Supporting Information for

Binding mechanism of uranyl to transferrin implicated by density functional theory study

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Content

1. The full citation of Gaussian 09

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2. Channel III for the first HTyr* binding to uranium tricarbonate following pathway YYD (Figures S1-S3).

We also considered the first ligand coordination process of the sequence YYD beginning with channel III. The optimized structures of the stationary points along with key geometrical parameters are given in Figures S1 and S2, and the free energy profiles in Figure S3.

Two possible reaction mechanisms (denoted as mechanism III-1 in Figure S1 and III-2 in Figure S2) for Channel III are considered here, which are both five-stepped, including the change of coordination mode of carbonate from κ^2 to η^1 with one coordination site release (TS1/TS1′), the binding of H_2O (TS2/TS2′), the proton migration (TS3/TS3′), the release of HCO_3^- (TS4/TS4′), and the binding of HTyr* accompanied with H_2O recovery (TS5/TS5′), differing in the steps 1 and 3.

As shown in Figures S1, prior to the proton transfer from water to one of the carbonate ligands in $UO_2(CO_3)_3^{4-}$ (**1a**), a complex forms with the approaching water molecule bridging the two neighboring carbonate groups via two hydrogen bonds (COM1). The transition state TS1 corresponds to the coordination mode change of one carbonate from κ^2 to η^1. This makes the way for the water to access the U atom, as seen from the shortening of U···O18 distance from 4.42 Å in INT1 to 2.80 Å in TS2 to 2.68 Å in INT2 to 2.48 Å in TS3 to 2.39 Å in INT3. This is accompanied by the lengthening of the U···O3 distance, and finally the HCO_3^- is replaced by the OH^- anion (INT4). The leaving of the HCO_3^- anion gives a penta-coordinated intermediate $UO_2(CO_3)_2(OH)^{3-}$ (**U-OH**) and offers room for the entry of a HTyr* ligand. The coordination of HTyr* to U and the proton transfer from HTyr* to the OH^- anion happen concertedly, and in the meantime, the replenished water molecule is repelled by the deprotonated Tyr* ligand, which produces **1b**.

Mechanism III-2 is similar to mechanism III-1 except that in the former the U-O2 but not U-O4 bond broken to release a coordination site in the first step, and the proton H20 migrated to O2 atom but not to O5 atom.

These two mechanisms for Channel III have similar free energy profile. The highest relative free energy (TS4′) along mechanism III-2 is a little higher than that in mechanism III-1 (9.5 kcal/mol vs. 6.8 kcal/mol), while both mechanisms are energetically accessible under physiological condition.

Compared with Channel I, the mechanism III-1 is just marginally lower in energy than Channel I with respect to the highest relative free energy, so the mechanism of Channel I for the first Tyr* binding to uranyl tricarbonate was adopted and discussed in the main text.

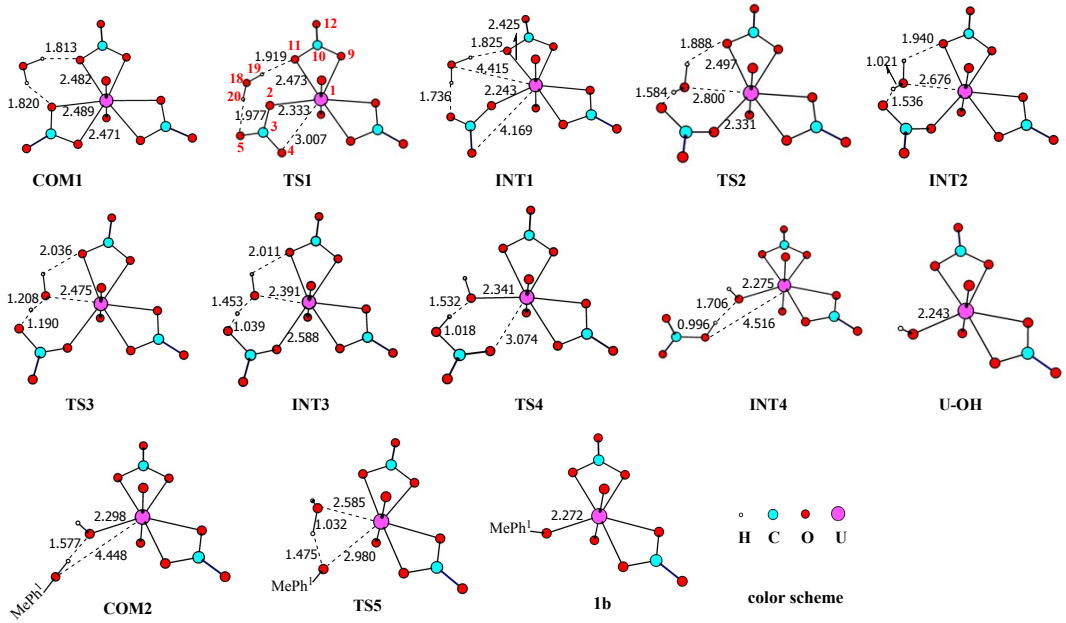


Figure S1. The schematic structures of stationary points following Channel III (mechanism III-1) along with the key geometrical parameters (bond lengths in Å, and bond angles and dihedral angles in degree).

