owater-30	2.698	0.137	0.692	0.0318	0.117	-5.41E-05	0.0901	2.603	0.187	0.839	0.0367	0.147	1.18E-03	0.151
Np-N-19	2.616	0.183	0.852	0.0424	0.151	-4.07E-04	0.192	2.619	0.209	0.869	0.0431	0.145	-8.04E-04	0.261
Np-N-20	2.643	0.156	0.837	0.0399	0.141	-6.22E-05	0.24	2.622	0.207	0.865	0.0428	0.145	-7.73E-04	0.191
Np-Ocarb-22	2.45	0.318	1.108	0.0536	0.215	-5.65E-04	0.253	2.477	0.267	1.076	0.0505	0.2	-1.58E-04	0.311
Np-Ocarb-25	2.543	0.205	0.942	0.0435	0.17	2.21E-04	0.297	2.482	0.262	1.079	0.0499	0.197	-1.26E-04	0.267
	$[NpO_2(PADA)(H_2O)_2]^-$_N													
	Gas							Aqueous(PCM)						

														
∠O-Np-O	179.182							179.692						
	d	MBO	δ	ρb	∇2ρb	Hb	ε	d	MBO	δ	ρb	∇2ρb	Hb	ε
Np-Oyl-27	1.807	0.235	2.82	0.277	0.241	-0.237	0.00554	1.812	0.0605	2.796	0.27	0.239	-0.226	0.00214
Np-Oyl-28	1.807	0.243	2.822	0.277	0.242	-0.236	0.00444	1.812	0.0607	2.796	0.27	0.239	-0.226	0.00216
Np-Owater-30	2.729	0.193	0.661	0.0293	0.107	9.58E-05	0.125	2.714	0.143	0.69	0.0298	0.106	-3.40E-04	0.355
Np-Owater-33	2.743	0.172	0.651	0.0286	0.102	5.27E-06	0.248	2.714	0.142	0.69	0.0298	0.106	-3.39E-04	0.355
Np-N-19	2.72	0.191	0.779	0.0336	0.118	5.30E-04	0.196	2.69	0.207	0.822	0.0369	0.12	2.84E-05	0.361
Np-N-20	2.72	0.191	0.78	0.0337	0.117	4.96E-04	0.233	2.689	0.207	0.822	0.0369	0.12	2.69E-05	0.361
Np-Ocarb-22	2.554	0.226	0.928	0.042	0.164	4.05E-04	0.291	2.524	0.239	0.976	0.045	0.174	3.85E-04	0.334
Np-Ocarb-25	2.553	0.23	0.93	0.0421	0.165	4.15E-04	0.295	2.523	0.239	0.977	0.045	0.175	3.84E-04	0.334

$[NpO_2(H_2O)_5]^+$

Gas: H = -1046.966757 Hartree

G = -1047.034288 Hartree

S = 142.131 Cal/Mol-Kelvin

O	-0.00124000	-0.00011700	-1.77958400
O	0.00023900	0.00045100	1.77959200
Np	-0.00052000	-0.00004400	0.00000100
O	2.16098500	-1.39755400	-0.00022500
H	2.74359800	-1.38577700	0.77757800
H	2.74311100	-1.38591100	-0.77839900
O	-0.66074800	-2.48696200	0.00023100
H	-0.46812300	-3.03756900	0.77757700
H	-0.47072300	-3.03657300	-0.77846100
O	-2.57012800	-0.13832600	0.00054100
H	-3.03508000	-0.48962500	0.77832800
H	-3.03538600	-0.48837200	-0.77762600
O	-0.92283500	2.40218100	-0.00010000
H	-1.39990800	2.73522100	0.77836800
H	-1.40188700	2.73460400	-0.77761300
O	1.99822900	1.62067700	-0.00053800
H	2.16968100	2.17591300	0.77845400
H	2.16704100	2.17939000	-0.77761600

Aqueous: H = -1047.062084 Hartree

G = -1047.125937 Hartree

S = 134.392 Cal/Mol-Kelvin

O	-0.00147300	-0.00095500	-1.79417400
O	-0.00044900	-0.00122300	1.79421700
Np	-0.00022300	-0.00063400	0.00001900
O	1.56432700	-2.02021600	-0.00024400
H	2.13644400	-2.15703300	0.77400600
H	2.13598900	-2.15697900	-0.77484000
O	-1.44327200	-2.10862800	0.00031700
H	-1.39806400	-2.69575700	0.77409900
H	-1.40088700	-2.69388200	-0.77503800
O	-2.45002900	0.72144100	0.00054400
H	-2.99433700	0.49807200	0.77473600
H	-2.99445200	0.49945000	-0.77396400
O	-0.07299600	2.55384500	-0.00032800
H	-0.45241900	3.00199300	0.77470000
H	-0.45505500	3.00155800	-0.77431300
O	2.40645100	0.86018300	-0.00062400
H	2.71256700	1.36044800	0.77494800
H	2.71045300	1.36552100	-0.77373700

$[NpO_2(H_2O)_6]^+$

Gas: H = -1123.384321 Hartree

G = -1123.456688 Hartree

S = 152.308 Cal/Mol-Kelvin

O	-0.00027300	0.00167700	1.79767300
O	0.00030000	-0.00157900	-1.79766000
Np	-0.00001000	-0.00000400	0.00001000

O	2.28703000	-1.26449000	-0.55593100
H	2.34530200	-1.34427100	-1.52409100
H	2.29055500	-2.17819400	-0.21987300
O	2.24008300	1.34246300	0.55665100
H	3.02944800	0.87923600	0.22491800
H	2.33664600	1.35935600	1.52487900
O	-0.04361900	2.61351700	-0.55596900
H	-0.00317000	2.70504300	-1.52408800
H	0.75012600	3.06674200	-0.22054000
O	-2.28702100	1.26451000	0.55579800
H	-2.29051400	2.17818400	0.21967200
H	-2.34517800	1.34438300	1.52395800
O	-2.24005800	-1.34250000	-0.55652100
H	-2.33672700	-1.35941200	-1.52473700
H	-3.02937000	-0.87922500	-0.22471000
O	0.04364600	-2.61353200	0.55587800
H	0.00320600	-2.70528200	1.52397100
H	-0.75012200	-3.06666600	0.22036000

Aqueous: H = -1123.475684 Hartree
G = -1123.546719 Hartree
S = 149.507 Cal/Mol-Kelvin

O	0.26507200	-0.23631100	1.76604700
O	-0.26912300	0.23329200	-1.76274400
Np	0.00006900	-0.00153900	0.00133100
O	0.10394900	-2.62398700	-0.38767300

H	0.55925300	-2.97269900	-1.17200400
H	-0.83354000	-2.87061700	-0.48840600
O	2.56132000	-1.07245400	0.23975600
H	2.99524800	-1.64845200	-0.41209900
H	2.61347200	-1.54733100	1.08630300
O	2.18376400	1.50861900	-0.37689700
H	2.37551600	1.77474500	-1.29198200
H	2.88482400	0.87564100	-0.12588600
O	-0.10330900	2.61802900	0.40144000
H	0.83602000	2.86532400	0.48247700
H	-0.54169700	2.96223400	1.19734500
O	-2.55935400	1.08530600	-0.24382700
H	-2.59563400	1.55976700	-1.09145200
H	-2.98688300	1.67095700	0.40363100
O	-2.18768800	-1.49877100	0.35341700
H	-2.38550300	-1.77780200	1.26338800
H	-2.88458800	-0.85845100	0.10876300

$[NpO_2(PA)(H_2O)_3]$_C

Gas: H = -1330.552683 Hartree

G = -1330.626489 Hartree

S = 155.339 Cal/Mol-Kelvin

C	5.02637900	1.23911800	0.12087800
C	5.82323800	0.09401200	0.00696700
C	5.19008900	-1.14338300	-0.11415800
C	3.79580000	-1.18336100	-0.11551700

C	3.08907600	0.02053500	0.00452300
N	3.69075600	1.21457800	0.12039900
H	5.76943000	-2.05853800	-0.20610400
H	5.48492000	2.22210100	0.21698300
H	6.90656400	0.17732500	0.01339300
H	3.24955700	-2.11527100	-0.20762800
C	1.57936600	0.00153200	0.00563600
O	0.98065700	-1.11994500	-0.09706400
O	0.92708600	1.08145400	0.10589800
O	-1.38289500	0.10803700	-1.78937700
O	-1.39836600	-0.13713000	1.78208100
Np	-1.31705300	-0.01714400	-0.00373400
O	-1.35349800	2.58960700	0.00957400
H	-0.44284300	2.69328400	0.35038100
H	-1.28823700	2.83731900	-0.92810900
O	-1.33237900	-2.61924200	-0.01153400
H	-1.36055500	-2.88743400	0.92202300
H	-0.38985200	-2.68783300	-0.26286200
O	-3.87574200	0.11268000	0.01401100
H	-4.39397200	0.31461000	0.80895900
H	-4.42693700	0.30237000	-0.76128500

Aqueous: H = -1330.594586 Hartree
G = -1330.666741 Hartree
S = 151.863 Cal/Mol-Kelvin

C	5.02039600	-1.33225100	-0.05758300

C	5.83472600	-0.19480400	-0.00258300
C	5.22236900	1.05709000	0.05649300
C	3.82782400	1.12061600	0.05655000
C	3.09955400	-0.07414700	-0.00050000
N	3.68302300	-1.28459700	-0.05607300
H	5.81590900	1.96573900	0.10132000
H	5.46510000	-2.32421500	-0.10511400
H	6.91571700	-0.29638500	-0.00617600
H	3.30445400	2.06880000	0.10034500
C	1.59042500	-0.02881800	-0.00169300
O	1.01202700	1.10455500	0.02572700
O	0.91039700	-1.09994700	-0.02958400
O	-1.36056700	0.07006200	1.80042400
O	-1.36406500	0.08719000	-1.80263300
Np	-1.34178700	0.08551100	-0.00105000
O	-1.40782300	-2.51766200	-0.03505600
H	-0.45902900	-2.72926500	0.04636000
H	-1.84810700	-2.97817200	0.69867800
O	-1.18186200	2.71718600	0.05173100
H	-1.55013400	3.21801100	-0.69535400
H	-0.21285400	2.80867200	-0.01717200
O	-3.79475500	-0.61517900	-0.00367500
H	-4.23393400	-1.01421200	-0.77314000
H	-4.27063300	-0.93510100	0.78081800

$[NpO_2(PA)(H_2O)_3]$_N

Gas: H = -1330.567199 Hartree
G = -1330.640047 Hartree
S = 153.321 Cal/Mol-Kelvin

C	-2.25698100	-1.79520100	0.02979000
C	-3.63559600	-1.99457900	-0.01617000
C	-4.46998500	-0.87484900	-0.06637000
C	-3.89412800	0.39386100	-0.06760900
C	-2.50234800	0.50851000	-0.01719800
N	-1.69816000	-0.57371800	0.03132400
H	-5.54997500	-0.99136200	-0.10504700
H	-1.56908100	-2.63627200	0.06456800
H	-4.03862100	-3.00286100	-0.01448800
H	-4.48224100	1.30403100	-0.10780000
C	-1.83967700	1.88608500	-0.02066300
O	-2.55162400	2.88641500	-0.07402500
O	-0.54760400	1.84844800	0.04241500
O	0.86886700	-0.16487600	-1.78349300
O	1.06248300	-0.13405500	1.81200100
Np	0.88140000	-0.07642000	0.01652900
O	1.08850800	-2.68599500	0.19420900
H	1.44014800	-2.93355900	1.06534500
H	1.62632800	-3.14779000	-0.46903500
O	3.46435500	-0.47716400	-0.45729400
H	3.54804800	-0.11432800	-1.35599600
H	4.12484300	-0.01511600	0.08303800
O	2.00299100	2.31558800	0.13724300

H	2.20909300	2.52341700	1.06315600
H	1.09688600	2.68709100	0.00067600

Aqueous: H = -1330.601111 Hartree
G = -1330.674171 Hartree
S = 153.768 Cal/Mol-Kelvin

C	2.24837800	-1.77226200	-0.01451400
C	3.62855000	-1.98033100	-0.01901000
C	4.47314300	-0.86972600	-0.01317700
C	3.90542200	0.40522900	-0.00355700
C	2.51524100	0.52889700	0.00018000
N	1.69844800	-0.54640300	-0.00495800
H	5.55218900	-0.99312300	-0.01622300
H	1.55484500	-2.60731500	-0.01869500
H	4.02217300	-2.99154700	-0.02685000
H	4.51389900	1.30212900	0.00105000
C	1.84699200	1.89576300	0.01003600
O	2.55468600	2.91665400	0.01358700
O	0.56102700	1.87145700	0.01362800
O	-0.92348100	-0.10801500	1.80908900
O	-0.93595800	-0.10833800	-1.79832800
Np	-0.90484500	-0.08395000	0.00554000
O	-0.91750600	-2.63623200	-0.00368300
H	-1.20320000	-3.14129300	-0.78359700
H	-1.19102800	-3.15385400	0.77234900
O	-3.42004700	-0.53172400	0.00680800

H	-3.98199300	-0.32652600	0.77270700
H	-3.97250300	-0.39258900	-0.78054800
O	-2.03923500	2.27094000	0.03554300
H	-2.58012400	2.53053300	-0.72869700
H	-1.19502500	2.76237700	-0.04486500

$[NpO_2(PA)(H_2O)_4]$_C

Gas: H = -1406.977875 Hartree

G = -1407.055638 Hartree

S = 163.665 Cal/Mol-Kelvin

C	-5.17537800	-1.22014500	-0.09253300
C	-5.97077200	-0.07249000	0.00531800
C	-5.33615700	1.16608100	0.10378700
C	-3.94176000	1.20488100	0.09899800
C	-3.23648500	-0.00128700	-0.00450700
N	-3.83977800	-1.19663900	-0.09796700
H	-5.91434900	2.08309600	0.18319600
H	-5.63504800	-2.20418500	-0.17019500
H	-7.05415500	-0.15490400	0.00441500
H	-3.39509100	2.13798300	0.17489900
C	-1.72645000	0.01435400	-0.01289900
O	-1.12341500	1.13342100	0.07462300
O	-1.07888400	-1.06839900	-0.10340800
O	1.26933400	0.08397300	-1.80100400
O	1.24215100	-0.07627100	1.80198600
Np	1.20492200	-0.00019200	0.00021000

O	0.99737900	-2.72859900	0.19725600
H	0.05906700	-2.68040700	-0.08037800
H	0.95701600	-2.85138600	1.16070400
O	3.39507800	-1.46445900	-0.29680900
H	3.79976300	-1.23055300	-1.14770600
H	2.97402400	-2.33459700	-0.42522900
O	3.42486000	1.42503100	0.33351200
H	3.82389700	1.16331400	1.17900800
H	3.02412600	2.30107000	0.48084500
O	1.04321000	2.71422200	-0.21966900
H	1.05206000	2.81737600	-1.18628500
H	0.09372200	2.64782200	0.01208500

Aqueous: H = -1407.014009 Hartree
G = -1407.093399 Hartree
S = 167.089 Cal/Mol-Kelvin

C	5.23848500	-1.20817500	0.07183400
C	6.01233300	-0.04356900	0.00552800
C	5.35601700	1.18509400	-0.06696800
C	3.96002000	1.19926600	-0.07000100
C	3.27360200	-0.01950100	-0.00067600
N	3.90025800	-1.20758100	0.06933500
H	5.91713700	2.11370400	-0.12009100
H	5.71776300	-2.18342600	0.12952000
H	7.09624600	-0.10698000	0.01102500
H	3.40392500	2.12801300	-0.12492600