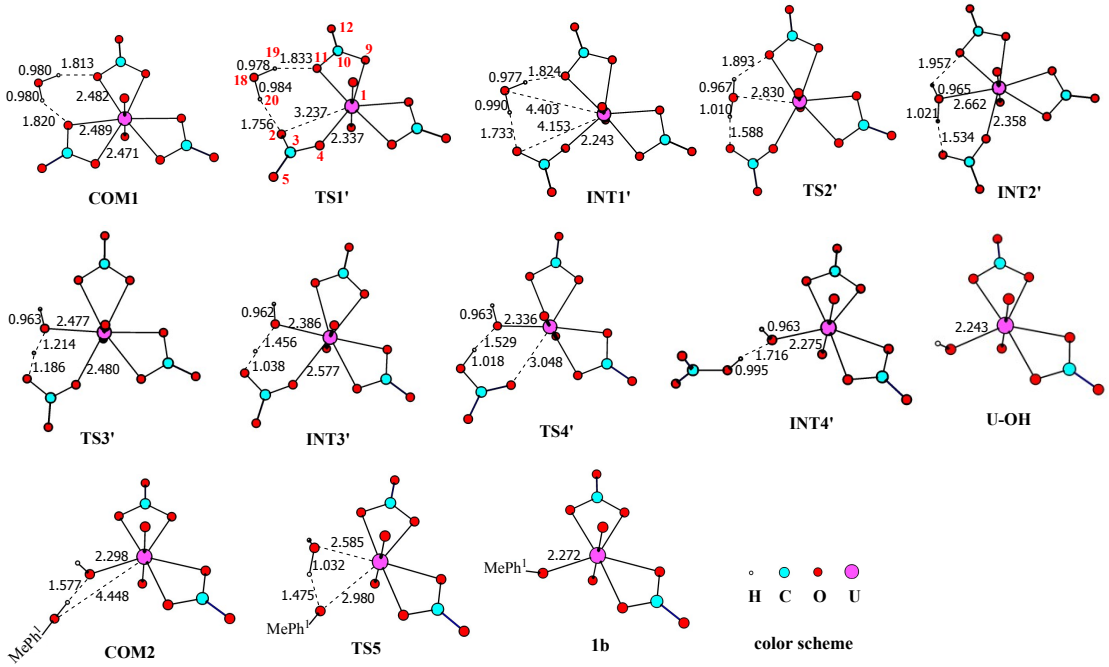


Figure S2. The schematic structures of the stationary points following channel III (mechanism III-2) for the first Tyr* ligand exchange with uranium tricarbonate of the YYD pathway along with the key geometrical parameters (bond lengths in Å, and bond angles and dihedral angles in degree).

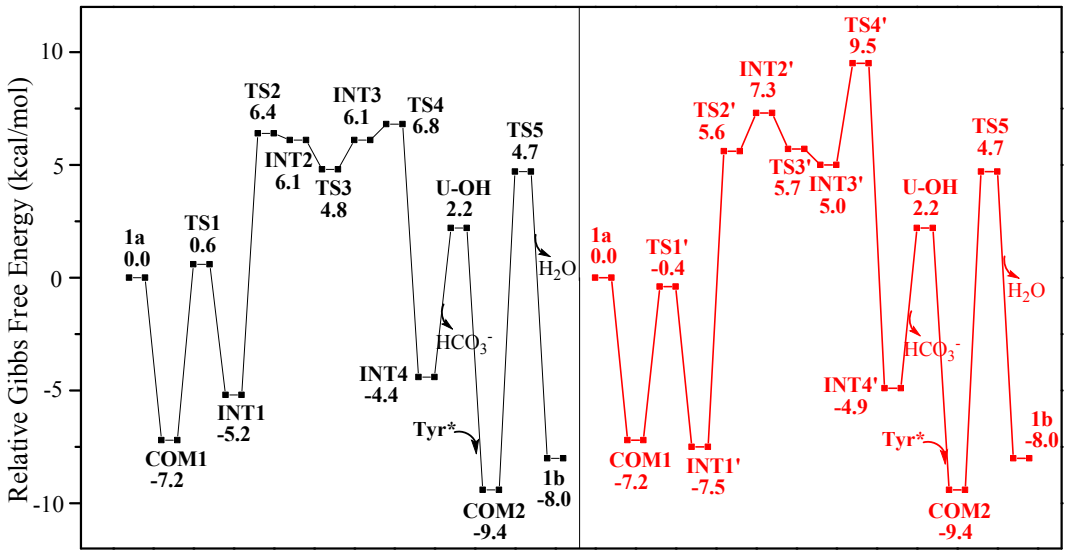


Figure S3. The Gibbs free energy profiles of mechanisms III-1(left) and III-2 (right) of channel III for the first Tyr* ligand exchange with uranium tricarbonate following YYD pathway.

3. Tables and figures

Table S1. The energies (with ZPE correction), enthalpies, and Gibbs free energies (in Hartree at 298 K) of the substances involved in Equation 1-7 and the changes of energies (ΔE), nthalpies (ΔH), and Gibbs free energies (ΔG) (in kcal/mol) for Equation 1-7.

	species	E	ΔE	H	ΔH	G	ΔG
	1a	-1420.02428		-1420.00761		-1420.04860	
	Tyr*	-346.76131		-346.75292		-346.77948	
	1b	-1502.16898		-1502.14797		-1502.20261	
	HCO_3^-	-264.62851		-264.62403		-264.63823	
	H_3O^+	-76.82034		-76.81651		-76.82703	
	U-H_2O	-1232.29602		-1232.28094		-1232.32215	
	H_2O	-76.445283		-76.44150		-76.44962	
	U-OH	-1231.840718		-1231.82607		-1231.85649	
	Asp*	-228.65884		-228.65353		-228.66978	
Eq. 1	**1a + Tyr***	-1766.78559	0.0	-1766.76053	0.0	-1766.82808	0.0
	1b + HCO_3^-	-1766.79749	-7.5	-1766.77200	-7.2	-1766.84084	-8.0
Eq. 2	**1a + H_3O^+**	-1496.84462	0.0	-1496.82412	0.0	-1496.87563	0.0
	U-H_2O + HCO_3^-	-1496.92453	-50.1	-1496.90497	-50.7	-1496.96038	-53.2
Eq. 3	**U-H_2O + Tyr***	-1579.05733	0.0	-1579.03386	0.0	-1579.10163	0.0
	1b + H_3O^+	-1578.98932	42.7	-1578.96448	43.5	-1579.02964	45.2
Eq. 4	**1a + H_2O**	-1496.469563	0.0	-1496.44911	0.0	-1496.49822	0.0
	U-OH + HCO_3^-	-1496.469228	0.2	-1496.45010	-0.6	-1496.49472	2.2
Eq. 5	**U-OH +Tyr***	-1578.602028	0.0	-1578.57899	0.0	-1578.63597	0.0
	1b + H_2O	-1578.614263	-7.7	-1578.58947	-6.6	-1578.65223	-10.2
Eq. 6	**1a + Asp***	-1648.68312	0.0	-1648.66114	0.0	-1648.71838	0.0
	U-3CO_3-Asp*	-1648.76122	-49.0	-1648.63647	15.5	-1648.69264	16.2
Eq. 7	**U-OH + Asp***	-1460.49956	0.0	-1460.47960	0.0	-1460.52627	0.0
	U-2CO_3-Asp*	-1460.58106	-51.1	-1460.46171	11.2	-1460.50834	11.3

Eq. 1 $UO_2(CO_3)_3^{4-}$ (**1a**)+ Tyr* → $UO_2(CO_3)_2(Tyr^*)^{3-}$ (**1b**)+ HCO_3^-

Eq. 2 $UO_2(CO_3)_3^{4-}$ (**1a**) + H_3O^+ → $UO_2(CO_3)_2(H_2O)^{2-}$ (**U-H_2O**) + HCO_3^-

Eq. 3 $UO_2(CO_3)_2(H_2O)^{2-}$ (**U-H_2O**) + Tyr* → $UO_2(CO_3)_2(Tyr^*)^{3-}$ (**1b**) + H_3O^+

Eq. 4 $UO_2(CO_3)_3^{4-}$ (**1a**) + H_2O → $UO_2(CO_3)_2(OH)^{3-}$ (**U-OH**) + HCO_3^-

Eq. 5 $UO_2(CO_3)_2(OH)^{3-}$ (**U-OH**)+ Tyr* → $UO_2(CO_3)_2(Tyr^*)^{3-}$ (**1b**)+ H_2O

Eq. 6 $UO_2(CO_3)_3^{4-}$ (**1a**)+ Asp^{*-}→ $UO_2(Asp^*)(CO_3)_3^{5-}$ (**U-3CO3-Asp***)

Eq. 7 $UO_2(CO_3)_2(OH)^{3-}$ + Asp^{*-} → $UO_2(CO_3)_2(OH)(Asp^*)^{4-}$ (**U-2CO3-Asp***)

Table S2. The natural charge of key atoms of the stationary points involved in the ligand exchange of two CO_3^{2-} by the first Tyr* and by the second Tyr* ligand.

	U1	O2	C3	O4	O5	O7
1a	1.305	-0.740	0.980	-0.740		
COM1a	1.318	-0.730	1.002	-0.722	-0.843	-0.755
TS1a	1.481	-0.752	0.996	-0.819	-0.864	-0.759
INT1a	1.433	-0.729	1.010	-0.841	-0.866	-0.755
TS2a	1.460	-0.719	1.024	-0.797	-0.799	-0.825
INT2a	1.466	-0.713	1.026	-0.782	-0.785	-0.855
TS3a	1.457	-0.707	1.015	-0.800	-0.796	-0.782
INT3a	1.362	-0.703	1.001	-0.817	-0.799	-0.729
TS4a	1.418	-0.732	0.985	-0.831	-0.808	-0.728
INT4a	1.461	-0.845	0.969	-0.842	-0.807	-0.726
	U1	**O9**	**C10**	**O11**	**O12**	**O14**
COM1b	1.450	-0.729	1.007	-0.742	-0.822	-0.751
TS1b	1.657	-0.827	1.003	-0.761	-0.856	-0.756
INT1b	1.660	-0.834	1.008	-0.754	-0.858	-0.755
TS2b	1.665	-0.783	1.025	-0.732	-0.790	-0.827
INT2b	1.667	-0.780	1.026	-0.731	-0.787	-0.833
TS3b	1.643	-0.778	1.025	-0.727	-0.783	-0.828
INT3b	1.411	-0.779	1.014	-0.708	-0.777	-0.777
TS4b	1.640	-0.834	0.973	-0.807	-0.805	-0.741
INT4b	1.686	-0.840	0.969	-0.845	-0.806	-0.746

Table S3. The Mayer atomic bond order of key bonds of the stationary points involved in the ligand exchange of two CO_3^{2-} by the first Tyr* and by the second Tyr* ligand.

	U1-O2	U1-O4	U1-O7	O5-H6	O7-H6
COM1a	0.447	0.401	-0.001	0.147	0.520
TS1a	0.489	0.076	0.002	0.136	0.526
INT1a	0.433	-0.005	-0.005	0.123	0.568
TS2a	0.396	-0.007	-0.001	0.378	0.235
INT2a	0.373	-0.004	0.001	0.515	0.177

TS3a	0.447	0.016	0.092	0.622	0.300
INT3a	0.350	0.019	0.366	0.744	0.249
TS4a	0.179	0.012	0.359	0.773	0.218
INT4a	0.002	0.002	0.385	0.820	0.044
	U1-O9	**U1-O11**	**U1-O14**	**O12-H13**	**O14-H13**
COM1b	0.364	0.435	0.000	0.136	0.546
TS1b	0.027	0.511	0.003	0.119	0.552
INT1b	0.000	0.509	0.001	0.124	0.556
TS2b	-0.002	0.360	0.003	0.446	0.236
INT2b	-0.003	0.361	0.017	0.473	0.221
TS3b	0.003	0.349	0.063	0.509	0.235
INT3b	0.013	0.332	0.341	0.712	0.211
TS4b	0.001	0.053	0.447	0.784	0.111
INT4b	0.002	0.000	0.428	0.817	0.044

Table S4. The total energies (E′), zero-point energy corrected total energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree at 298 K) of the stationary points following pathway YYD and the corresponding relative energies (ΔE′, ΔE, ΔH, and ΔG in kcal/mol) (corresponding to Figure 3).

species	E′	ΔE′	E	ΔE	H	ΔH	G	ΔG
1a	-1420.07717		-1420.02428		-1420.00761		-1420.04860	
HTyr*	-346.89242		-346.76131		-346.75292		-346.77948	
1a+ HTyr*	-1766.96959	0.0	-1766.78559	0.0	-1766.76053	0.0	-1766.82808	0.0
COM1a	-1766.98664	-10.7	-1766.80161	-10.1	-1766.77599	-9.7	-1766.83984	-7.4
TS1a	-1766.97688	-4.6	-1766.79294	-4.6	-1766.76793	-4.6	-1766.83201	-2.5
INT1a	-1766.98183	-7.7	-1766.79782	-7.7	-1766.77194	-7.2	-1766.83916	-7.0
TS2a	-1766.97838	-5.5	-1766.79827	-8.0	-1766.77284	-7.7	-1766.83683	-5.5
INT2a	-1766.97856	-5.6	-1766.79603	-6.6	-1766.77010	-6.0	-1766.83592	-4.9
TS3a	-1766.96271	4.3	-1766.77886	4.2	-1766.75410	4.0	-1766.81499	8.2
INT3a	-1766.96765	1.2	-1766.78243	2.0	-1766.75689	2.3	-1766.82087	4.5
TS4a	-1766.96608	2.2	-1766.78109	2.8	-1766.75614	2.8	-1766.81811	6.3
INT4a	-1766.98361	-8.8	-1766.79937	-8.7	-1766.77297	-7.8	-1766.84081	-8.0
1b	-1502.32600		-1502.16898		-1502.14797		-1502.20261	
HCO_3^-	-264.65443		-264.62851		-264.62403		-264.63823	