C	1.76235200	-0.02946600	-0.00240000
O	1.14501300	1.08158600	-0.06284300
O	1.12540000	-1.12376200	0.05583800
O	-1.21629000	0.06078500	1.80845200
O	-1.22661500	-0.06140300	-1.80888700
Np	-1.20887400	0.00004100	-0.00024700
O	-1.07780600	-2.67983300	-0.09632300
H	-0.11299900	-2.74003900	0.04393300
H	-1.22324400	-3.04925800	-0.98419900
O	-3.46251500	-1.38458100	0.17597900
H	-4.10214800	-1.09699500	0.84896400
H	-3.20603700	-2.28924300	0.42752700
O	-3.43945200	1.41989500	-0.16701200
H	-4.08574400	1.14312900	-0.83816300
H	-3.16948300	2.32069600	-0.41832200
O	-1.03435200	2.67935300	0.09546200
H	-1.16598900	3.04932700	0.98524800
H	-0.06988200	2.72214400	-0.05212500

$[NpO_2(PA)(H_2O)_4]$_N

Gas: H = -1406.983437 Hartree

G = -1407.061197 Hartree

S = 163.659 Cal/Mol-Kelvin

C	-2.44494700	-1.75901600	-0.03371600
C	-3.83463900	-1.86033100	-0.08896900
C	-4.59103600	-0.68648700	-0.11770600

C	-3.92927600	0.53965200	-0.09449000
C	-2.53318700	0.55461200	-0.04711700
N	-1.80267600	-0.57903900	-0.01296300
H	-5.67634500	-0.72787800	-0.15920700
H	-1.81700100	-2.64502200	-0.00836000
H	-4.30552300	-2.83857100	-0.10850600
H	-4.45404600	1.48840500	-0.11363100
C	-1.77998000	1.87862200	-0.03467500
O	-2.41093800	2.93107700	0.03122000
O	-0.48831700	1.75904000	-0.09542500
O	0.85842900	-0.51656700	-1.79711100
O	0.91236900	-0.12191200	1.79091500
Np	0.81030600	-0.24116500	-0.00969300
O	0.52969900	-2.81577400	0.67668800
H	0.51512000	-2.69788500	1.64250300
H	1.40477900	-3.19109200	0.47591500
O	3.05313900	-1.76920100	-0.24738500
H	3.18285600	-1.71980500	-1.21021900
H	3.84829100	-1.38204400	0.15487400
O	1.38021200	3.66994800	0.34406300
H	1.32575900	4.05139500	1.23288600
H	0.52205400	3.19122600	0.19347800
O	2.69250000	1.48064000	-0.36681600
H	2.37365200	2.35219600	0.01799900
H	2.80227800	1.66035900	-1.31469500

Aqueous: H = -1407.031045 Hartree
G = -1407.109774 Hartree
S = 165.699 Cal/Mol-Kelvin

C	-2.46046000	-1.76275300	-0.05282900
C	-3.85222500	-1.86853900	-0.06180100
C	-4.61219800	-0.69896100	-0.02768900
C	-3.95172000	0.52960700	0.01320400
C	-2.55584100	0.54896800	0.02074900
N	-1.82050800	-0.58269300	-0.01110000
H	-5.69739600	-0.74185600	-0.03374200
H	-1.83300300	-2.64807900	-0.07994400
H	-4.31941800	-2.84739200	-0.09538300
H	-4.49225500	1.46858500	0.03880300
C	-1.79816800	1.86583800	0.06055400
O	-2.43299000	2.93195100	0.06510800
O	-0.51155600	1.76538200	0.08747200
O	0.81267500	-0.27015000	-1.80825800
O	0.85391800	-0.37593400	1.81120900
Np	0.82435400	-0.29771800	0.00257900
O	0.71051800	-2.85945000	0.01704000
H	0.67115800	-3.42106700	0.80906700
H	0.78696900	-3.45721300	-0.74535300
O	3.29338200	-1.21580300	-0.00733000
H	3.84065200	-0.98957400	-0.77839200
H	3.38264300	-2.17749000	0.10308600
O	2.59683000	1.56386300	0.01118800

H	3.20272600	1.54793900	0.77012200
H	2.23081300	2.49066700	-0.03398700
O	1.19346000	3.86719900	-0.04125900
H	1.16128300	4.32804000	-0.89504800
H	0.39827700	3.27261300	-0.01586500

$[NpO_2(PA)_2(H_2O)]^-$_ C_C

Gas: H = -1614.030988 Hartree

G = -1614.112874 Hartree

S = 172.344 Cal/Mol-Kelvin

C	-6.02831900	2.13252600	-0.17922400
C	-7.03159800	1.16196600	-0.09790100
C	-6.64338100	-0.17506100	0.01848100
C	-5.28313500	-0.47589200	0.04813700
C	-4.35173000	0.57135100	-0.03997100
N	-4.72017800	1.85724600	-0.15214700
H	-7.38693700	-0.96661600	0.08548700
H	-6.29025900	3.18691600	-0.27083700
H	-8.07995600	1.44984700	-0.12494700
H	-4.91428300	-1.49149000	0.13864100
C	-2.86525000	0.23843400	-0.00393800
O	-2.55501000	-0.98982300	0.10409100
O	-2.01339100	1.16603400	-0.07837200
C	6.54718900	-0.05862200	-0.08950100
C	6.97563000	1.27228400	-0.08278700
C	6.00382900	2.27523100	-0.04668900

C	4.66094000	1.90437800	-0.01921600
C	4.33233800	0.53946900	-0.02719100
N	5.26228900	-0.42814900	-0.06219600
H	6.28785300	3.32540900	-0.04019500
H	7.27483100	-0.86993100	-0.11801100
H	8.03671000	1.50901600	-0.10518900
H	3.85784100	2.63230900	0.00827100
C	2.86415500	0.13562200	0.00473500
O	2.01241300	1.07514200	0.00558800
O	2.55307800	-1.08783700	0.03126500
O	-0.01006900	-0.35913800	1.87001300
O	-0.05490600	-0.58736200	-1.73016200
Np	-0.04368400	-0.42915400	0.07286800
O	0.61724000	-3.00802900	-0.25256500
H	1.55133800	-2.72827500	-0.14901300
H	0.45180800	-2.94155700	-1.20898700

Aqueous: H = -1614.122431 Hartree
G = -1614.207221 Hartree
S = 178.455 Cal/Mol-Kelvin

C	-5.21311900	2.95317100	0.01513000
C	-6.42275500	2.24942600	0.01055000
C	-6.37741000	0.85519500	-0.00961900
C	-5.13133500	0.22608800	-0.02245400
C	-3.97498500	1.01681000	-0.01640300
N	-4.01239000	2.36142900	0.00111200

H	-7.29170500	0.26843200	-0.01458400
H	-5.21132700	4.04134300	0.03096500
H	-7.36703200	2.78541400	0.02259400
H	-5.04214500	-0.85406500	-0.03680600
C	-2.61398200	0.35262200	-0.02625300
O	-2.56202300	-0.91924800	-0.00630000
O	-1.55848700	1.05575800	-0.05105300
C	6.28695000	0.78813000	-0.05470500
C	6.45985200	2.17563700	0.00415600
C	5.32318200	2.98288400	0.05785000
C	4.06787700	2.37235800	0.04914100
C	3.99661600	0.97456900	-0.00882800
N	5.08873200	0.19091800	-0.05958900
H	5.41031800	4.06473300	0.10536300
H	7.15159500	0.12872300	-0.09904900
H	7.45832700	2.60234200	0.00764000
H	3.15441600	2.95447400	0.08822300
C	2.64451800	0.29313500	-0.01231100
O	1.60085300	1.02239500	-0.03685200
O	2.56551700	-0.97201800	0.01238200
O	-0.00866000	-0.91913000	1.81308200
O	0.00721700	-1.01437200	-1.80755900
Np	-0.00032400	-0.93862900	0.00215700
O	-0.01487500	-3.49000500	0.07615800
H	-0.14420800	-4.03016200	0.87302300
H	-0.13127000	-4.08231900	-0.68500100

$[NpO_2(PA)_2(H_2O)]^-$_ C_N

Gas: H = -1614.039223 Hartree

G = -1614.119340 Hartree

S = 168.621 Cal/Mol-Kelvin

C	-5.98995400	0.13041400	0.00477700
C	-6.29294500	1.49550800	-0.00418300
C	-5.23162400	2.40342500	-0.01169000
C	-3.92891900	1.90849300	-0.00953100
C	-3.72769500	0.51935600	-0.00262400
N	-4.74490900	-0.35677000	0.00464700
H	-5.41621400	3.47553400	-0.01910000
H	-6.79012000	-0.60980300	0.01183600
H	-7.32753100	1.82996300	-0.00531400
H	-3.06309400	2.56075600	-0.01385800
C	-2.30484900	-0.02591400	-0.00445000
O	-1.36257000	0.82378400	0.04017100
O	-2.11752800	-1.27137100	-0.05266500
C	1.29254000	2.58716100	0.09339000
C	2.04181300	3.76346900	0.12499700
C	3.43647200	3.66778200	0.10051600
C	4.02435900	2.40590200	0.04631100
C	3.20292900	1.27300700	0.01954400
N	1.86028000	1.37224200	0.04276400
H	4.05272000	4.56444200	0.12360200
H	0.20608600	2.59629300	0.10750600

H	1.53969300	4.72633400	0.16710100
H	5.09846100	2.25706400	0.02458300
C	3.80792300	-0.13900700	-0.03607300
O	5.04530300	-0.22798400	-0.04891200
O	2.94662300	-1.08282900	-0.05983200
O	0.53060100	-0.82389700	-1.84415400
O	0.51657300	-1.09702400	1.75954700
Np	0.54229500	-0.91724400	-0.04580400
O	-0.42310400	-3.41380400	0.24314700
H	-0.29544800	-3.36900400	1.20658900
H	-1.31306300	-3.02875700	0.10062400

Aqueous: H = -1614.143272 Hartree
G = -1614.221973 Hartree
S = 165.639 Cal/Mol-Kelvin

C	5.94944200	0.14162200	0.03862500
C	6.25645800	1.50695600	0.02734900
C	5.20373200	2.42178700	-0.00514800
C	3.89490800	1.93650300	-0.02491800
C	3.68799200	0.55114200	-0.00951500
N	4.69899700	-0.33549900	0.02167000
H	5.39585200	3.49097100	-0.01445200
H	6.74548600	-0.60003900	0.06280300
H	7.29158400	1.83451400	0.04388400
H	3.04343000	2.60672800	-0.05044900
C	2.27761400	-0.00020300	-0.02381700

O	1.30885100	0.82297300	-0.07328100
O	2.08111500	-1.25141500	0.01766800
C	-1.25298700	2.58502900	-0.05160300
C	-1.97940800	3.77720700	-0.03520900
C	-3.37281800	3.71208600	0.00250600
C	-3.98604700	2.45845200	0.02120300
C	-3.18815700	1.31224500	0.00246300
N	-1.84021600	1.37685000	-0.03280300
H	-3.97062300	4.61898700	0.01734700
H	-0.16821500	2.58369700	-0.07873800
H	-1.45717500	4.72860000	-0.05085900
H	-5.06424000	2.35039600	0.05028400
C	-3.80639400	-0.08129900	0.02360000
O	-5.04836200	-0.18445400	0.04384900
O	-2.97070600	-1.05272300	0.01658200
O	-0.51716800	-0.83638400	1.81738400
O	-0.53789500	-1.05858400	-1.81592100
Np	-0.53602400	-0.94313500	0.00097900
O	0.46431000	-3.43378200	0.10166600
H	0.28452700	-4.02340200	-0.64905700
H	1.39096400	-3.14252100	-0.00064700

$[NpO_2(PA)_2(H_2O)]^-$_N_N

Gas: H = -1614.048421 Hartree

G = -1614.126996 Hartree

S = 165.373 Cal/Mol-Kelvin

C	-2.29508200	2.22620000	-0.03236000
C	-3.50477700	2.92147400	-0.05220200
C	-4.69626500	2.19133600	-0.03127700
C	-4.63613800	0.79915700	0.00607200
C	-3.38478700	0.17410800	0.02141600
N	-2.24136700	0.88514300	0.00406500
H	-5.65725500	2.70161600	-0.04488900
H	-1.33309600	2.73380300	-0.04746100
H	-3.50425200	4.00744600	-0.08328200
H	-5.52188100	0.17353900	0.02238100
C	-3.27417400	-1.35732200	0.05013000
O	-4.32580600	-2.01202500	0.06610700
O	-2.07188100	-1.80356500	0.04700500
C	3.55141400	-1.25225200	0.11440200
C	4.93428400	-1.07319000	0.10993400
C	5.43344100	0.23058700	0.03231800
C	4.53536300	1.29317400	-0.03480600
C	3.16033000	1.02812500	-0.02440200
N	2.68567200	-0.23011000	0.04686200
H	6.50623000	0.41193400	0.02644000
H	3.11380500	-2.24675800	0.17660500
H	5.59551400	-1.93342400	0.16729400
H	4.85335400	2.32832100	-0.09373200
C	2.14339500	2.18176300	-0.08823100
O	2.60120000	3.33361400	-0.14794700
O	0.91710800	1.82354200	-0.07114500

O	0.05121400	-0.43301000	1.84600800
O	0.06041000	-0.55497900	-1.77081900
Np	0.02056300	-0.43908600	0.04114800
O	0.22213900	-3.10954900	-0.37516600
H	0.22621600	-2.92760700	-1.33182100
H	-0.73825100	-3.13030000	-0.15307200

Aqueous: H = -1614.137434 Hartree
G = -1614.214862 Hartree
S = 162.960 Cal/Mol-Kelvin

C	-2.23232300	2.26170000	-0.01480700
C	-3.42163100	2.99313600	-0.02229100
C	-4.63377100	2.30229900	-0.01763700
C	-4.61037500	0.90694000	-0.00582500
C	-3.37919500	0.24859000	0.00116000
N	-2.20660300	0.91837700	-0.00316300
H	-5.57869700	2.83804400	-0.02313700
H	-1.26287200	2.74990100	-0.01804800
H	-3.38819900	4.07790200	-0.03146600
H	-5.52163400	0.32008000	-0.00187100
C	-3.30282200	-1.27188500	0.01453600
O	-4.35862200	-1.93011000	0.01783900
O	-2.11353400	-1.75440400	0.02163800
C	3.58669100	-1.18664300	0.00952600
C	4.96588200	-0.97115500	0.00428300
C	5.43472500	0.34372500	-0.00391100

C	4.50970800	1.38886500	-0.00598500
C	3.14616900	1.08731900	-0.00010800
N	2.69497900	-0.18356500	0.00741200
H	6.50086800	0.55148600	-0.00845100
H	3.18002500	-2.19469100	0.01615300
H	5.64708600	-1.81587800	0.00643800
H	4.82104200	2.42708800	-0.01208700
C	2.08817700	2.18431500	-0.00168000
O	2.45914800	3.37348900	-0.00875100
O	0.87294900	1.77543100	0.00487000
O	0.04112100	-0.51892800	1.81955800
O	0.04650000	-0.52358500	-1.80702400
Np	0.03818800	-0.50383600	0.00651500
O	0.08040800	-3.18928500	0.01704100
H	0.40114900	-3.62460600	-0.78983700
H	-0.90010600	-3.20036000	-0.03827700

$[NpO_2(PA)_2(H_2O)_2]^-$_ lC_C

Gas: H = -1690.441392 Hartree

G = -1690.527922 Hartree

S = 182.118 Cal/Mol-Kelvin

C	-6.32278100	1.12184800	-0.05358400
C	-6.39745100	2.51683000	0.00264800
C	-5.20208300	3.23670000	0.07390100
C	-3.99868300	2.53454700	0.08570900
C	-4.02931100	1.13205100	0.02588500