1b+ HCO_3^-	-1766.98043	-6.8	-1766.79749	-7.5	-1766.77200	-7.2	-1766.84084	-8.0
1a+2HTyr*-HCO_3^-	-1849.20760	0.0	-1848.91838	0.0	-1848.88943	0.0	-1848.96933	0.0
COM1b	-1849.23398	-16.6	-1848.94502	-16.7	-1848.91479	-15.9	-1848.99171	-14.0
TS1b	-1849.21929	-7.3	-1848.93110	-8.0	-1848.90155	-7.6	-1848.97644	-4.5
INT1b	-1849.21982	-7.7	-1848.93171	-8.4	-1848.90126	-7.4	-1848.97839	-5.7
TS2b	-1849.21572	-5.1	-1848.93041	-7.5	-1848.90070	-7.1	-1848.97555	-3.9
INT2b	-1849.21572	-5.1	-1848.92969	-7.1	-1848.89928	-6.2	-1848.97535	-3.8
TS3b	-1849.21462	-4.4	-1848.92785	-5.9	-1848.89847	-5.7	-1848.97137	-1.3
INT3b	-1849.22970	-13.9	-1848.94009	-13.6	-1848.91014	-13.0	-1848.98430	-9.4
TS4b	-1849.21786	-6.4	-1848.92890	-6.6	-1848.89919	-6.1	-1848.97406	-3.0
INT4b	-1849.22104	-8.4	-1848.93232	-8.7	-1848.90164	-7.7	-1848.97921	-6.2
1c	-1661.03359		-1660.74744		-1660.71917		-1660.79039	
1c-H_2O+ HCO_3^-	-1849.22154	-8.7	-1848.93067	-7.7	-1848.90170	-7.7	-1848.97900	-6.1
Asp*	-228.70704		-228.65884		-228.65353		-228.66978	
H_2O	-76.46648		-76.445283		-76.44150		-76.44962	
1a+2HTyr*+Asp* +H_2O - 2HCO_3^-	-1889.72668	0.0	-1889.39398	0.0	-1889.36043	0.0		0.0
TS1c	-1889.73811	-7.2	-1889.40313	-5.7	-1889.36926	-5.5	-1889.45264	-1.4
INT1c	-1889.75253	-16.2	-1889.41716	-14.5	-1889.38280	-14.0	-1889.46694	-10.3
Prod	-1813.27556		-1812.96464		-1812.93323		-1813.01227	
Prod+H_2O	-1889.74204	-9.6	-1889.40992	-10.0	-1889.37473	-9.0	-1889.46189	-7.2

Table S5. The total energies (E′), zero-point energy corrected total energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree at 298 K) of the stationary points following pathway YDY and the corresponding relative energies (ΔE′, ΔE, ΔH, and ΔG in kcal/mol) (corresponding to Figure 6).

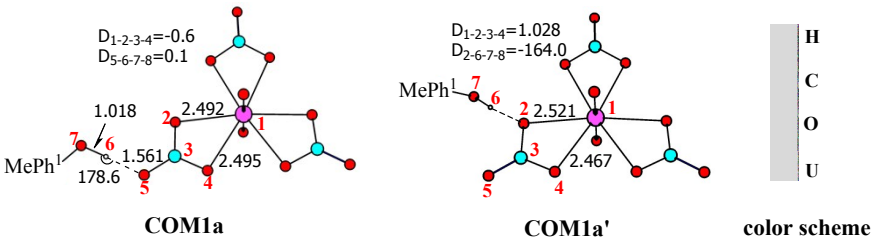
species	E′	ΔE′	E	ΔE	H	ΔH	G	ΔG
1a	-1420.07717		-1420.02428		-1420.00761		-1420.04860	
HTyr*	-346.89242		-346.76131		-346.75292		-346.77948	
1a+ HTyr*	-1766.96959	0.0	-1766.78559	0.0	-1766.76053	0.0	-1766.82808	0.0
1b	-1502.32600		-1502.16898		-1502.14797		-1502.20261	
HCO_3^-	-264.65443		-264.62851		-264.62403		-264.63823	
1b+ HCO_3^-	-1766.98043	-6.8	-1766.79749	-7.5	-1766.77200	-7.2	-1766.84084	-8.0
Asp*	-228.70704		-228.65884		-228.65353		-228.66978	

1a+ HTyr*+ Asp*- HCO_3^-	-1731.02220	0.0	-1730.81592	0.0	-1730.79003	0.0	-1730.85963	0.0
TS1b′	-1731.00736	9.3	-1730.80085	9.5	-1730.77460	9.7	-1730.84042	12.1
INT1b′	-1731.00928	8.1	-1730.80296	8.1	-1730.77563	9.0	-1730.84412	9.7
1a+ 2HTyr*+ Asp*- HCO_3^-	-2077.91462	0.0	-2077.57723	0.0	-2077.54295	0.0	-2077.63911	0.0
COM1c′	-2077.91936	-3.0	-2077.58040	-2.0	-2077.54452	-1.0	-2077.63263	4.0
TS1c′	-2077.91494	-0.2	-2077.57690	0.2	-2077.54162	0.8	-2077.62932	6.1
INT1c′	-2077.93034	-9.9	-2077.59222	-9.4	-2077.55621	-8.3	-2077.64420	-3.2
TS2c′	-2077.92834	-8.6	-2077.59404	-10.5	-2077.55842	-9.7	-2077.64468	-3.5
INT2c′	-2077.92973	-9.5	-2077.59231	-9.5	-2077.55609	-8.2	-2077.64518	-3.8
TS3c′	-2077.91391	0.4	-2077.57583	0.9	-2077.54023	1.7	-2077.62810	6.9
INT3c′	-2077.93330	-11.7	-2077.59435	-10.7	-2077.55802	-9.5	-2077.64682	-4.9
Prod	-1813.27556		-1812.96464		-1812.93323		-1813.01227	
Prod+ HCO_3^-	-2077.92999	-9.6	-2077.59315	-10.0	-2077.55726	-9.0	-2077.65050	-7.2

Table S6. The total energies (E′), zero-point energy corrected total energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree at 298 K) of the stationary points following mechanism III-1 and III-2 of channel III for the first Tyr* ligand exchange with uranium tricarbonate following YYD pathway and the corresponding relative energies (ΔE′, ΔE, ΔH, and ΔG in kcal/mol) (corresponding to Figure S3).