N	-5.17495300	0.43542300	-0.04295200
H	-5.20863000	4.32370700	0.11884400
H	-7.23337200	0.52491900	-0.11036600
H	-7.36289600	3.01721000	-0.00974800
H	-3.03562400	3.03010800	0.13890700
C	-2.71038700	0.37041800	0.03744100
O	-1.65170700	1.05939000	0.09299500
O	-2.71449700	-0.89227300	-0.00652800
C	5.15890400	3.17905900	-0.03413800
C	6.40004300	2.53466100	-0.03947900
C	6.41345500	1.13797700	-0.04031400
C	5.19704200	0.45786800	-0.03442600
C	4.00248000	1.19600000	-0.02972000
N	3.98586200	2.53825300	-0.03028000
H	7.35363700	0.59029900	-0.04533800
H	5.10528700	4.26797600	-0.03320600
H	7.32113300	3.11270400	-0.04324900
H	5.14032200	-0.62473900	-0.03477000
C	2.67043600	0.45360400	-0.02311000
O	2.72826200	-0.81998900	0.01214100
O	1.59573000	1.09762200	-0.05673000
O	-0.06613300	-0.95008700	-1.80198200
O	0.05561900	-0.98477800	1.80603000
Np	-0.00949700	-0.89478800	0.00235100
O	-1.42500300	-3.22207800	-0.25635000
H	-2.22362500	-2.65263100	-0.25868800

H	-1.20453100	-3.36524900	-1.19065200
O	1.47924500	-3.18475400	0.26690800
H	2.23582500	-2.56105000	0.29319200
H	1.21720600	-3.31750400	1.19230700

Aqueous: H = -1690.545771 Hartree
G = -1690.633438 Hartree
S = 184.510 Cal/Mol-Kelvin

C	6.23815300	1.15636200	0.00140900
C	6.32532400	2.55299000	0.00496600
C	5.14070900	3.29007000	0.00699700
C	3.92534400	2.60362800	0.00513000
C	3.93977300	1.20280700	0.00097200
N	5.07862500	0.48693100	-0.00074700
H	5.16098400	4.37627800	0.00982500
H	7.14190000	0.54998600	-0.00002300
H	7.29580200	3.04009100	0.00603500
H	2.97752800	3.12941600	0.00658400
C	2.63045000	0.44055100	-0.00330500
O	1.54669800	1.10092000	0.00542500
O	2.63066100	-0.82874800	-0.01702400
C	-5.04475300	3.24315300	-0.02280000
C	-6.29293600	2.61232100	0.02805600
C	-6.32884800	1.21804100	0.05928900
C	-5.12210300	0.51659600	0.03871800
C	-3.92175000	1.23713800	-0.01127700

N	-3.88117100	2.58144600	-0.04215800
H	-7.27547200	0.68642200	0.09919100
H	-4.97929300	4.32920600	-0.04857400
H	-7.20382200	3.20320200	0.04268700
H	-5.09681400	-0.56674300	0.06166500
C	-2.60006500	0.49620100	-0.02920300
O	-2.62398200	-0.77800700	-0.00594300
O	-1.50960100	1.13454500	-0.06195300
O	-0.02538100	-0.90209100	1.81528600
O	0.02623700	-1.04595200	-1.81990300
Np	0.00154700	-0.95436800	-0.00308600
O	1.41712500	-3.21694700	0.03304800
H	2.28886500	-2.78665900	0.12300300
H	1.31450800	-3.78614700	0.81331800
O	-1.44329900	-3.18561500	0.02900600
H	-2.30951400	-2.75461600	-0.09923000
H	-1.32417100	-3.78686800	-0.72436600

$[NpO_2(PA)_2(H_2O)_2]^-$_ dC_C

Gas: H = -1690.442760 Hartree

G = -1690.531520 Hartree

S = 186.811 Cal/Mol-Kelvin

C	-6.51144900	1.16376900	-0.24872500
C	-7.25530600	-0.01688700	-0.16248100
C	-6.56173400	-1.22062400	-0.01387000
C	-5.16984600	-1.18772000	0.03912000

C	-4.51375000	0.05044500	-0.05270600
N	-5.17592100	1.20982100	-0.19394100
H	-7.09618500	-2.16552700	0.05921400
H	-7.01577100	2.12310800	-0.36690300
H	-8.34132800	0.01180600	-0.21004500
H	-4.57085200	-2.08470600	0.15069200
C	-2.99131100	0.08086500	0.01088500
O	-2.39582200	-1.03425900	0.04168500
O	-2.38990400	1.19110900	0.03874100
C	6.53675000	-1.10004700	-0.25114900
C	7.25694400	0.09426000	-0.15289800
C	6.53917100	1.28307700	0.00079200
C	5.14796900	1.22254800	0.04666300
C	4.51660300	-0.02756400	-0.05626700
N	5.20216500	-1.17268600	-0.20246500
H	7.05460000	2.23774800	0.08300400
H	7.06030800	-2.04843600	-0.37397600
H	8.34352700	0.08717900	-0.19539800
H	4.53124300	2.10708500	0.16078300
C	2.99456300	-0.08887400	0.00136100
O	2.37765000	1.01515700	0.01897200
O	2.41670000	-1.21040200	0.03839700
O	-0.00354500	-0.07998100	1.91572900
O	-0.00814600	0.04472100	-1.69552800
Np	-0.00580400	-0.01371600	0.11909000
O	-0.14459100	2.65839100	-0.13373200

H	-1.11422400	2.56848100	-0.23676300
H	0.21928600	2.69481300	-1.03276000
O	0.18668500	-2.67690300	-0.21354100
H	1.15958500	-2.56627900	-0.25549200
H	-0.11794000	-2.73179300	-1.13299700

Aqueous: H = -1690.534245 Hartree
G = -1690.621495 Hartree
S = 183.633 Cal/Mol-Kelvin

C	-6.78761900	-0.26546000	-0.08407600
C	-7.33216100	-1.55437900	-0.06536400
C	-6.45833400	-2.64107200	-0.01764100
C	-5.08462900	-2.39467900	0.00880400
C	-4.63458700	-1.06819200	-0.01286600
N	-5.47228400	-0.01688100	-0.05836000
H	-6.83694300	-3.65924600	-0.00120800
H	-7.43939500	0.60534600	-0.12116200
H	-8.40883700	-1.69345700	-0.08751400
H	-4.36427300	-3.20374100	0.04593200
C	-3.14715600	-0.78040200	0.01578100
O	-2.34359700	-1.76636000	0.05201700
O	-2.72640200	0.41521500	0.00601000
C	6.33198700	-0.28955800	0.04885000
C	6.87727200	0.99829300	-0.00317700
C	6.00409500	2.08564200	-0.04375200
C	4.62974300	1.84138700	-0.03000300

C	4.17937800	0.51606500	0.02342600
N	5.01628500	-0.53617600	0.06175400
H	6.38340400	3.10279600	-0.08495300
H	6.98346900	-1.16068300	0.08165300
H	7.95430800	1.13587200	-0.01118800
H	3.91022700	2.65150800	-0.05927400
C	2.69270700	0.22896200	0.04106100
O	1.88693200	1.21240800	0.02005200
O	2.27195400	-0.96539200	0.07890100
O	-0.26032900	-0.24695800	1.87619800
O	-0.23699200	-0.31601200	-1.75079200
Np	-0.25201200	-0.28174300	0.06308500
O	-0.57677100	2.31855600	0.03857500
H	-1.20701700	2.64563000	-0.62432200
H	0.30314800	2.64010600	-0.22817400
O	0.33781100	-2.83767500	0.12977200
H	1.28502900	-2.82532400	-0.09904100
H	-0.10418900	-3.38330600	-0.54126300

$[NpO_2(PA)_2(H_2O)_2]^-$_ lC_N

Gas: H = -1690.452914 Hartree

G = -1690.538580 Hartree

S = 180.299 Cal/Mol-Kelvin

C	6.06066200	-0.01901200	0.05271400
C	6.40541100	1.33425900	-0.01766400
C	5.37232000	2.27140200	-0.09040800

C	4.05538400	1.81570500	-0.08808200
C	3.81101900	0.43528500	-0.01657100
N	4.80155900	-0.46856800	0.05266200
H	5.58953200	3.33592400	-0.14737200
H	6.83761600	-0.78142700	0.11153000
H	7.44956800	1.63761400	-0.01538300
H	3.21056000	2.49279300	-0.14119500
C	2.37193600	-0.06940200	-0.01690100
O	1.45336400	0.80484400	-0.02669500
O	2.15100600	-1.30735100	-0.01305700
C	-0.83354600	2.77676500	0.05138800
C	-1.38825400	4.05794000	0.05183900
C	-2.77929300	4.18640400	0.03881400
C	-3.55734000	3.03105000	0.02593600
C	-2.92220700	1.78388400	0.03043100
N	-1.58157900	1.66196900	0.04286300
H	-3.24642000	5.16928000	0.03767300
H	0.23969100	2.61612500	0.05601600
H	-0.73815400	4.92893900	0.06090200
H	-4.64159400	3.05260300	0.01225600
C	-3.74915500	0.49655200	0.01763600
O	-4.98399200	0.59451300	-0.02741600
O	-3.04920800	-0.57482100	0.05777100
O	-0.48754200	-0.99268500	1.79779600
O	-0.62163200	-0.83861200	-1.80663000
Np	-0.55905900	-0.87453200	-0.00335100

O	0.48797000	-3.38999900	0.07096300
H	1.37287400	-2.98184500	0.16648700
H	0.19204900	-3.62033400	0.96572400
O	-2.28932800	-3.02805600	-0.12081300
H	-2.99555500	-2.33806500	-0.10293300
H	-2.18431000	-3.28161700	-1.05092000

Aqueous: H = -1690.551395 Hartree
G = -1690.637297 Hartree
S = 180.797 Cal/Mol-Kelvin

C	-6.02509300	-0.02856300	0.01200600
C	-6.37409200	1.32659700	0.01339400
C	-5.34969800	2.27369700	0.01003700
C	-4.02652600	1.82899300	0.00567100
C	-3.77662800	0.45053500	0.00502600
N	-4.76018500	-0.46698000	0.00788700
H	-5.57459700	3.33657200	0.01094200
H	-6.79824800	-0.79447500	0.01435600
H	-7.41898400	1.62202900	0.01701400
H	-3.19560600	2.52501600	0.00310900
C	-2.34864900	-0.05627700	0.00160400
O	-1.40806100	0.79876400	-0.00244000
O	-2.11134300	-1.29885100	0.00560300
C	0.82786500	2.79139100	-0.02526600
C	1.38764800	4.07125300	-0.02433200
C	2.77673100	4.19696900	-0.01136600

C	3.55091900	3.03634700	0.00015600
C	2.91228400	1.79399700	-0.00387000
N	1.56822400	1.66974000	-0.01630400
H	3.24742200	5.17603000	-0.00994400
H	-0.24631300	2.64624200	-0.03260600
H	0.74040900	4.94266100	-0.03326200
H	4.63419500	3.07160000	0.01152400
C	3.72065000	0.50668200	0.00536900
O	4.96349900	0.57165500	0.03557100
O	3.02575400	-0.57150600	-0.02202300
O	0.52928600	-0.94746500	-1.81927400
O	0.55419100	-0.83665200	1.81587600
Np	0.54446700	-0.87867500	-0.00196800
O	-0.45046900	-3.36230800	0.04715600
H	-1.37993100	-3.13153600	-0.13785000
H	-0.15030300	-3.92476200	-0.68503300
O	2.26323600	-3.02524400	-0.02276600
H	3.01405200	-2.39661600	0.05884300
H	2.25502300	-3.55218600	0.79266900

$[NpO_2(PA)_2(H_2O)_2]^-$_ dC_N

Gas: H = -1690.457400 Hartree

G = -1690.542457 Hartree

S = 179.018 Cal/Mol-Kelvin

C	-6.01762200	1.21638900	0.06196100
C	-7.03980400	0.28151500	0.25224900

C	-6.68766000	-1.06819900	0.32858200
C	-5.34343200	-1.41620400	0.21056200
C	-4.38908100	-0.40204400	0.02842100
N	-4.72410500	0.89552700	-0.04527200
H	-7.44667000	-1.83378700	0.47633300
H	-6.25045700	2.27925300	-0.00586000
H	-8.07427600	0.60580000	0.33737300
H	-5.00490600	-2.44511600	0.25573600
C	-2.91296200	-0.78462100	-0.09096500
O	-2.66826400	-2.02675200	-0.14413000
O	-2.06435500	0.14513500	-0.12864000
C	3.00310900	-2.19314400	0.04207400
C	4.26630700	-2.77974900	0.12627600
C	5.38570500	-1.94668700	0.20416600
C	5.19722800	-0.56649700	0.19850400
C	3.89614600	-0.05671700	0.11779700
N	2.82068000	-0.86303600	0.03610800
H	6.38664300	-2.36817400	0.27060800
H	2.09753800	-2.79078500	-0.02279500
H	4.36209500	-3.86214800	0.13143500
H	6.01879600	0.13899800	0.25730300
C	3.65654000	1.45833400	0.13049200
O	4.64905500	2.19993900	0.15102600
O	2.42203600	1.79803300	0.12137500
O	0.33900900	0.10020300	1.76438800
O	0.48279200	0.48167400	-1.82830000

Np	0.40938100	0.32024800	-0.02122700
O	0.08508600	2.97027800	-0.08755000
H	-0.13469600	3.10715900	-1.02277600
H	1.06784100	3.03361700	-0.03483900
O	-0.08563100	-2.17286900	-0.63092900
H	-0.06102900	-2.06364700	-1.59586700
H	-1.07395300	-2.23105000	-0.40706700

Aqueous: H = -1690.536373 Hartree
G = -1690.621745 Hartree
S = 179.681 Cal/Mol-Kelvin

C	-6.26333200	0.85391200	-0.11137000
C	-6.96481800	-0.35434300	-0.03208400
C	-6.23401200	-1.53804800	0.07310600
C	-4.84013500	-1.46490200	0.09274100
C	-4.22754400	-0.20754700	0.01185000
N	-4.92737700	0.93703000	-0.08862900
H	-6.73705700	-2.49877900	0.13813900
H	-6.80109500	1.79626700	-0.19614800
H	-8.05045400	-0.35857400	-0.05255700
H	-4.22775400	-2.35579400	0.17152100
C	-2.71535100	-0.10629600	0.03672400
O	-2.04215400	-1.18641000	0.04397500
O	-2.15086200	1.02335600	0.05602900
C	3.18434200	-2.12821300	0.13138900
C	4.50126100	-2.59230500	0.15311600

C	5.54013200	-1.66597700	0.06231800
C	5.21826100	-0.31208900	-0.03410200
C	3.87430900	0.06877700	-0.03956800
N	2.86613100	-0.82629600	0.03147900
H	6.57718300	-1.98920100	0.07155600
H	2.35125600	-2.81861900	0.20031200
H	4.69644600	-3.65661700	0.23827000
H	5.98189300	0.45438400	-0.09900300
C	3.48452100	1.53669600	-0.10218700
O	4.37805400	2.39523200	-0.22821500
O	2.22815100	1.77028500	-0.00469100
O	0.34073300	0.03615500	1.82426700
O	0.26612900	0.34246600	-1.78294200
Np	0.30483800	0.20287400	0.02226000
O	-0.09841500	2.80517300	0.32708500
H	-0.74176000	3.15729200	-0.30904800
H	0.79237600	3.08741700	0.03840800
O	0.22822500	-2.42822600	-0.43289500
H	0.44390600	-2.63925000	-1.35663400
H	-0.75084800	-2.42320500	-0.38746700