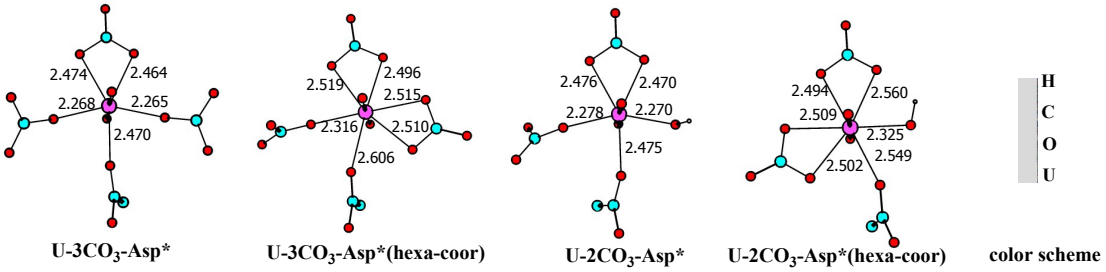
species	E′	ΔE′	E	ΔE	H	ΔH	G	ΔG
1a	-1420.07717		-1420.02428		-1420.00761		-1420.04860	
H_2O	-76.46648		-76.445283		-76.44150		-76.44962	
1a + H_2O	-1496.54365	0.0	-1496.469563	0.0	-1496.44911	0.0	-1496.49822	0.0
COM1	-1496.56023	-10.4	-1496.48219	-7.9	-1496.46299	-8.7	-1496.50963	-7.2
TS1	-1496.54753	-2.4	-1496.46993	-0.2	-1496.45139	-1.4	-1496.49727	0.6
INT1	-1496.55820	-9.1	-1496.48081	-7.1	-1496.46145	-7.7	-1496.50647	-5.2
TS2	-1496.53912	2.8	-1496.46182	4.9	-1496.44342	3.6	-1496.48802	6.4
INT2	-1496.53926	2.8	-1496.46172	4.9	-1496.44281	4.0	-1496.48850	6.1
TS3	-1496.53695	4.2	-1496.46341	3.9	-1496.44478	2.7	-1496.49061	4.8
INT3	-1496.53808	3.5	-1496.46100	5.4	-1496.44204	4.4	-1496.48847	6.1
TS4	-1496.53652	4.5	-1496.45929	6.4	-1496.44114	5.0	-1496.48745	6.8
INT4	-1496.55155	-5.0	-1496.47486	-3.3	-1496.45523	-3.8	-1496.50529	-4.4
U-OH	-1231.88969		-1231.840718		-1231.82607		-1231.85649	

HCO_3^-	-264.65443		-264.62851		-264.62403		-264.63823	
U-OH + HCO_3^-	-1496.54412	-0.3	-1496.46923	0.2	-1496.45010	-0.6	-1496.49472	2.2
HTyr*	-346.89242		-346.76131		-346.75292		-346.77948	
1a + H_2O + HTyr*- HCO_3^-	-1578.78164	0.0	-1578.602363	0.0	-1578.57800	0.0	-1578.63947	0.0
COM2	-1578.79839	-10.5	-1578.61687	-9.1	-1578.59329	-9.6	-1578.65452	-9.4
TS5	-1578.77782	2.4	-1578.59669	3.6	-1578.57427	2.3	-1578.63192	4.7
1b	-1502.32600		-1502.16898		-1502.14797		-1502.20261	
1b + H_2O	-1578.79248	-6.8	-1578.61426	-7.5	-1578.58947	-7.2	-1578.65223	-8.0
TS1′	-1496.54965	-3.8	-1496.47252	-1.9	-1496.45381	-2.9	-1496.49893	-0.4
INT1′	-1496.55819	-9.1	-1496.48077	-7.0	-1496.46146	-7.7	-1496.51010	-7.5
TS2′	-1496.53905	2.9	-1496.46164	5.0	-1496.44332	3.6	-1496.48935	5.6
INT2′	-1496.53924	2.8	-1496.46179	4.9	-1496.44276	4.0	-1496.48653	7.3
TS3′	-1496.53708	4.1	-1496.46337	3.9	-1496.44489	2.6	-1496.48912	5.7
INT3′	-1496.53812	3.5	-1496.46132	5.2	-1496.44221	4.3	-1496.49020	5.0
TS4′	-1496.53640	4.5	-1496.45943	6.4	-1496.44107	5.0	-1496.48308	9.5
INT4′	-1496.55150	-4.9	-1496.47480	-3.3	-1496.45517	-3.8	-1496.50605	-4.9



species	E	Δ E	H	Δ H	G	Δ G
COM1a	-1766.801608	0.0	-1766.775988	0.0	-1766.839840	0.0
COM1a′	-1766.799484	1.3	-1766.773945	1.3	-1766.837300	1.6