$[NpO_2(PA)_2(H_2O)_2]^-$_ lN_N

Gas: H = -1690.458296 Hartree

G = -1690.543559 Hartree

S = 179.451 Cal/Mol-Kelvin

C	5.08153600	-0.82725000	0.01375500

C	6.22568100	-0.04093800	-0.12549000
C	6.06377000	1.34492000	-0.21225800
C	4.77747500	1.87641900	-0.15869400
C	3.68109000	1.01147600	-0.02670700
N	3.84125400	-0.32154500	0.06034500
H	6.92759900	1.99757400	-0.31997400
H	5.15578000	-1.91123000	0.08870600
H	7.20834000	-0.50352500	-0.16353200
H	4.58182600	2.94139500	-0.21568100
C	2.25858000	1.59723900	0.01547200
O	2.16547300	2.83920200	0.03817100
O	1.31434300	0.75063900	0.01484500
C	-1.38826700	2.58815300	0.03448900
C	-2.17878800	3.73927700	0.05341300
C	-3.56844000	3.60188400	0.03482200
C	-4.11750100	2.32105800	-0.00332200
C	-3.26015100	1.21649600	-0.02131400
N	-1.91998800	1.35411800	-0.00230000
H	-4.21283100	4.47881000	0.04965900
H	-0.30236100	2.64591700	0.04848000
H	-1.70259400	4.71528900	0.08273200
H	-5.18677800	2.14033300	-0.01962800
C	-3.82813600	-0.20586500	-0.06545200
O	-5.05863300	-0.34431200	-0.09526400
O	-2.93781000	-1.13018000	-0.07230100
O	-0.51496600	-0.87041700	1.82476700

O	-0.36690000	-0.99563300	-1.78919400
Np	-0.46604300	-0.86883600	0.01467800
O	1.75754700	-2.20282900	0.49525600
H	2.44652000	-1.50523700	0.31491900
H	1.64157100	-2.20296800	1.45979200
O	-1.53094600	-3.33218600	-0.27764700
H	-2.39840000	-2.86585000	-0.20566600
H	-1.37150100	-3.40828000	-1.23256000

Aqueous: H = -1690.555975 Hartree
G = -1690.639338 Hartree
S = 175.453 Cal/Mol-Kelvin

C	-3.56941100	-1.17958100	-0.00602000
C	-4.95583400	-1.01976300	0.02557800
C	-5.47850200	0.27352000	0.07016400
C	-4.59595000	1.35463600	0.08455000
C	-3.22153700	1.10933400	0.05228500
N	-2.71756100	-0.14161100	0.00487100
H	-6.55200900	0.43725900	0.09504900
H	-3.11895500	-2.16704300	-0.03663800
H	-5.60137800	-1.89212400	0.01558700
H	-4.94808200	2.37899900	0.12145500
C	-2.21268000	2.25121300	0.07633100
O	-2.63408100	3.42304600	0.10969100
O	-0.98058700	1.89627700	0.06234000
C	2.11571400	2.50703700	0.05486500

C	3.27855200	3.27987400	0.06934700
C	4.51416500	2.63244300	0.04204000
C	4.54051600	1.23750700	0.00298800
C	3.33285600	0.53689900	-0.00817500
N	2.13816800	1.16446200	0.01624800
H	5.43937800	3.20139400	0.05182500
H	1.12949700	2.96027200	0.07495700
H	3.20720900	4.36237300	0.10147700
H	5.47233900	0.68431700	-0.01741700
C	3.31158400	-0.98309100	-0.03998900
O	4.38669900	-1.60590600	-0.03601600
O	2.13862400	-1.51595100	-0.06289800
O	-0.05831600	-0.24912700	-1.86027400
O	-0.05594300	-0.46476200	1.76219200
Np	-0.05090200	-0.33798900	-0.04762700
O	-0.74112000	-2.82142000	-0.26372700
H	-0.90927200	-3.06995500	-1.18795700
H	-0.00938600	-3.42811800	0.04108400
O	1.53237400	-4.11422300	0.39772200
H	1.97285500	-3.23190800	0.27298700
H	1.64938800	-4.34612600	1.33301700

$[NpO_2(PA)_2(H_2O)_2]^-$_ dN_N

Gas: H = -1690.461351 Hartree

G = -1690.547366 Hartree

S = 181.033 Cal/Mol-Kelvin

C	-2.45212000	-2.05114900	-0.41385700
C	-3.69894600	-2.65719500	-0.56755900
C	-4.84104500	-1.85399500	-0.52233100
C	-4.69591800	-0.48119600	-0.32750900
C	-3.41149600	0.05167400	-0.18146700
N	-2.31447900	-0.72931300	-0.22725900
H	-5.82983400	-2.29339300	-0.63567300
H	-1.53044300	-2.62683000	-0.43692400
H	-3.76380700	-3.73166100	-0.71203600
H	-5.54070000	0.19726500	-0.28217700
C	-3.20979800	1.55756200	0.03677300
O	-4.21442400	2.27977000	0.05829500
O	-1.98414000	1.91608900	0.17449500
C	3.48447100	1.40484200	0.18442300
C	4.86847500	1.31375900	0.03885200
C	5.42016400	0.07586200	-0.30363800
C	4.57170800	-1.01465100	-0.48156800
C	3.19353500	-0.84119000	-0.30947400
N	2.66711100	0.35478200	0.01540000
H	6.49526100	-0.03463500	-0.42758400
H	3.00415300	2.34544200	0.44529700
H	5.49069500	2.19138300	0.19029900
H	4.93284700	-2.00232800	-0.74609200
C	2.23503200	-2.03050900	-0.47349500
O	2.72695700	-3.11909100	-0.79564400
O	1.00006300	-1.77259700	-0.22919800

O	0.11144500	0.77062000	-1.71641100
O	-0.04360100	0.16979100	1.85715100
Np	0.00685100	0.44073500	0.06165700
O	0.39202700	3.11006100	0.04209700
H	-0.57697900	3.17284500	0.21585700
H	0.44445100	3.10016700	-0.92982000
O	0.07948900	-2.72486600	2.46826500
H	0.46957400	-2.81001000	1.57914900
H	-0.02769000	-1.75597000	2.54129800

Aqueous: H = -1690.547909 Hartree
G = -1690.633095 Hartree
S = 179.290 Cal/Mol-Kelvin

C	-3.39631800	-1.62836000	-0.12717300
C	-4.79121200	-1.65345700	-0.17195000
C	-5.48346900	-0.44259000	-0.13461900
C	-4.75309000	0.74420100	-0.06387800
C	-3.35853600	0.68244800	-0.02816900
N	-2.68848500	-0.48931400	-0.05152200
H	-6.56897500	-0.42232600	-0.16422500
H	-2.82161200	-2.54782100	-0.16109600
H	-5.31246500	-2.60319200	-0.23453400
H	-5.23849100	1.71305700	-0.03921800
C	-2.52475000	1.95202000	0.02329500
O	-3.09838800	3.05273500	0.08548400
O	-1.24838100	1.77855600	-0.00885300

C	2.81260200	1.90273200	-0.07241500
C	4.12635900	2.37417200	-0.10933600
C	5.17033100	1.44875300	-0.11881600
C	4.86087200	0.08793800	-0.08877700
C	3.52080200	-0.30249500	-0.05175400
N	2.51141600	0.59265700	-0.04579200
H	6.20472700	1.77890200	-0.14789000
H	1.97733100	2.59796900	-0.06102700
H	4.31595800	3.44274400	-0.12953100
H	5.63202400	-0.67348800	-0.09273100
C	3.13059500	-1.77272700	-0.01174300
O	4.02577500	-2.63633100	-0.01566400
O	1.86693400	-1.99628800	0.02553800
O	-0.03411300	-0.44464800	-1.78876200
O	0.00236500	-0.26536500	1.82746000
Np	-0.00831200	-0.34543500	0.01840600
O	-0.54659200	-2.92792400	0.24500600
H	-0.82274600	-3.19811700	1.13708400
H	0.41602200	-3.12846700	0.19907100
O	0.17946500	4.16677900	0.13799200
H	-0.44007800	4.90546300	0.24306700
H	-0.39081600	3.36142500	0.08687300

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

Gas: H = Hartree

G = Hartree

S = Cal/Mol-Kelvin

Aqueous: H = -1974.054737 Hartree
G = -1974.150959 Hartree
S = 202.517 Cal/Mol-Kelvin

C	-5.90509200	-2.93607500	-0.06678200
C	-6.95915500	-2.01643600	-0.04537900
C	-6.64882300	-0.65660800	-0.00124500
C	-5.30585600	-0.27700000	0.01902700
C	-4.31870000	-1.27155000	-0.00374000
N	-4.61309000	-2.58361400	-0.04575300
H	-7.43485100	0.09328400	0.01671600
H	-6.10980000	-4.00447700	-0.10235900
H	-7.98817500	-2.36287000	-0.06311500
H	-5.01251200	0.76590800	0.05220700
C	-2.85262800	-0.87405600	0.01836800
O	-2.57098100	0.36509900	0.03186500
O	-1.94922700	-1.75929200	0.02126200
O	0.00202400	0.01568800	1.83783800
O	-0.01342100	-0.02860400	-1.80538500
Np	-0.00500700	-0.00564900	0.01623100
C	0.39829800	6.56750400	-0.02616600
C	1.72016600	7.02586400	-0.02239600
C	2.74710800	6.08110200	-0.01483800
C	2.41046500	4.72661200	-0.01143400
C	1.05699600	4.36349500	-0.01573300

N	0.06355100	5.27067300	-0.02296200
H	3.78848900	6.39107700	-0.01174600
H	-0.42796500	7.27608100	-0.03209600
H	1.92995300	8.09129600	-0.02539400
H	3.16998200	3.95339700	-0.00562800
C	0.67397000	2.89410000	-0.01182600
O	1.60816100	2.03261400	-0.00472900
O	-0.54454600	2.55301300	-0.01466300
C	5.51135600	-3.59622200	-0.06308500
C	5.26100500	-4.97242700	-0.03858600
C	3.93405600	-5.40172200	0.00721100
C	2.92031200	-4.44249900	0.02549700
C	3.26912500	-3.08548900	-0.00069800
N	4.54711500	-2.66696500	-0.04381300
H	3.69235700	-6.46081500	0.02802000
H	6.53392200	-3.22502900	-0.09980000
H	6.08542900	-5.67902800	-0.05491100
H	1.87419300	-4.72424000	0.05975600
C	2.17807100	-2.02914600	0.01789900
O	0.96866500	-2.41916000	0.02625500
O	2.47902100	-0.80018100	0.02255800

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

Gas: H = -1973.770432 Hartree

G = -1973.868592 Hartree

S = 206.594 Cal/Mol-Kelvin

C	6.81149000	-0.15285900	-0.00120600
C	7.17596900	-1.50197100	-0.00304400
C	6.15036600	-2.45408300	-0.00387900
C	4.82968900	-2.01409100	-0.00282800
C	4.56216900	-0.63152100	-0.00097800
N	5.54661900	0.28364300	-0.00019300
H	6.37981600	-3.51897100	-0.00531600
H	7.58097100	0.62189700	-0.00050600
H	8.22548000	-1.79159400	-0.00379100
H	3.98235700	-2.69147100	-0.00336000
C	3.09538700	-0.17386500	0.00019700
O	2.23888300	-1.10882000	-0.00032400
O	2.81760200	1.04565400	0.00156600
O	0.11525800	0.43290400	1.80262000
O	0.11536800	0.43623800	-1.79970500
Np	0.14419800	0.43936500	0.00146000
C	-3.09568100	-5.50255500	-0.00253200
C	-4.48239900	-5.32794900	-0.00104800
C	-4.97235100	-4.01800500	0.00096900
C	-4.06198400	-2.96449500	0.00132900
C	-2.68149900	-3.23891800	-0.00029800
N	-2.21173200	-4.49875100	-0.00218900
H	-6.04428900	-3.82471800	0.00221400
H	-2.67131900	-6.50847900	-0.00415300
H	-5.14916600	-6.18828900	-0.00145300
H	-4.37477100	-1.92656900	0.00284700

C	-1.68623400	-2.06446100	0.00009200
O	-2.21172500	-0.90589100	0.00125000
O	-0.46285500	-2.29438600	-0.00070100
C	-3.45380800	1.75294000	-0.00250900
C	-4.52698100	2.64772300	-0.00541100
C	-4.25387200	4.01961800	-0.00587500
C	-2.92469200	4.43382700	-0.00341300
C	-1.90667200	3.46768300	-0.00058100
N	-2.17232700	2.15082000	-0.00012700
H	-5.06448900	4.74843800	-0.00812900
H	-3.59728500	0.67702300	-0.00209600
H	-5.54816800	2.27140400	-0.00729000
H	-2.62982100	5.47796300	-0.00356100
C	-0.42708300	3.88793200	0.00219900
O	-0.20139800	5.12095600	0.00258700
O	0.39530400	2.92993900	0.00386200

Aqueous: H = -1974.056920 Hartree
G = -1974.151502 Hartree
S = 199.066 Cal/Mol-Kelvin

C	-6.69928200	0.20199800	-0.00059700
C	-7.12093700	1.53580000	-0.00127600
C	-6.14790100	2.53618800	-0.00154400
C	-4.80327400	2.16224700	-0.00108400
C	-4.47724400	0.79915100	-0.00034900
N	-5.41208400	-0.16867000	-0.00013500

H	-6.42917800	3.58574300	-0.00209800
H	-7.43034500	-0.60448600	-0.00034800
H	-8.18021100	1.77503600	-0.00159900
H	-4.00941600	2.90031900	-0.00127700
C	-3.01788300	0.37465300	0.00007800
O	-2.13136400	1.28373900	-0.00000700
O	-2.71114000	-0.85122600	0.00049100
O	-0.09130000	-0.36889100	1.82167100
O	-0.09127300	-0.36971700	-1.82071300
Np	-0.10004800	-0.37161900	0.00048200
C	3.24691200	5.34197500	-0.00040100
C	4.63192100	5.14455000	-0.00000600
C	5.11213800	3.83442800	0.00051300
C	4.19274200	2.78429700	0.00060600
C	2.82307400	3.08084600	0.00016500
N	2.35560900	4.34237200	-0.00032900
H	6.17986700	3.63314500	0.00083900
H	2.83631800	6.35000200	-0.00081700
H	5.30619800	5.99576200	-0.00010300
H	4.51639600	1.74989000	0.00101000
C	1.80606900	1.95253800	0.00026700
O	2.24393100	0.75744400	0.00087800
O	0.57053700	2.20251700	-0.00023000
C	3.32503500	-1.97708300	-0.00148400
C	4.31215200	-2.96578600	-0.00252500
C	3.92140700	-4.30514000	-0.00241100

C	2.55795000	-4.60023800	-0.00127500
C	1.63552600	-3.54981300	-0.00028100
N	2.01011200	-2.25456900	-0.00036400
H	4.66074900	-5.10137000	-0.00320100
H	3.58107500	-0.92397300	-0.00155800
H	5.36018000	-2.68198200	-0.00340400
H	2.19375800	-5.62127600	-0.00116100
C	0.13816500	-3.81989700	0.00093200
O	-0.25472600	-5.00808700	0.00134700
O	-0.60663600	-2.78508900	0.00140700

$[NpO_2(PA)_3^{2-}$_C_N_N

Gas: H = -1973.796069 Hartree

G = -1973.890829 Hartree

S = 199.439 Cal/Mol-Kelvin

C	4.17098900	0.03090000	-0.10916200
C	5.51088000	-0.35949200	-0.03433900
C	5.80767700	-1.72079000	0.08400900
C	4.75510400	-2.63229300	0.11926200
C	3.43783800	-2.15620400	0.03947000
N	3.15579800	-0.84739300	-0.07010400
H	6.84132200	-2.06198500	0.14578700
H	3.86961700	1.07009500	-0.20940100
H	6.29491700	0.39391100	-0.06948600
H	4.90254500	-3.70375600	0.20561700
C	2.24938500	-3.13017100	0.07009700

O	2.52804600	-4.34980300	0.13679600
O	1.11071000	-2.58222100	0.01807800
C	-1.84005800	3.08582800	0.39186800
C	-2.17165900	4.43275200	0.56885200
C	-1.16093600	5.39178100	0.44787700
C	0.13305500	4.96473300	0.15827900
C	0.37621500	3.59165200	0.00129000
N	-0.59525100	2.67324700	0.11376400
H	-1.38076200	6.45134100	0.57806500
H	-2.57771200	2.29160700	0.46407100
H	-3.19781900	4.71493400	0.79612800
H	0.96899800	5.64785800	0.04934300
C	1.78727800	3.07563700	-0.30507800
O	2.68952100	3.93491300	-0.44639300
O	1.89257300	1.81710300	-0.37964400
C	-5.95015200	-2.60951100	0.59046900
C	-6.81680700	-1.88106700	-0.22848600
C	-6.28358300	-0.80518000	-0.94690800
C	-4.93046900	-0.51162000	-0.80389600
C	-4.13233900	-1.31593800	0.03208900
N	-4.64265000	-2.35415500	0.71667200
H	-6.91468300	-0.20626900	-1.60216000
H	-6.32722400	-3.45073300	1.17509000
H	-7.86922900	-2.14981700	-0.29818200
H	-4.46010700	0.32049000	-1.31686700
C	-2.63738300	-0.99546200	0.14992100

O	-2.33161200	0.22662600	-0.02193400
O	-1.82497900	-1.91597000	0.36074000
O	0.17194100	-0.31496100	-1.83239100
O	0.52308500	-0.03141900	1.75737300
Np	0.34968200	-0.20029100	-0.03586100

Aqueous: H = -1974.068183 Hartree
G = -1974.164712 Hartree
S = 203.163 Cal/Mol-Kelvin

C	-4.18106500	-0.09125300	-0.16199900
C	-5.48767400	-0.55090200	-0.34767600
C	-5.71227600	-1.92700400	-0.40819600
C	-4.62014400	-2.78566600	-0.28099900
C	-3.34519100	-2.23921600	-0.10248100
N	-3.12502600	-0.91190100	-0.04268900
H	-6.71436100	-2.32258300	-0.55032800
H	-3.95073400	0.96657400	-0.09655900
H	-6.30330000	0.16004500	-0.43988000
H	-4.73235000	-3.86331000	-0.31779800
C	-2.11950300	-3.12964200	0.03412600
O	-2.28117400	-4.37198100	0.03004200
O	-1.00575000	-2.52151700	0.14446100
C	1.76936900	3.10942100	-0.34171200
C	2.06619200	4.46338500	-0.52031100
C	1.03577900	5.39713600	-0.40211900
C	-0.24862500	4.93761900	-0.11008800

C	-0.45752400	3.56369000	0.04660400
N	0.53438800	2.65972100	-0.06589500
H	1.22790800	6.45850900	-0.53373500
H	2.53677300	2.34689300	-0.41450700
H	3.08350300	4.76913700	-0.74556000
H	-1.08799700	5.61548400	-0.00469100
C	-1.83992100	3.00957300	0.35366000
O	-2.77617900	3.81576200	0.55386900
O	-1.93093900	1.73776700	0.37964400
C	5.74647700	-2.88870800	-0.14622600
C	6.75625400	-1.92727300	-0.03242800
C	6.38228300	-0.58770500	0.08096500
C	5.02329400	-0.26944900	0.07698000
C	4.08298000	-1.30213900	-0.04080200
N	4.43971100	-2.59487700	-0.15181400
H	7.13205300	0.19355400	0.17138400
H	6.00103400	-3.94316600	-0.23666200
H	7.80011900	-2.22664200	-0.03333800
H	4.68277600	0.75576700	0.16485500
C	2.59712700	-0.97702200	-0.04189200
O	2.25955600	0.24383000	0.07983400
O	1.74273800	-1.89454800	-0.15606100
O	-0.19621500	-0.18659400	1.91946500
O	-0.44015800	-0.05383000	-1.72403200
Np	-0.32560200	-0.12861300	0.09795000

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

Gas: H = -1973.799076 Hartree

G = -1973.892297 Hartree

S = 196.202 Cal/Mol-Kelvin

C	-3.89664500	-0.62333500	0.00076200
C	-5.12218400	-1.29764400	-0.00135300
C	-5.12025500	-2.69563300	-0.00379900
C	-3.89600200	-3.36162200	-0.00403500
C	-2.71497800	-2.60588600	-0.00185900
N	-2.71814300	-1.26402100	0.00049300
H	-6.05646700	-3.25389900	-0.00549600
H	-3.82348600	0.46124900	0.00273400
H	-6.05033800	-0.73011600	-0.00109400
H	-3.81284300	-4.44356000	-0.00586800
C	-1.34506900	-3.28728000	-0.00212700
O	-1.32089000	-4.54042700	-0.00424200
O	-0.35666800	-2.49469200	-0.00010800
C	1.40826000	3.68596000	-0.00257500
C	1.43696400	5.08442800	-0.00656300
C	0.22532300	5.78171400	-0.00782400
C	-0.96360200	5.05450900	-0.00501800
C	-0.89956000	3.65388700	-0.00107500
N	0.26413700	2.98569800	0.00012000
H	0.20997200	6.87163900	-0.01093300
H	2.31084900	3.08016100	-0.00139900
H	2.39251800	5.60448300	-0.00862900

H	-1.94224200	5.52330500	-0.00576500
C	-2.17480200	2.80838200	0.00217600
O	-3.27197600	3.41435100	0.00148200
O	-1.98273900	1.55610100	0.00546400
C	2.48774100	-3.06248100	-0.00305300
C	3.68427800	-3.78690600	-0.00437700
C	4.89421200	-3.08655100	-0.00347700
C	4.85930600	-1.69330500	-0.00133400
C	3.61447300	-1.04803400	-0.00014500
N	2.45383200	-1.72150500	-0.00095600
H	5.84560000	-3.61856200	-0.00442100
H	1.51156900	-3.54084200	-0.00360200
H	3.65669800	-4.87447300	-0.00604900
H	5.75495700	-1.08065600	-0.00053800
C	3.51986400	0.47915200	0.00217000
O	4.59314400	1.12647600	0.00240700
O	2.33933100	0.93897000	0.00361000
O	0.00062300	-0.00214100	1.80348000
O	-0.00010100	0.00222700	-1.79902400
Np	0.00015800	-0.00003200	0.00225700

Aqueous: H = -1974.057266 Hartree
G = -1974.148574 Hartree
S = 192.175 Cal/Mol-Kelvin

C	2.42451300	3.14792500	0.00152200
C	2.83786500	4.48351800	0.00114800

C	1.86708700	5.48640000	-0.00038400
C	0.52280500	5.11221100	-0.00137500
C	0.20074700	3.75124200	-0.00066500
N	1.13365600	2.78181800	0.00068700
H	2.14996700	6.53561200	-0.00079700
H	3.13424900	2.32738000	0.00251800
H	3.89723400	4.72260800	0.00199700
H	-0.27486600	5.84642700	-0.00262800
C	-1.24317100	3.27947000	-0.00125400
O	-2.15711400	4.13492800	-0.00359100
O	-1.40694700	2.01473200	0.00089600
C	1.51572900	-3.67657500	-0.00267000
C	2.46643100	-4.70167700	-0.00420900
C	3.82016700	-4.36145400	-0.00454900
C	4.16750400	-3.00987700	-0.00335700
C	3.14905900	-2.05142300	-0.00180600
N	1.84342600	-2.37550000	-0.00141500
H	4.58788400	-5.13053700	-0.00569000
H	0.45018100	-3.88145300	-0.00241200
H	2.14458300	-5.73891200	-0.00499900
H	5.20198800	-2.68546500	-0.00361900
C	3.46011600	-0.56454600	-0.00016500
O	4.65713200	-0.19847400	-0.00084900
O	2.44488700	0.20725600	0.00194200
C	-3.94419800	0.52281700	-0.00304300
C	-5.30691300	0.21028900	-0.00517400

C	-5.68743600	-1.13272300	-0.00427500
C	-4.68915600	-2.10771800	-0.00115000
C	-3.35038300	-1.70330800	0.00071900
N	-2.97980300	-0.40998200	-0.00027700
H	-6.73694500	-1.41447300	-0.00590200
H	-3.59056200	1.54863400	-0.00347000
H	-6.04514000	1.00681500	-0.00749900
H	-4.92332300	-3.16620000	-0.00019600
C	-2.21729700	-2.71512800	0.00414800
O	-2.49762700	-3.93516300	0.00775500
O	-1.04178200	-2.22082800	0.00315600
O	0.00142900	0.00178600	1.82215600
O	0.00150900	0.00203000	-1.81994400
Np	0.00054900	0.00202600	0.00114800

$[NpO_2(DPA)(H_2O)_3]^-$_C

Gas: H = -1518.591458 Hartree

G = -1518.673020 Hartree

S = 171.661 Cal/Mol-Kelvin

O	2.05599800	0.05349200	1.79885700
O	1.94091300	-0.39444000	-1.77573600
Np	1.88109500	-0.17269400	0.01396200
O	2.40582100	2.45061500	-0.00397200
H	1.46933100	2.58646100	-0.26541000
H	2.39305800	2.59409600	0.95754800
O	1.28441300	-2.72064700	0.09443100

H	1.25817100	-3.02288400	-0.82845800
H	0.34444200	-2.53714800	0.31015200
O	4.51211400	-0.07594600	-0.05960800
H	4.83065900	0.39453100	-0.84678700
H	4.88894700	0.37633600	0.71151100
C	-4.55600400	-0.01044000	-0.00821600
C	-5.04970500	1.31046800	-0.08558100
C	-4.16228800	2.37684800	-0.18561200
C	-2.79011500	2.11280600	-0.16747700
C	-2.38689200	0.77654900	-0.05958600
N	-3.23867100	-0.26052500	0.00031600
H	-4.52582200	3.40031500	-0.26631400
H	-6.12557000	1.44548800	-0.05475000
H	-2.04886600	2.90245400	-0.23096700
C	-0.92431600	0.45390700	-0.01645100
O	-0.51470400	-0.73911000	0.12287400
O	-0.05574400	1.39969600	-0.12279800
C	-5.57840800	-1.18451200	0.06903100
O	-5.17779700	-2.30258400	-0.31909800
O	-6.70965100	-0.82972500	0.50706700

Aqueous: H = -1518.716972 Hartree
G = -1518.795530 Hartree
S = 165.340 Cal/Mol-Kelvin

O	1.94577000	-0.07909900	1.80649300
O	1.93718400	-0.27454600	-1.79289700

Np	1.91976700	-0.18005000	0.00697100
O	2.40997800	2.37715700	-0.15634300
H	1.50630400	2.73719200	-0.08299900
H	2.92237700	2.79397000	0.55644400
O	1.30625900	-2.73205900	0.15669500
H	1.57907600	-3.31553700	-0.57102600
H	0.33676000	-2.64521300	0.08159000
O	4.44139000	0.12531000	0.00749800
H	4.95811500	0.38797400	-0.77238000
H	4.95178800	0.40770000	0.78463000
C	-4.61073600	0.02560100	-0.00449200
C	-5.08827100	1.34812100	0.00275500
C	-4.17808900	2.40290800	-0.01478200
C	-2.81333800	2.11221800	-0.02451600
C	-2.42339800	0.76739100	-0.01715300
N	-3.29831800	-0.25087300	-0.01405400
H	-4.52301500	3.43340600	-0.01837300
H	-6.15769300	1.52188600	0.01973800
H	-2.06365400	2.89502100	-0.03543600
C	-0.95505000	0.41792900	-0.01303000
O	-0.57472600	-0.78952400	0.06352300
O	-0.09854700	1.35970700	-0.08463900
C	-5.61176600	-1.15078300	-0.00393200
O	-5.15874200	-2.30538700	-0.22611400
O	-6.81809700	-0.83855300	0.21813700

$[NpO_2(DPA)(H_2O)_2]^-$_N

Gas: H = -1442.240329 Hartree

G = -1442.308184 Hartree

S = 142.812 Cal/Mol-Kelvin

C	2.16941100	1.16498800	0.05129900
C	3.56602100	1.20458900	0.05301000
C	4.27000000	-0.00021100	0.00012000
C	3.56592600	-1.20495100	-0.05268500
C	2.16931400	-1.16525500	-0.05045200
N	1.50387400	-0.00012800	0.00069100
H	5.35816100	-0.00024800	-0.00001200
H	4.05781600	2.17046600	0.09538600
H	4.05763400	-2.17085300	-0.09550900
C	1.31678600	-2.43515900	-0.10284700
O	0.04945900	-2.20868300	-0.09480700
O	1.88696400	-3.53179900	-0.14353000
C	1.31702700	2.43499500	0.10334600
O	0.04967300	2.20855000	0.09748600
O	1.88728500	3.53167300	0.14166400
O	-1.12246900	0.07488000	-1.79934900
O	-1.12555200	-0.07472000	1.79912800
Np	-1.04615900	0.00006800	-0.00008300
O	-2.57843800	-2.19476400	0.24638900
H	-1.75110500	-2.69122900	0.03945900
H	-2.60423300	-2.17971500	1.21798900
O	-2.57771100	2.19468800	-0.24784600

H	-2.60223000	2.18238800	-1.21956500
H	-1.75094700	2.69118700	-0.03868200

Aqueous: H = -1442.339414 Hartree
G = -1442.407399 Hartree
S = 143.088 Cal/Mol-Kelvin

C	2.19701300	-1.16214700	-0.00980000
C	3.59341600	-1.20349300	-0.01018800
C	4.30046000	0.00002100	0.00008400
C	3.59340500	1.20353000	0.01026200
C	2.19700300	1.16217000	0.00980500
N	1.52302100	0.00000800	-0.00001100
H	5.38658600	0.00002600	0.00009800
H	4.09728400	-2.16324200	-0.01851200
H	4.09726400	2.16328200	0.01858300
C	1.34339100	2.42192500	0.02071500
O	0.07668600	2.20617300	0.02020500
O	1.89995800	3.53333000	0.02914500
C	1.34342100	-2.42191500	-0.02081100
O	0.07671200	-2.20620100	-0.02028500
O	1.90002000	-3.53330600	-0.02928100
O	-1.08518700	-0.00395300	1.81144200
O	-1.08531100	0.00393900	-1.81144800
Np	-1.07047300	-0.00000200	-0.00000200
O	-2.54522400	2.21177400	0.02006900
H	-1.74567500	2.77768700	-0.03799000

H	-3.07266300	2.40664800	-0.77196100
O	-2.54520300	-2.21180700	-0.01992600
H	-3.07255400	-2.40663900	0.77217400
H	-1.74565200	-2.77772200	0.03807700

$[NpO_2(DPA)(H_2O)_4]^-$_C

Gas: H = -1595.046361 Hartree

G = -1595.125602 Hartree

S = 166.777 Cal/Mol-Kelvin

O	-2.56550200	0.05948400	-1.69189700
O	-1.59514400	-0.00696600	1.77158500
Np	-1.99143800	0.03122300	0.01150500
O	-1.99626100	2.56809800	0.32356300
H	-1.04388200	2.78145400	0.02399200
H	-1.97966800	2.74858500	1.27694400
O	1.26215600	-2.19889200	-0.75651700
H	1.41209300	-1.22995500	-0.66231500
H	2.13135800	-2.52965700	-0.35886900
O	-3.50966200	-2.02357400	0.85007000
H	-3.32088500	-1.98027800	1.80214400
H	-2.80431200	-2.60415800	0.48264600
C	4.13835700	-0.23700500	0.07389300
C	5.11060200	0.77480300	0.18549600
C	4.72181200	2.10997500	0.11330300
C	3.36921000	2.41662200	-0.05539300
C	2.46761100	1.35474100	-0.16796400