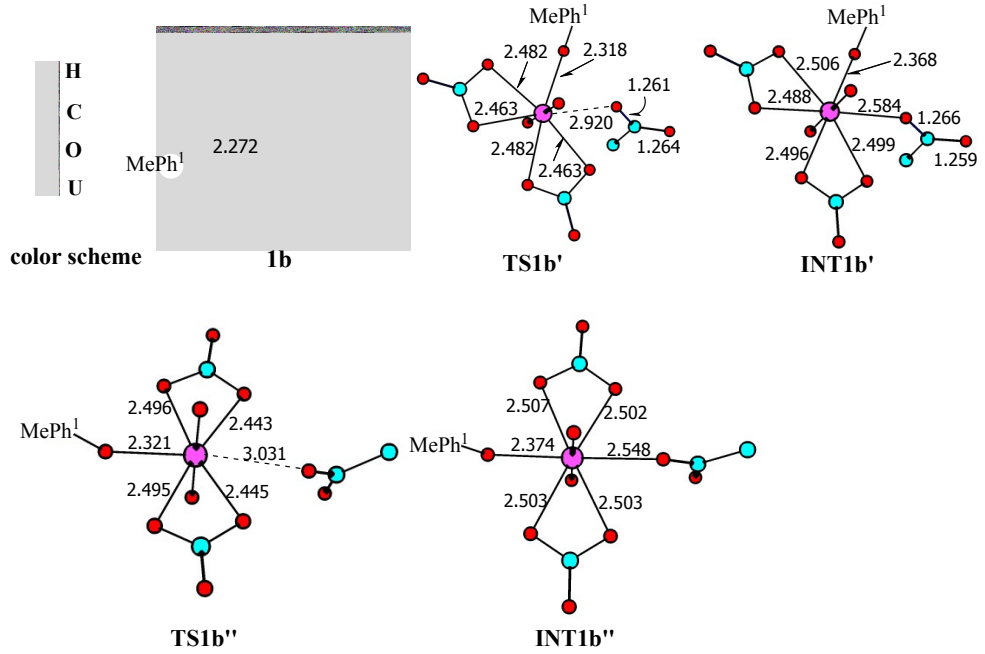
Figure S4. The schematic structures of COM1a and COM1a′ with the key geometrical parameters (bond lengths in Å, and bond angles and dihedral angles in degree). The energies (with ZPE correction), enthalpies, and Gibbs free energies (in Hartree at 298 K) of these two structures and the corresponding relative values (in kcal/mol) are listed in the followed table. The aromatic C atom of p-cresol that is bonded to its hydroxyl group is numbered as 8.



U-3CO$_3$-Asp* U-3CO$_3$-Asp*(hexa-coor) U-2CO$_3$-Asp* U-2CO$_3$-Asp*(hexa-coor) color scheme

species	E	ΔE	H	ΔH	G	ΔG
U-3CO$_3$-Asp*	-1648.659281	0.0	-1648.636469	0.0	-1648.692640	0.0
U-3CO$_3$-Asp*(hexa-coor)	-1648.647071	7.7	-1648.624257	7.7	-1648.680090	7.9
U-2CO$_3$-Asp*	-1460.48229	0.0	-1460.461705	0.0	-1460.50834	0.0
U-2CO$_3$-Asp*(hexa-coor)	-1460.474246	5.0	-1460.453974	4.9	-1460.50212	3.9

Figure S5. The schematic structures of penta- and hexa-coordinated (in the equatorial plane) U-3CO$_3$-Asp* and U-2CO$_3$-Asp* with the key geometrical parameters (bond lengths in Å). The energies (with ZPE correction), enthalpies, and Gibbs free energies (in Hartree at 298 K) of these structures and the corresponding relative values (in kcal/mol) are listed in the followed table.



color scheme 1b TS1b' INT1b' TS1b'' INT1b''

Figure S6. The schematic structures of the stationary points involved in Asp* binding to

uranium of 1b in the YDY pathway along with the key geometrical parameters (bond length in Å, and bond angle and dihedral angle in degree). There are two possible attacking sites, i. e., between Tyr* and carbonate groups (top), and between two carbonate groups (below).

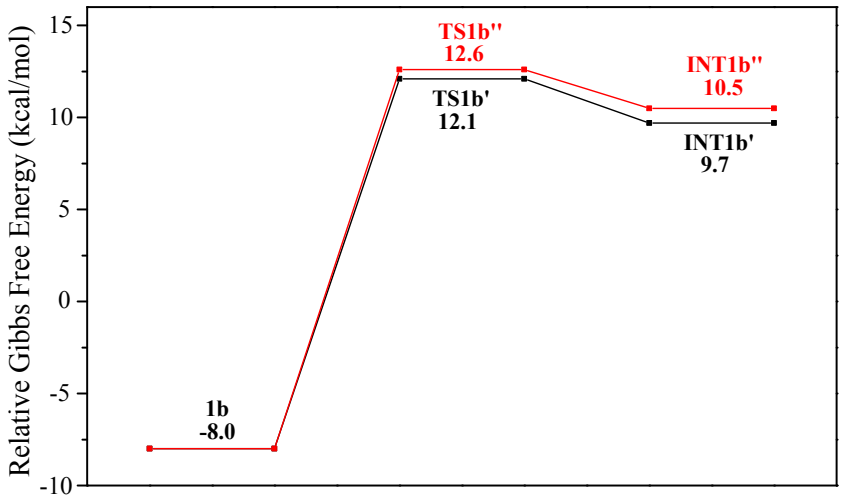


Figure S7. The Gibbs free energy profiles for the Asp* binding to uranium of 1b in the YDY pathway. There are two possible attacking sites, i. e., between Tyr* and carbonate groups (black), and between two carbonate groups (red).

4. Coordinates and energies of stationary points

1a

E(B3LYP)= -1420.077172 Hartree

Zero-point correction= 0.052894(Hartree/Particle)

Sum of electronic and zero-point Energies= -1420.024278 Hartree

Sum of electronic and thermal Enthalpies= -1420.00761 Hartree

Sum of electronic and thermal Free Energies= -1420.04860 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.000494	0.000219	-0.000058
2	8	0.589726	2.396605	0.000057
3	8	-1.986685	1.462434	0.000124
4	8	2.260373	0.986672	0.000237
5	8	-2.370135	-0.690224	-0.000688
6	8	1.780813	-1.704709	0.000485
7	8	-0.273095	-2.45245	0.00026
8	6	-2.885811	0.512116	-0.000092
9	6	1.88879	2.240936	0.000009
10	6	0.999886	-2.75405	0.000507
11	8	1.431074	-3.935047	-0.000381
12	8	2.700316	3.201287	0.000005
13	8	-4.123879	0.732811	0.000389
14	8	-0.002158	0.000506	-1.818329
15	8	-0.002818	0.000344	1.818193

Tyr*

E(B3LYP)= -346.8924241Hartree

Zero-point correction= 0.131119 (Hartree/Particle)

Sum of electronic and zero-point Energies= -346.761305 Hartree

Sum of electronic and thermal Enthalpies = -346.752924 Hartree

Sum of electronic and thermal Free Energies= -346.779480 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	6	1.434045	0.014563	0.000011
2	6	0.727704	1.223546	0.000001
3	6	0.750365	-1.205452	-0.00001
4	1	1.274467	2.16051	-0.000028
5	1	1.295633	-2.145162	-0.000038
6	6	-0.670438	1.204139	-0.00001
7	6	-0.653155	-1.206867	0.000003