N	2.84599500	0.06728200	-0.11578400
H	5.45929900	2.90619700	0.19793300
H	6.14111600	0.47098100	0.33127100
H	3.00357600	3.43691300	-0.09591200
C	0.98428400	1.62460500	-0.30663100
O	0.22736300	0.61404300	-0.51567700
O	0.56852700	2.80788200	-0.19152100
C	4.58355100	-1.72415100	0.20417400
O	3.68646400	-2.61574200	0.14904900
O	5.81355600	-1.88135000	0.37125300
O	-1.19755200	-2.36998700	-0.51055100
H	-1.39082500	-2.50245800	-1.45339700
H	-0.13026400	-2.41382200	-0.48005500

Aqueous: H = -1595.136688 Hartree
G = -1595.224078 Hartree
S = 183.928 Cal/Mol-Kelvin

O	-1.87320200	0.06239200	-1.78740200
O	-1.69977800	-0.23644100	1.81506900
Np	-1.77382500	-0.08325300	0.01349500
O	-2.06147900	2.54272200	0.24268800
H	-1.11850500	2.77513100	0.14423100
H	-2.53353700	3.03323400	-0.44981400
O	-1.09243000	-2.62550500	-0.24813400
H	-1.40711000	-3.31751800	0.35561600
H	-0.13232300	-2.54275200	-0.09625800

O	-4.39509100	0.82097200	-0.21570900
H	-4.79187900	1.41322100	0.44542900
H	-4.63443000	1.19310900	-1.08128500
C	4.80055800	-0.04430800	-0.00608600
C	5.32033000	1.26200800	0.01568100
C	4.44367200	2.34449100	0.04713300
C	3.07044100	2.09692300	0.03952600
C	2.63715700	0.76568900	0.00418500
N	3.47997400	-0.27914900	-0.01068300
H	4.82076100	3.36331800	0.07467000
H	6.39492500	1.40211000	0.01018100
H	2.34573700	2.90266700	0.05963200
C	1.15649000	0.46569400	-0.01299900
O	0.73594600	-0.72783900	-0.08469300
O	0.33545700	1.43675700	0.04622100
C	5.76348200	-1.25131500	-0.02152500
O	5.27860600	-2.39092800	0.21123400
O	6.97517600	-0.97749700	-0.26433700
O	-3.82296900	-1.76892400	0.04810000
H	-3.97096500	-2.31736300	0.83584200
H	-4.56148500	-1.12930800	0.02175800

$[NpO_2(DPA)(H_2O)_3]^-$_N

Gas: H = -1518.661702 Hartree

G = -1518.734136 Hartree

S = 152.451 Cal/Mol-Kelvin

C	2.48797600	-0.76288500	-0.16469000
C	3.86191300	-0.50915200	-0.16402700
C	4.29972400	0.80592400	0.00554400
C	3.36028300	1.82662500	0.16494300
C	2.00307900	1.49474800	0.15088800
N	1.59424700	0.22663600	-0.00901000
H	5.36370300	1.03368300	0.01161200
H	4.54359900	-1.34267700	-0.29480200
H	3.63955700	2.86642900	0.29627600
C	0.90541900	2.54818200	0.29636300
O	-0.29368000	2.07252700	0.25520300
O	1.23371100	3.73408100	0.41806200
C	1.91771000	-2.17120700	-0.34012800
O	0.63099400	-2.21282400	-0.31788700
O	2.70136700	-3.11708900	-0.48135800
O	-0.80567500	-0.56170700	1.87719200
O	-1.14242300	-0.05434200	-1.68724600
Np	-0.90503400	-0.31395900	0.09231700
O	-2.37547100	2.56153100	-1.53436400
H	-1.60485400	2.81111300	-0.97519500
H	-2.02656200	1.76748400	-1.99463000
O	-1.89141000	-2.80354700	0.12170800
H	-1.90319400	-2.94817500	1.08204800
H	-0.98509400	-3.08219400	-0.15426500
O	-3.16077000	0.89989000	0.44500700
H	-3.09284400	1.60834700	-0.25734700

H	-3.11565600	1.35611000	1.30003800

Aqueous: H = -1518.757243 Hartree
G = -1518.832608 Hartree
S = 158.620 Cal/Mol-Kelvin

C	2.61594800	-0.44149300	-0.04993200
C	3.93931700	0.00478400	-0.01287300
C	4.18331300	1.37716200	0.06102000
C	3.10158500	2.25897000	0.09263600
C	1.80749200	1.73418000	0.05334200
N	1.57986300	0.41246100	-0.01457000
H	5.20136700	1.75416600	0.09208000
H	4.74560000	-0.71918700	-0.04180800
H	3.23976900	3.33272500	0.14618000
C	0.57198500	2.61768500	0.07631400
O	-0.54790800	1.97791900	0.05939600
O	0.70192400	3.85197100	0.10229900
C	2.25406200	-1.91715600	-0.13442500
O	0.99156400	-2.15372100	-0.16122400
O	3.16274700	-2.76438200	-0.17277600
O	-0.77729000	-0.57437600	1.82812900
O	-0.96298700	-0.41324900	-1.78513600
Np	-0.85301500	-0.49074000	0.02013500
O	-2.98265800	3.08860200	-0.35573000
H	-2.01356000	2.89873500	-0.24571400
H	-3.10533600	3.34275300	-1.28456500

O	-1.46240600	-3.06536900	-0.07186900
H	-1.85583100	-3.45879700	0.72441800
H	-0.51509500	-3.32189300	-0.06465000
O	-3.28337600	0.46293200	0.21998300
H	-3.33938900	1.42412800	-0.03722000
H	-3.64527400	0.41156300	1.11966400

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

Gas: H = -1989.913633 Hartree

G = -1990.010884 Hartree

S = 204.681 Cal/Mol-Kelvin

C	-4.32575300	0.76164100	-0.12450700
C	-4.53651200	2.14465600	-0.23377000
C	-5.84958400	2.61728900	-0.23511200
C	-6.89125300	1.70089700	-0.12766900
C	-6.59903200	0.32323600	-0.06804900
N	-5.33171300	-0.12998100	-0.06570400
H	-6.05211700	3.68698900	-0.30693700
H	-3.67734300	2.80218800	-0.30651300
H	-7.93130300	2.00848000	-0.07721100
C	-7.79978500	-0.65948100	-0.01681200
O	-7.73039300	-1.68671300	-0.73079200
O	-8.75369900	-0.26513100	0.72093100
C	-2.87867800	0.27528600	-0.06826400
O	-2.59587700	-0.91897700	0.22199200
O	-1.97103100	1.14711900	-0.30917800

C	6.56426000	0.39024200	-0.07324100
C	6.83377900	1.77367400	-0.06369700
C	5.77617900	2.67793100	-0.09404700
C	4.47049100	2.18530300	-0.08978200
C	4.28422000	0.79530600	-0.05677700
N	5.30416300	-0.08171700	-0.06925300
H	5.96104700	3.75294200	-0.10985200
H	7.87062300	2.09217500	-0.02245500
H	3.60038900	2.83238200	-0.10485300
C	2.84961600	0.27579700	-0.00698000
O	2.61129100	-0.94870200	0.19766300
O	1.91920600	1.13339500	-0.16356600
C	7.77962600	-0.57942400	-0.09996800
O	7.66290200	-1.62800800	-0.77458400
O	8.78594100	-0.15610600	0.54691000
O	-0.05271300	-0.08531500	1.87871600
O	-0.03538000	-0.88119600	-1.65063500
Np	-0.05733200	-0.42911300	0.10821000
O	0.82390400	-2.99688500	0.13389000
H	1.71601600	-2.59046100	0.21608900
H	0.65881600	-2.99726400	-0.82577100

Aqueous: H = -1990.365705 Hartree
G = -1990.461398 Hartree
S = 201.405 Cal/Mol-Kelvin

C	-4.03442700	1.00778600	0.01602700

C	-4.11458900	2.40592000	0.05051400
C	-5.37793600	2.99743100	0.03615200
C	-6.50212800	2.17569400	-0.01357800
C	-6.33362400	0.78061400	-0.04577300
N	-5.11700000	0.21462200	-0.03037500
H	-5.48192700	4.07894800	0.06296300
H	-3.20777600	2.99832400	0.08806700
H	-7.50530200	2.58489100	-0.02830000
C	-7.57576100	-0.13681700	-0.09856000
O	-7.38763400	-1.38260500	-0.11221100
O	-8.69173200	0.46061600	-0.12265900
C	-2.67450500	0.34083600	0.03117500
O	-2.57781500	-0.92375500	0.04260700
O	-1.63832800	1.08351800	0.03187200
C	6.28589900	0.83244500	-0.04577500
C	6.44296200	2.22889000	-0.01317700
C	5.31179800	3.04168700	0.02573600
C	4.05299200	2.44022500	0.03006200
C	3.98470400	1.04151100	-0.00327700
N	5.07382000	0.25702100	-0.04002000
H	5.40692300	4.12401900	0.05230200
H	7.44303000	2.64592700	-0.01897400
H	3.14119100	3.02544500	0.05958800
C	2.63166000	0.36223700	0.00464000
O	2.54493700	-0.90285000	0.01740500
O	1.58720100	1.09418700	0.00066800

C	7.53496500	-0.07600600	-0.08777100
O	7.35548900	-1.32306700	-0.10707500
O	8.64684500	0.52927900	-0.09837500
O	0.00331300	-0.86776200	1.84384800
O	-0.02158200	-0.89081200	-1.78110100
Np	-0.01016900	-0.85574900	0.03110500
O	0.43051400	-3.39804300	0.03508800
H	0.82959200	-3.82942800	0.80900300
H	0.82048000	-3.82933000	-0.74353100

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

Gas: H = -1913.506749 Hartree

G = -1913.592161 Hartree

S = 179.766 Cal/Mol-Kelvin

C	-3.74775500	-0.58493200	-0.00966700
C	-4.12820800	-1.93230800	0.10707400
C	-5.48631700	-2.23814200	0.19347200
C	-6.41128500	-1.19809100	0.15976200
C	-5.95578800	0.12463300	-0.00668600
N	-4.64329200	0.41786700	-0.08739800
H	-5.81493000	-3.27419100	0.29662600
H	-3.35216400	-2.68921000	0.13181700
H	-7.47867400	-1.36860300	0.26724800
C	-7.03449700	1.23475400	-0.11054100
O	-6.91327200	2.06979800	-1.03842800
O	-7.97143800	1.12819600	0.73993600

C	-2.23919600	-0.29022500	-0.04394300
O	-1.79797900	0.88395900	0.05976500
O	-1.47734000	-1.30831500	-0.15990200
C	4.01601200	1.28526500	0.05884500
C	5.41383400	1.37345800	0.04510200
C	6.15954800	0.19458400	-0.02228200
C	5.49539000	-1.03301800	-0.07237700
C	4.09502600	-1.04052600	-0.05410200
N	3.39201500	0.09944300	0.00882000
H	7.25004300	0.23225000	-0.03490200
H	5.86706100	2.35863500	0.08818900
H	6.01426500	-1.98479500	-0.12520500
C	3.28323800	-2.34798300	-0.10285600
O	2.02735600	-2.19515200	-0.07149100
O	3.94200600	-3.41536700	-0.16478500
C	3.11926200	2.53541000	0.13391900
O	1.87557100	2.29875400	0.12856000
O	3.70718800	3.64258000	0.19301000
O	0.78440400	0.13160700	-1.80035000
O	0.72170800	-0.09069500	1.81780900
Np	0.72701200	0.01553300	0.00687000

Aqueous: H = -1913.983934 Hartree
G = -1914.068945 Hartree
S = 178.921 Cal/Mol-Kelvin

C	3.67362100	-0.71611800	-0.00078400

C	4.11972900	-2.04397700	-0.00448400
C	5.49460300	-2.28177300	-0.00107200
C	6.36437400	-1.19276800	0.00073200
C	5.83405400	0.10871100	0.01457800
N	4.51114600	0.33315000	0.01571000
H	5.87934800	-3.29828600	-0.00231000
H	3.39990000	-2.85426400	-0.00992700
H	7.43997900	-1.32524300	-0.00600300
C	6.78617500	1.32392500	0.03218200
O	6.29263800	2.45315500	0.29682000
O	8.00063400	1.06882700	-0.21962600
C	2.18437700	-0.42701600	-0.01054500
O	1.76972500	0.77158700	-0.02479300
O	1.37951300	-1.41295000	-0.00338100
C	-4.00522900	1.19211700	-0.00410000
C	-5.40272200	1.20126500	0.00772200
C	-6.08005200	-0.02019600	0.02871300
C	-5.34718700	-1.20923400	0.03676600
C	-3.95179200	-1.13500800	0.02340200
N	-3.31183000	0.04374400	0.00378500
H	-7.16607800	-0.04514600	0.03875300
H	-5.93177500	2.14746100	0.00094400
H	-5.83136400	-2.17916900	0.05327000
C	-3.05070700	-2.36545300	0.03022900
O	-1.79437300	-2.11561500	0.01306400
O	-3.57911100	-3.49511700	0.05112600

C	-3.16250700	2.46378800	-0.02595100
O	-1.89585800	2.27209200	-0.02558400
O	-3.74396400	3.56724900	-0.04190900
O	-0.70945300	0.11971400	1.81054100
O	-0.72813100	0.08539800	-1.83539500
Np	-0.71891000	0.09690400	-0.01228400

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

Gas: H = -2066.325678 Hartree

G = -2066.431406 Hartree

S = 222.524 Cal/Mol-Kelvin

C	-4.03868800	1.10005200	0.03419200
C	-3.97366600	2.49849000	0.12067100
C	-5.17074300	3.21412500	0.16650100
C	-6.37276200	2.51327900	0.12887500
C	-6.35403000	1.10986100	0.00093500
N	-5.19815700	0.42240100	-0.04572500
H	-5.16122300	4.30244900	0.24111700
H	-3.00153100	2.97799600	0.15509300
H	-7.33646200	3.00682900	0.20492600
C	-7.72211600	0.37688000	-0.09618200
O	-7.78919000	-0.61637700	-0.85620300
O	-8.64201600	0.91633900	0.59201200
C	-2.71984900	0.33297700	0.02857800
O	-2.70261700	-0.93126100	0.08275000
O	-1.64759000	1.01502000	-0.01682400

C	6.35816500	1.10653500	-0.04790400
C	6.36934700	2.51398800	-0.12144300
C	5.16696700	3.20351500	-0.24963600
C	3.97440500	2.47901900	-0.25758200
C	4.04451200	1.08245400	-0.14611000
N	5.20696300	0.40996500	-0.06578500
H	5.15300900	4.29133500	-0.32949400
H	7.32750400	3.02047000	-0.06288200
H	3.00150800	2.95114200	-0.33889800
C	2.72745300	0.31193000	-0.11606800
O	2.71287900	-0.94708800	0.00601300
O	1.65453500	0.98783400	-0.21430100
C	7.73044000	0.37888200	0.04695500
O	7.83432500	-0.73159300	-0.52229700
O	8.61627700	1.03773700	0.67361700
O	0.07708900	-0.87219000	1.83357000
O	-0.08144800	-1.14179300	-1.77634100
Np	-0.00240000	-0.92293200	0.02209500
O	-1.49605700	-3.28537300	-0.30186400
H	-1.22951500	-3.20677200	-1.23361300
H	-2.26218800	-2.67594200	-0.21867700
O	1.47588100	-3.22254300	0.65973900
H	1.21477300	-3.03491200	1.57745000
H	2.24253300	-2.62810600	0.50103100

Aqueous: H = -2066.787168 Hartree

G = -2066.888342 Hartree

S = 212.939 Cal/Mol-Kelvin

C	-3.91421200	1.20701500	0.02582500
C	-3.89685100	2.60763000	0.04269800
C	-5.11627800	3.28513500	0.02799000
C	-6.29563500	2.54329700	-0.00093300
C	-6.22453600	1.13983300	-0.02597500
N	-5.04968300	0.49159500	-0.01336700
H	-5.14470800	4.37153400	0.04076500
H	-2.95065600	3.13574300	0.06744100
H	-7.26788800	3.02191600	-0.00525200
C	-7.52590200	0.30890200	-0.07100900
O	-7.42561000	-0.93052200	-0.27625900
O	-8.59584000	0.96375800	0.10040700
C	-2.60412700	0.44648900	0.04791900
O	-2.60007800	-0.82441700	0.08075900
O	-1.51921100	1.10460100	0.03224200
C	6.22469200	1.14138400	-0.03153700
C	6.29450300	2.54524200	-0.02616100
C	5.11445600	3.28621300	-0.04546700
C	3.89531600	2.60796400	-0.05240700
C	3.91377700	1.20738200	-0.04720200
N	5.05035000	0.49245500	-0.04547500
H	5.14208000	4.37268800	-0.05118800
H	7.26540100	3.02626900	-0.00789500
H	2.94856000	3.13556200	-0.06102400

C	2.60400200	0.44606700	-0.04500900
O	2.60059000	-0.82522600	-0.04272900
O	1.51878300	1.10388000	-0.04351600
C	7.52586800	0.31027500	-0.02164500
O	7.44069200	-0.91912300	-0.28607200
O	8.58079800	0.95503500	0.25141300
O	0.04653300	-0.97423000	1.84505000
O	-0.04607500	-1.02113800	-1.80239500
Np	0.00022800	-0.97545000	0.02100900
O	-1.43214300	-3.22309000	0.09718900
H	-1.33680600	-3.82710700	-0.65723800
H	-2.29966200	-2.78818600	-0.00945100
O	1.43244600	-3.22458800	-0.00317900
H	1.33991300	-3.80924400	0.76670200
H	2.30033500	-2.78720000	0.08941900

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

Gas: H = -2066.332108 Hartree

G = -2066.432217 Hartree

S = 210.698 Cal/Mol-Kelvin

C	-4.38303600	0.63266800	-0.29977200
C	-4.64854900	1.98437000	-0.56489900
C	-5.97939700	2.38455300	-0.69329600
C	-6.98203800	1.43033400	-0.55089300
C	-6.63161700	0.08309100	-0.32823200
N	-5.34755900	-0.30040000	-0.20558400

H	-6.22597700	3.42889700	-0.88962700
H	-3.81811000	2.67575900	-0.65466900
H	-8.03633500	1.68566800	-0.59423800
C	-7.78687100	-0.95102700	-0.24044900
O	-7.61622400	-2.05095600	-0.81502200
O	-8.81011500	-0.52349500	0.37566700
C	-2.92371300	0.22855700	-0.11571500
O	-2.60133900	-0.92447300	0.28370500
O	-2.04095400	1.12226600	-0.37212400
C	6.50929900	0.05429400	-0.40009600
C	6.85064900	1.36777800	-0.78162400
C	5.85813400	2.33981800	-0.86237900
C	4.53832600	1.97622500	-0.59261000
C	4.27634300	0.64435700	-0.24045700
N	5.23742800	-0.29008200	-0.13133800
H	6.10192400	3.36561700	-1.14090500
H	7.89101100	1.57171100	-1.01186300
H	3.71658800	2.68104200	-0.65379000
C	2.82854000	0.24898700	0.01712100
O	2.51485400	-0.94436200	0.27480900
O	1.94436000	1.17521400	-0.05521000
C	7.66168000	-0.99435500	-0.29538000
O	7.46529300	-1.99806000	0.42416200
O	8.69971800	-0.67734200	-0.95428200
O	-0.12300900	0.14574700	1.95311400
O	-0.04929700	-0.88652000	-1.52272400

Np	-0.10204700	-0.34363600	0.20301000
O	0.64911900	-2.91248500	0.46546600
H	1.57328000	-2.57964600	0.48422600
H	0.47187900	-3.06415200	-0.47888900
O	1.33878500	2.65420300	2.43858200
H	0.73514600	1.89204300	2.55365200
H	1.75587600	2.41880700	1.58755300

Aqueous: H = -2066.789465 Hartree
G = -2066.890838 Hartree
S = 213.357 Cal/Mol-Kelvin

C	-4.48453500	-0.42751100	-0.03494300
C	-5.12381700	-1.67263500	-0.10051900
C	-6.51680100	-1.70062700	-0.16604100
C	-7.21205500	-0.49326300	-0.16166600
C	-6.49437900	0.71325000	-0.09443400
N	-5.15383300	0.73684800	-0.03421100
H	-7.04868800	-2.64699500	-0.21896100
H	-4.53455500	-2.58223000	-0.09965800
H	-8.29395600	-0.46025100	-0.20867000
C	-7.25996200	2.05503300	-0.08792300
O	-6.58531400	3.11887100	-0.05872300
O	-8.52246500	1.96025900	-0.11257100
C	-2.97081800	-0.37438600	0.03631800
O	-2.36381000	0.73488100	0.09068300
O	-2.33303500	-1.47818600	0.03517400

C	6.50115100	0.69221200	-0.09364700
C	7.20566000	-0.52179700	-0.16384500
C	6.49710000	-1.72146500	-0.17402800
C	5.10450900	-1.67839300	-0.10983800
C	4.47896500	-0.42640700	-0.04018900
N	5.16086300	0.73038500	-0.03532900
H	7.01853100	-2.67346500	-0.22997100
H	8.28799000	-0.50061400	-0.20846800
H	4.50517800	-2.58136400	-0.11289800
C	2.96599100	-0.35857300	0.03195400
O	2.36982000	0.75963200	0.08909400
O	2.31793200	-1.45272800	0.02881000
C	7.28007400	2.02591800	-0.08067100
O	6.61532400	3.09613100	-0.05566100
O	8.54170000	1.91886900	-0.09654800
O	0.00005900	-0.40661500	-1.74684800
O	-0.01058900	-0.28330000	1.89773500
Np	-0.00550800	-0.34689800	0.07548900
O	0.09717100	2.27374700	0.00633500
H	1.01567700	2.45809700	0.27304300
H	-0.47657100	2.73035400	0.64320700
O	-0.06134100	-2.97139600	0.13806600
H	-0.94530200	-3.19904700	-0.19962200
H	0.58458100	-3.38303000	-0.45919800

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

Gas: H = -1989.931103 Hartree
G = -1990.024474 Hartree
S = 196.516 Cal/Mol-Kelvin

C	3.90856600	0.21500400	-0.02532000
C	3.75178000	1.60843900	-0.08822100
C	4.89339900	2.40837900	-0.02680700
C	6.13846300	1.79657600	0.09628100
C	6.21776500	0.39022200	0.11194800
N	5.11507100	-0.37929700	0.05057900
H	4.80663900	3.49538200	-0.06333200
H	2.75228300	2.01998400	-0.17482400
H	7.05818500	2.36578600	0.19256300
C	7.63242700	-0.24931600	0.19320200
O	7.84317300	-1.28030000	-0.48933800
O	8.44934100	0.39088900	0.92597000
C	2.63658300	-0.64971700	-0.04453300
O	2.73265900	-1.88982800	0.13867700
O	1.54820800	-0.01514600	-0.24648300
C	-4.44829700	-0.39432600	0.21857100
C	-5.77482000	0.03238700	0.35753200
C	-6.04215800	1.40310800	0.35697900
C	-4.98508500	2.30536000	0.22172800
C	-3.68481100	1.80244200	0.08906000
N	-3.44263800	0.48340100	0.08817400
H	-7.06600800	1.76514900	0.46194600
H	-6.54886200	-0.72116400	0.46149500

H	-5.12264900	3.38181800	0.21493300
C	-2.46372200	2.72766600	-0.06010400
O	-1.35293700	2.12708400	-0.16178100
O	-2.69133000	3.96076600	-0.06619900
C	-4.06729200	-1.88540300	0.21222100
O	-2.83205100	-2.11814300	0.06274800
O	-5.00691000	-2.70575100	0.35490300
O	-1.06514300	-0.40338900	-1.96584000
O	-0.83844400	-0.40452800	1.65853400
Np	-0.93578700	-0.38622400	-0.15620000
O	0.21688700	-2.75058100	0.01337500
H	-0.05819000	-2.97119000	0.91655900
H	1.19531500	-2.49914700	0.07419600

Aqueous: H = -1990.399258 Hartree
G = -1990.489801 Hartree
S = 190.565 Cal/Mol-Kelvin

C	3.67228700	0.79745100	0.02532900
C	4.03028000	2.15144400	0.06844000
C	5.38608500	2.47971400	0.09149800
C	6.32670700	1.45129200	0.07028000
C	5.88442700	0.11865100	0.01887200
N	4.57906700	-0.19255300	-0.00184800
H	5.70230700	3.51913000	0.12603900
H	3.25824800	2.91210000	0.08372500
H	7.39110100	1.65364600	0.09111900

C	6.91669300	-1.02996200	-0.01928800
O	6.48850400	-2.20036200	-0.20839100
O	8.12415200	-0.68344600	0.14139600
C	2.20346400	0.40886800	0.00331800
O	1.86724700	-0.81067200	0.01038700
O	1.33640400	1.33825200	-0.02318700
C	-4.24768700	-0.70223900	0.04683700
C	-5.62061600	-0.43953600	0.06067500
C	-6.04939500	0.88849800	0.03633500
C	-5.09614800	1.90700300	0.00332600
C	-3.74129900	1.56120700	-0.00570100
N	-3.33459100	0.28212000	0.01272800
H	-7.10961700	1.12564500	0.04440300
H	-6.32097900	-1.26647300	0.08999300
H	-5.37728200	2.95377500	-0.01422800
C	-2.63339200	2.60767200	-0.03209900
O	-1.44505000	2.14573800	-0.02592600
O	-2.96104900	3.81536300	-0.05496500
C	-3.69484800	-2.11966600	0.07420700
O	-2.41764900	-2.19881900	0.03739400
O	-4.49265000	-3.07705300	0.12964300
O	-0.74149300	-0.26775900	-1.85891000
O	-0.70162200	-0.28653900	1.80543100
Np	-0.71959700	-0.26893400	-0.02684500
O	0.04518100	-2.86551700	-0.12543100
H	0.66830100	-3.06857600	0.58989300

H	-0.83610700	-3.20124700	0.13779400

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

Gas: H = -1913.476315 Hartree

G = -1913.562902 Hartree

S = 182.239 Cal/Mol-Kelvin

C	3.53033800	1.15975300	-0.00935600
C	4.93046600	1.20228700	0.05364400
C	5.63857200	0.00000400	0.08921400
C	4.93049500	-1.20230200	0.05390400
C	3.53036400	-1.15982600	-0.00912600
N	2.85647900	-0.00004700	-0.03379600
H	6.72988700	0.00002200	0.14015100
H	5.41023000	2.17589300	0.07042000
H	5.41028100	-2.17589300	0.07090900
C	2.68728500	-2.44485300	-0.06575000
O	1.44513400	-2.25782500	-0.10668200
O	3.33169700	-3.53116900	-0.07173100
C	2.68723100	2.44474400	-0.06619300
O	1.44507600	2.25767300	-0.10694400
O	3.33159800	3.53107800	-0.07247400
C	-3.53054100	-1.15987300	0.00918400
C	-4.93066400	-1.20240700	-0.05403900
C	-5.63876800	-0.00011400	-0.08945700
C	-4.93071200	1.20220100	-0.05379900
C	-3.53058400	1.15971400	0.00939400

N	-2.85672700	-0.00007200	0.03395300
H	-6.73007700	-0.00012900	-0.14055600
H	-5.41042900	-2.17600700	-0.07111700
H	-5.41052400	2.17578200	-0.07066000
C	-2.68750800	2.44473200	0.06625100
O	-1.44534200	2.25772300	0.10698600
O	-3.33192600	3.53104500	0.07253900
C	-2.68736500	-2.44485900	0.06580900
O	-1.44522700	-2.25778700	0.10667100
O	-3.33174200	-3.53120900	0.07181500
O	-0.11006400	0.00009200	-1.80899100
O	0.11038700	0.00007600	1.80899200
Np	0.00015000	0.00009000	0.00000200

Aqueous: H = -1913.989414 Hartree
G = -1914.071996 Hartree
S = 173.809 Cal/Mol-Kelvin

C	-3.46510600	-1.15654000	-0.01110000
C	-4.86167400	-1.20150800	0.04750300
C	-5.57073200	-0.00000100	0.08043400
C	-4.86166800	1.20150300	0.04750500
C	-3.46510100	1.15652800	-0.01109900
N	-2.78591000	-0.00000800	-0.03488300
H	-6.65631700	0.00000100	0.12871200
H	-5.36241100	-2.16288200	0.06698700
H	-5.36240100	2.16287900	0.06699000

C	-2.60478500	2.40861500	-0.05668800
O	-1.35177200	2.19774400	-0.07718600
O	-3.17644700	3.52555400	-0.07340100
C	-2.60479300	-2.40863000	-0.05668900
O	-1.35178000	-2.19776500	-0.07716600
O	-3.17646200	-3.52556600	-0.07341900
C	3.46511100	1.15652200	0.00978200
C	4.86159000	1.20149000	-0.05094800
C	5.57059700	-0.00001700	-0.08495400
C	4.86158300	-1.20152000	-0.05094800
C	3.46510400	-1.15654400	0.00978100
N	2.78595000	-0.00001000	0.03460200
H	6.65610800	-0.00002000	-0.13487800
H	5.36230200	2.16286200	-0.07120100
H	5.36228900	-2.16289500	-0.07120100
C	2.60486600	-2.40863700	0.05671000
O	1.35188700	-2.19779500	0.07917200
O	3.17658100	-3.52556900	0.07257300
C	2.60488200	2.40862000	0.05671500
O	1.35190100	2.19778500	0.07919400
O	3.17660100	3.52554800	0.07256600
O	0.07058800	0.00001700	-1.82154200
O	-0.07066800	0.00001800	1.82304300
Np	-0.00002700	0.00001200	0.00075100

$[NpO_2(PADA)(H_2O)_3]^-$_C

Gas: H = -1841.833804 Hartree
G = -1841.927775 Hartree
S = 197.780 Cal/Mol-Kelvin

C	0.97778600	-3.03284800	-0.03975100
C	2.24485300	-3.57798200	-0.04514400
C	3.37853000	-2.73295600	-0.02159900
C	3.14923100	-1.31741500	0.00755300
C	0.86192300	-1.62327700	-0.00252400
C	4.71366900	-3.24741700	-0.02984200
C	4.29394600	-0.40437200	0.02280300
C	5.60229400	-0.97311400	0.00655100
C	5.78062000	-2.39151000	-0.01575600
C	6.69817700	-0.07185800	0.00471500
H	7.71382600	-0.46705800	-0.00992700
C	6.45831200	1.28003800	0.00554700
C	5.11408700	1.75782900	0.04422500
H	4.86124700	-4.32565900	-0.05000700
H	0.08431500	-3.64709100	-0.06224900
H	2.38737600	-4.65724800	-0.06968800
H	6.79742300	-2.78269500	-0.02543400
H	7.26724400	2.00367100	-0.02953200
N	1.90323300	-0.80334300	0.02048200
N	4.07174800	0.92642400	0.05726700
C	-0.49953800	-0.98570900	0.01194100
O	-0.61829500	0.26964000	0.10882100
O	-1.54580100	-1.72599000	-0.07724900