8	1	-1.211984	2.146401	-0.000022
9	1	-1.178379	-2.157945	-0.000025
10	6	-1.388919	-0.009337	0.000009
11	6	-2.903502	-0.015296	0.000003
12	1	-3.306765	0.497528	0.882587
13	1	-3.306765	0.497578	-0.882547
14	1	-3.29462	-1.037743	-0.000017
15	8	2.835858	0.098338	0.000005
16	1	3.264957	-0.779645	0.000014

H_3O^+

E(B3LYP)= -76.8552263 Hartree

Zero-point correction= 0.034885 (Hartree/Particle)

Sum of electronic and zero-point Energies= -76.820342 Hartree

Sum of electronic and thermal Enthalpies= -76.816513 Hartree

Sum of electronic and thermal Free Energies= -76.827030 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	8	0.00000	0.00000	0.083075
2	1	0.00000	0.929627	-0.221533
3	1	-0.80508	-0.464813	-0.221533
4	1	0.80508	-0.464813	-0.221533

HCO_3^-

E(B3LYP)= -264.6544267 Hartree

Zero-point correction= 0.025915 (Hartree/Particle)

Sum of electronic and zero-point Energies= -264.628512 Hartree

Sum of electronic and thermal Enthalpies= -264.624030 Hartree

Sum of electronic and thermal Free Energies= -264.638230 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	8	1.02429	0.85776	0.00000
2	6	0.00000	0.15197	0.00000
3	8	-1.208264	0.476207	0.00000
4	8	0.259395	-1.238913	0.00000
5	1	-0.60339	-1.672271	0.00000

U-H_2O

E(B3LYP)= -1232.3580936 Hartree

Zero-point correction= 0.062077 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1232.296016 Hartree

Sum of electronic and thermal Enthalpies= -1232.280939 Hartree

Sum of electronic and thermal Free Energies= -1232.322150 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.01139	-0.09929	0.011469
2	8	-2.20948	0.872441	0.004895
3	8	-2.026934	-1.309952	-0.020832
4	8	2.057554	-1.282255	-0.021465
5	8	2.196125	0.905291	0.001138
6	6	-2.848594	-0.27728	-0.025273
7	6	2.857635	-0.230565	-0.024543
8	8	4.097299	-0.313153	-0.048915
9	8	-4.085917	-0.38356	-0.054481
10	8	0.008452	-0.096479	1.812666
11	8	0.007443	-0.036861	-1.787644
12	8	-0.117137	2.460073	0.097213
13	1	0.496827	2.971084	-0.443366
14	1	-1.018415	2.686324	-0.173426

COM1a

E(B3LYP)= -1766.986639 Hartree

Zero-point correction= 0.185031 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.801608 Hartree

Sum of electronic and thermal Enthalpies = -1766.775988 Hartree

Sum of electronic and thermal Free Energies= -1766.839840 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	1.934159	0.023408	-0.000502
2	8	-0.474846	-0.615455	-0.020818
3	8	-0.052325	1.533063	-0.026471
4	8	2.554019	2.402422	-0.004315
5	8	4.203809	0.969100	0.022592
6	6	-0.94498	0.593466	-0.029853
7	6	3.851587	2.229585	0.01426
8	8	4.674783	3.178224	0.023456
9	8	-2.194635	0.844717	-0.041171
10	8	1.942712	0.019002	-1.815752
11	8	1.902433	0.030811	1.814609
12	6	-6.272533	-1.471869	-0.002391
13	6	-7.587399	-1.014697	0.006822
14	6	-5.202811	-0.564504	-0.011399
15	1	-8.395633	-1.740342	0.010581
16	6	-7.890658	0.35363	0.009035
17	6	-5.490282	0.808542	-0.013854

18	1	-4.673966	1.52142	-0.026734
19	6	-6.814868	1.247645	-0.004581
20	1	-7.010742	2.316008	-0.009794
21	1	-6.058005	-2.535131	-0.006583
22	6	-9.32112	0.839864	0.050697
23	1	-9.976068	0.208553	-0.555923
24	1	-9.718919	0.830076	1.071977
25	1	-9.402539	1.864428	-0.32001
26	8	-3.941116	-1.053395	-0.022377
27	1	-3.240696	-0.314528	-0.029721
28	8	3.675085	-1.710777	0.02233
29	6	2.871249	-2.743393	0.012192
30	8	1.60515	-2.410977	-0.000403
31	8	3.273033	-3.93344	0.014166

COM1a-2

E(B3LYP)= -1766.9847444 Hartree

Zero-point correction= 0.185260 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.799484 Hartree

Sum of electronic and thermal Enthalpies = -1766.773945 Hartree

Sum of electronic and thermal Free Energies= -1766.837300 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	1.608404	-0.00595	0.018407
2	8	2.280125	2.347579	0.278263
3	8	0.14281	1.953956	0.049073
4	8	-0.820069	-0.602429	-0.300779
5	8	0.61519	-2.249495	-0.238921
6	6	1.076254	2.856095	0.219993
7	6	-0.633104	-1.907637	-0.376544
8	8	-1.568162	-2.719061	-0.561626
9	8	0.838123	4.085319	0.318741
10	8	1.425204	-0.156335	1.818204
11	8	1.776307	0.137277	-1.783505
12	6	-5.25068	1.138558	-0.915437
13	6	-6.507105	0.870175	-0.381292
14	6	-4.155932	0.316748	-0.606782
15	1	-7.337021	1.522803	-0.637094
16	6	-6.723831	-0.21685	0.477527
17	6	-4.355533	-0.775932	0.246637
18	1	-3.522045	-1.434603	0.463222
19	6	-5.623385	-1.026391	0.775654
20	1	-5.755147	-1.881498	1.432378

21	1	-5.100883	1.986449	-1.57528
22	6	-8.094983	-0.500431	1.046998
23	1	-8.474894	0.349024	1.623776
24	1	-8.824691	-0.702378	0.255889
25	1	-8.074597	-1.369255	1.708622
26	8	-2.956283	0.612924	-1.161185
27	1	-2.19276	0.06944	-0.783471
28	8	3.307342	-1.788963	0.032064
29	6	4.347857	-1.010398	0.187742
30	8	4.03552	0.258379	0.266902
31	8	5.527827	-1.436177	0.254208

TS1a

E(B3LYP)= -1766.976882 Hartree

Zero-point correction= 0.183939 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.792943 Hartree