C	4.88960400	3.27493200	0.04627600
O	4.45950800	3.77047400	1.11246000
O	5.22789000	3.82431800	-1.03595300
O	-3.05530900	0.48488600	-1.80906000
O	-3.29970500	0.17140300	1.77093700
Np	-3.06903200	0.30880600	-0.01624000
O	-1.94526300	2.65128600	0.07623300
H	-1.07084400	2.37115600	0.41597600
H	-1.75963800	2.94542700	-0.83114200
O	-5.60560200	0.96821700	-0.08119100
H	-6.10023900	0.64859700	-0.85249000
H	-6.11058400	0.71790800	0.70831300
O	-4.22325400	-2.09599700	0.05462600
H	-3.35287800	-2.48336700	-0.17783200
H	-4.25648000	-2.17609900	1.02311400

Aqueous: H = -1841.976318 Hartree
G = -1842.067348 Hartree
S = 191.590 Cal/Mol-Kelvin

C	-1.01056200	-2.97725100	-0.00815800
C	-2.26842300	-3.54524600	-0.00392400
C	-3.41188500	-2.71505100	-0.00421600
C	-3.20395300	-1.30172300	-0.01329200
C	-0.90932700	-1.56745300	-0.01140900
C	-4.74195200	-3.25381700	0.00659500
C	-4.36865400	-0.41628900	-0.01763000

C	-5.66773400	-1.00050600	0.00312100
C	-5.82665400	-2.42733800	0.01222700
C	-6.77586900	-0.12185800	0.01586900
H	-7.78312400	-0.53176600	0.03101000
C	-6.56386700	1.24055800	0.01591000
C	-5.23504200	1.73222600	-0.02789200
H	-4.86586700	-4.33368800	0.01287300
H	-0.11195000	-3.58274000	-0.00674100
H	-2.39153900	-4.62532800	0.00112400
H	-6.83399300	-2.83625900	0.02434900
H	-7.38755200	1.94422800	0.04442100
N	-1.96615200	-0.76145200	-0.01546900
N	-4.17908200	0.92337600	-0.04806600
C	0.45783000	-0.91992600	-0.00630500
O	0.57407000	0.34042300	0.00738900
O	1.48866200	-1.67316800	-0.01292200
C	-4.99594400	3.25505700	-0.05038900
O	-3.91055500	3.67220000	-0.53586400
O	-5.93716100	3.95621000	0.42417300
O	3.06716900	0.34692100	1.83154900
O	3.17544600	0.28639500	-1.78717800
Np	3.10711700	0.30500300	0.02175000
O	2.42047300	2.78148800	0.03504800
H	1.86677700	3.10853300	-0.69388900
H	2.01000200	3.12175000	0.84766400
O	5.70094100	0.66953600	-0.05689000

H	6.29237100	0.40505700	0.66728300
H	6.19444200	0.51024500	-0.87843400
O	4.17692200	-2.08168100	0.05072300
H	3.37063200	-2.61717700	-0.07092700
H	4.77901900	-2.33646400	-0.66799600

$[NpO_2(PADA)(H_2O)]^-$_N

Gas: H = -1689.094987 Hartree

G = -1689.168363 Hartree

S = 154.435 Cal/Mol-Kelvin

C	-3.19582000	2.47202400	-0.02582400
C	-4.09524300	1.42512700	-0.03970900
C	-3.62203500	0.08933800	-0.04066000
C	-2.21615200	-0.09233300	-0.02859100
C	-1.80845700	2.19299500	-0.01460900
C	-4.47465000	-1.06587800	-0.05017800
C	-1.66252000	-1.42739100	-0.02301600
C	-2.53288100	-2.54723800	-0.02835000
C	-3.95241300	-2.32988200	-0.04396500
C	-1.92916700	-3.82839800	-0.01536600
H	-2.55918800	-4.71625900	-0.01867100
C	-0.55367200	-3.93729500	0.00262700
C	0.23456200	-2.76227600	0.00660900
H	-5.55239200	-0.91642400	-0.06060200
H	-3.50321900	3.51204200	-0.02306400
H	-5.16794900	1.61110400	-0.04891100

H	-4.61003700	-3.19673000	-0.04944200
H	-0.03994700	-4.89216300	0.01398700
N	-1.35034700	0.94612100	-0.01745200
N	-0.31411300	-1.55167800	-0.00821100
C	-0.75741800	3.31759600	0.00218300
O	0.44895200	2.90426900	0.01243500
O	-1.18427900	4.48326900	0.00130000
C	1.76898800	-2.84137900	0.02740100
O	2.34970600	-1.70295400	0.04552900
O	2.28106200	-3.97032500	0.02125200
O	1.16111400	0.56163200	1.84004900
O	1.36713700	0.60994500	-1.76987200
Np	1.24033200	0.58580200	0.03853700
O	3.92237400	0.41388500	-0.19586000
H	3.79346600	-0.55537500	-0.06714400
H	3.95236600	0.52532900	-1.16043100

Aqueous: H = -1689.198164 Hartree
G = -1689.273080 Hartree
S = 157.674 Cal/Mol-Kelvin

C	-1.78953800	3.58513100	0.00371100
C	-3.06016500	3.04004300	0.00512100
C	-3.22006300	1.63440900	0.00405100
C	-2.03807600	0.85083600	-0.00040200
C	-0.67124000	2.72501000	-0.00112300
C	-4.49822300	0.97709500	0.00815000

C	-2.13442700	-0.58979900	0.00073400
C	-3.41055300	-1.20836600	0.00770400
C	-4.58946800	-0.38625300	0.01019300
C	-3.43964200	-2.62273600	0.01218400
H	-4.39541200	-3.14019000	0.01774000
C	-2.25311800	-3.33241300	0.00954400
C	-1.02986400	-2.62934900	-0.00006700
H	-5.39624900	1.58864000	0.01033200
H	-1.62805300	4.65665300	0.00586100
H	-3.93832800	3.68025200	0.00782100
H	-5.56099100	-0.87255800	0.01409700
H	-2.23697000	-4.41589400	0.01343100
N	-0.80103300	1.39982100	-0.00448300
N	-0.98150900	-1.29859900	-0.00429500
C	0.76104500	3.25575300	-0.00091600
O	1.67322000	2.35879100	-0.01487200
O	0.93318100	4.49065500	0.01140500
C	0.31897800	-3.34704600	-0.00716600
O	1.34200100	-2.57909200	-0.03139900
O	0.32584300	-4.59364800	0.00838400
O	1.32951100	-0.11218100	1.81003600
O	1.40235800	-0.08234500	-1.83369400
Np	1.34849200	-0.09708400	-0.01167600
O	3.94765400	-0.01940000	0.10568900
H	4.41472100	-0.22415900	0.93276700
H	4.50531400	-0.36859600	-0.60945400

$[NpO_2(PADA)(H_2O)_4]^-$_C

Gas: H = -1918.242492 Hartree

G = -1918.339639 Hartree

S = 204.463 Cal/Mol-Kelvin

C	1.29267100	-3.11946500	0.18321800
C	2.58954500	-3.58231600	0.27068200
C	3.67027800	-2.67055300	0.23763800
C	3.35718100	-1.27666400	0.11410000
C	1.09472200	-1.72495300	0.05286400
C	5.03378200	-3.09665400	0.32243000
C	4.44189600	-0.29415900	0.09279500
C	5.78184300	-0.77577400	0.17499700
C	6.04586000	-2.17678500	0.28873700
C	6.81855000	0.19205600	0.13437900
H	7.85666600	-0.13535400	0.18918600
C	6.49489000	1.52117900	0.01165000
C	5.12319300	1.91214300	-0.03041000
H	5.24747200	-4.16016100	0.41202600
H	0.43772000	-3.78636900	0.20993500
H	2.79592600	-4.64711600	0.36682200
H	7.08382200	-2.50230900	0.34941600
H	7.25587500	2.29191500	-0.06232000
N	2.08461200	-0.84426900	0.01907700
N	4.13567200	1.01801200	0.01264800
C	-0.29688700	-1.16917200	-0.05455500

O	-0.47095100	0.07358100	-0.22505900
O	-1.30830700	-1.95206600	0.03094200
C	4.80340400	3.40956000	-0.15220700
O	4.17375100	3.92615300	0.79794100
O	5.27476800	3.92595900	-1.20135200
O	-2.93981100	-0.08402000	-2.00114500
O	-2.99136700	0.24947100	1.59103900
Np	-2.89562300	0.05770500	-0.21758100
O	-1.81839900	2.41628700	-0.33806200
H	-1.64776500	2.76765300	0.55205700
H	-0.93235700	2.14849700	-0.65692300
O	-4.94368000	1.98064600	2.38953900
H	-5.57207100	1.59983700	3.02059300
H	-4.17492800	1.35325200	2.35035100
O	-3.97272400	-2.32427800	-0.21773000
H	-4.11163200	-2.52373200	-1.15834000
H	-3.08726800	-2.69615600	-0.01205300
O	-5.06090200	1.40541700	-0.22797400
H	-5.22263100	2.09516900	-0.88911600
H	-5.22246600	1.78426800	0.67829100

Aqueous: H = -1918.380920 Hartree
G = -1918.476917 Hartree
S = 202.042 Cal/Mol-Kelvin

C	1.29068000	-3.02924300	0.17403400
C	2.57264000	-3.53446900	0.24978400

C	3.67597500	-2.65241600	0.21856700
C	3.40424900	-1.25397000	0.11003700
C	1.12633100	-1.62964700	0.06710800
C	5.02860900	-3.12639700	0.29156800
C	4.52751800	-0.31653700	0.07737800
C	5.85130700	-0.83761300	0.15421700
C	6.07448500	-2.25204600	0.25986600
C	6.91704300	0.09084400	0.12259000
H	7.94184300	-0.26925900	0.17788500
C	6.64302800	1.43894600	0.02427900
C	5.29383600	1.86692000	-0.04989000
H	5.20092900	-4.19661000	0.37212100
H	0.42093400	-3.67521900	0.19419600
H	2.74512200	-4.60450600	0.33274300
H	7.09862700	-2.61282800	0.31477000
H	7.43199600	2.18087800	0.00143800
N	2.14358900	-0.77522400	0.03683900
N	4.27764700	1.00866900	-0.02507800
C	-0.26788000	-1.05570900	-0.02153200
O	-0.45219300	0.19654300	-0.11533600
O	-1.25883400	-1.85547600	-0.00333600
C	4.98523400	3.37786900	-0.16290000
O	3.78492000	3.72484800	-0.32462700
O	5.99085300	4.14305900	-0.08195000
O	-2.88302400	-0.04371800	-2.02110000
O	-3.09450000	0.14067800	1.58694400

Np	-2.97332500	0.03107800	-0.22600100
O	-2.01498700	2.43444400	-0.32462900
H	-2.27528100	3.07241800	0.36096000
H	-1.05905600	2.28489200	-0.20111900
O	-5.01934200	2.00455500	2.42409900
H	-5.77411700	1.63724900	2.91204200
H	-4.33213300	1.29863100	2.41060500
O	-3.92291000	-2.41170000	-0.12449900
H	-4.42046600	-2.74773200	-0.88899400
H	-3.08029800	-2.90381800	-0.11677700
O	-4.96768900	1.57935000	-0.24063700
H	-5.18308500	2.26694900	-0.89074500
H	-5.18114600	1.92474500	0.66661400

$[NpO_2(PADA)(H_2O)_2]^-$_N

Gas: H = -1765.509565 Hartree

G = -1765.588552 Hartree

S = 166.243 Cal/Mol-Kelvin

C	-2.19826500	3.47846800	0.02196000
C	-3.42442700	2.84922400	0.01370300
C	-3.48474900	1.43529000	0.00939200
C	-2.25016400	0.73221200	0.01650000
C	-1.02106200	2.69458300	0.03102600
C	-4.71772600	0.70154100	-0.00350900
C	-2.25614400	-0.71550400	0.00489200
C	-3.49647300	-1.40826400	-0.00847100

C	-4.72335700	-0.66427300	-0.01149100
C	-3.44772500	-2.82263700	-0.01988100
H	-4.37734200	-3.38921800	-0.02988800
C	-2.22683700	-3.46206900	-0.01840500
C	-1.04309300	-2.68804100	-0.00789600
H	-5.65271200	1.25810400	-0.00771400
H	-2.08828900	4.55714800	0.02139900
H	-4.34933300	3.42351000	0.00841400
H	-5.66292100	-1.21298700	-0.02176700
H	-2.12578700	-4.54159900	-0.02559900
N	-1.05298500	1.36528000	0.03099200
N	-1.06425100	-1.35859900	0.00381300
C	0.35588600	3.36761300	0.03415300
O	1.33219400	2.54659600	0.06589600
O	0.38893500	4.60726500	0.00462800
C	0.32845100	-3.37240200	-0.00878300
O	1.31159400	-2.55934300	-0.02090600
O	0.35049800	-4.61262500	0.00444200
O	1.38641700	-0.06587500	1.80142000
O	1.23146400	0.05317400	-1.80716800
Np	1.29606100	-0.00642900	-0.00208200
O	3.62824100	-1.42372100	0.01109300
H	3.92808700	-1.24311900	0.91555700
H	3.07079700	-2.23526300	0.05877800
O	3.64216100	1.41307000	-0.08549800
H	3.07983100	2.22322600	-0.07562200

H	3.92669200	1.28855800	-1.00400200

Aqueous: H = -1765.597221 Hartree
G = -1765.675744 Hartree
S = 165.265 Cal/Mol-Kelvin

C	-2.20296000	3.46919800	0.00182000
C	-3.42804900	2.83239100	0.00084700
C	-3.47820500	1.42005100	0.00027000
C	-2.24061000	0.72232400	0.00060500
C	-1.02620400	2.69274800	0.00357000
C	-4.70996700	0.68154000	-0.00031100
C	-2.24035600	-0.72301200	-0.00123900
C	-3.47767300	-1.42123100	-0.00068700
C	-4.70971700	-0.68319700	-0.00037800
C	-3.42694500	-2.83355500	-0.00051900
H	-4.35124600	-3.40497800	0.00004800
C	-2.20160800	-3.46989400	-0.00076100
C	-1.02515700	-2.69298100	-0.00293200
H	-5.64579200	1.23354600	-0.00040200
H	-2.11865500	4.54951200	0.00189700
H	-4.35257300	3.40345300	0.00042900
H	-5.64534100	-1.23554400	-0.00034100
H	-2.11689800	-4.55017800	0.00001700
N	-1.04523800	1.35964400	0.00322900
N	-1.04476900	-1.35988600	-0.00364700
C	0.34747700	3.34688000	0.00646900

O	1.32805000	2.52334300	0.01879500
O	0.42454300	4.58888900	-0.00282600
C	0.34883000	-3.34645800	-0.00492800
O	1.32896100	-2.52244500	-0.01952300
O	0.42652400	-4.58840800	0.00711900
O	1.28020600	-0.01936500	1.81144300
O	1.28037500	0.01952300	-1.81241600
Np	1.27541500	0.00009900	-0.00045900
O	3.61861400	-1.36785400	-0.07260800
H	4.16664200	-1.24667600	0.71953900
H	3.15095800	-2.22378000	0.03581200
O	3.61795700	1.36924000	0.07373100
H	3.14865900	2.22450600	-0.03311900
H	4.16570500	1.25038800	-0.71895200