Sum of electronic and thermal Enthalpies = -1766.767929 Hartree

Sum of electronic and thermal Free Energies= -1766.832010 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	1.713353	0.039877	-0.034221
2	8	-0.500679	-0.344735	0.66578
3	8	0.058673	-2.348006	1.470196
4	8	2.751708	-2.091734	-0.431243
5	8	4.00406	-0.342917	-0.8387
6	6	-0.802664	-1.424845	1.364773
7	6	3.920645	-1.647458	-0.844917
8	8	4.84967	-2.405005	-1.205022
9	8	-1.970837	-1.489212	1.905126
10	8	2.312305	0.059346	1.673096
11	8	1.123261	0.026517	-1.746792
12	6	-5.716823	1.080315	0.753105
13	6	-6.721846	0.914821	-0.196862
14	6	-4.648675	0.173109	0.828695
15	1	-7.534214	1.635065	-0.232114
16	6	-6.709052	-0.152483	-1.104383
17	6	-4.619355	-0.896526	-0.080861
18	1	-3.797426	-1.601817	-0.040235
19	6	-5.63556	-1.046693	-1.024221
20	1	-5.585772	-1.882517	-1.716343
21	1	-5.744782	1.915206	1.445229
22	6	-7.822577	-0.345331	-2.108174
23	1	-8.64539	-0.935127	-1.687683

24	1	-8.242234	0.612126	-2.427503
25	1	-7.468916	-0.872006	-2.998044
26	8	-3.695182	0.366992	1.764294
27	1	-2.969794	-0.367335	1.750598
28	8	2.798961	2.179194	-0.430256
29	6	1.783057	2.933434	-0.084984
30	8	0.729404	2.241306	0.280082
31	8	1.8133	4.185459	-0.101391

INT1a

E(B3LYP)= -1766.981836 Hartree

Zero-point correction= 0.184081 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.797754 Hartree

Sum of electronic and thermal Enthalpies = -1766.771914 Hartree

Sum of electronic and thermal Free Energies= -1766.839160 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	1.664091	0.070875	-0.069562
2	8	-0.242363	-2.802161	1.957366
3	8	-0.206149	-1.023732	0.592398
4	8	0.611666	2.142315	0.559007
5	8	2.642584	2.28905	-0.267308
6	6	-0.759906	-1.715019	1.59354
7	6	1.609315	2.934239	0.220418
8	8	1.569591	4.176541	0.353733
9	8	-1.823515	-1.221426	2.122658
10	8	0.96904	0.222693	-1.738467
11	8	2.346583	-0.085082	1.602127
12	6	-4.603389	-0.917422	0.27084
13	6	-5.757404	-1.21251	-0.454336
14	6	-4.248988	0.417214	0.525467
15	1	-6.00994	-2.25383	-0.633229
16	6	-6.595764	-0.208124	-0.951861
17	6	-5.084087	1.432656	0.036232
18	1	-4.822001	2.466756	0.232776
19	6	-6.233058	1.11843	-0.686051
20	1	-6.861801	1.926058	-1.049693
21	1	-3.973527	-1.712948	0.651879
22	6	-7.825868	-0.541126	-1.764614
23	1	-8.585253	0.239744	-1.67526
24	1	-7.588376	-0.642582	-2.829894
25	1	-8.272655	-1.485141	-1.442114
26	8	-3.147066	0.764549	1.2254

27	1	-2.594229	-0.046905	1.524481
28	8	3.863306	-0.345155	-1.008627
29	6	3.733042	-1.648634	-1.097845
30	8	2.570413	-2.087355	-0.662452
31	8	4.621921	-2.40147	-1.552086

TS2a

E(B3LYP)= -1766.978382Hartree

Zero-point correction = 0.180108 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.798274 Hartree

Sum of electronic and thermal Enthalpies = -1766.772838 Hartree

Sum of electronic and thermal Free Energies= -1766.836830 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	1.598609	0.097865	-0.075665
2	8	-0.054329	-2.834207	2.027317
3	8	-0.264675	-1.057965	0.671371
4	8	0.531803	2.118575	0.645532
5	8	2.517462	2.33189	-0.267437
6	6	-0.668089	-1.815874	1.66092
7	6	1.493948	2.943906	0.28172
8	8	1.432178	4.17996	0.445963
9	8	-1.789808	-1.460823	2.262932
10	8	0.816335	0.262865	-1.699179
11	8	2.355036	-0.084529	1.55638
12	6	-4.406606	-1.011959	0.116399
13	6	-5.484491	-1.174626	-0.752233
14	6	-4.107786	0.248033	0.693203
15	1	-5.676859	-2.161266	-1.16682
16	6	-6.325094	-0.11071	-1.103111
17	6	-4.964189	1.31867	0.336857
18	1	-4.768555	2.297435	0.764457
19	6	-6.036143	1.136927	-0.533322
20	1	-6.667023	1.989217	-0.773931
21	1	-3.781843	-1.863027	0.366196
22	6	-7.469855	-0.292616	-2.074032
23	1	-8.285359	0.405322	-1.864963
24	1	-7.15725	-0.120766	-3.111224
25	1	-7.876769	-1.306469	-2.025392
26	8	-3.099041	0.4394	1.524916
27	1	-2.359896	-0.57631	1.835514
28	8	3.743808	-0.267622	-1.125384
29	6	3.63054	-1.572652	-1.227342

30	8	2.495432	-2.032778	-0.742476
31	8	4.50682	-2.305054	-1.732056

INT2a

E(B3LYP)= -1766.978564 Hartree

Zero-point correction = 0.182534 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.79603 Hartree

Sum of electronic and thermal Enthalpies = -1766.770099 Hartree

Sum of electronic and thermal Free Energies= -1766.835920 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	1.559476	0.105433	-0.075651
2	8	0.102966	-2.799227	2.266037
3	8	-0.217968	-1.094548	0.837528
4	8	0.52391	2.092084	0.764502
5	8	2.398586	2.357618	-0.346591
6	6	-0.555373	-1.833591	1.853291
7	6	1.427412	2.942235	0.316771
8	8	1.361425	4.17347	0.508541
9	8	-1.701085	-1.516419	2.462716
10	8	0.617527	0.251878	-1.612164
11	8	2.471062	-0.061851	1.475435
12	6	-4.244283	-1.010112	0.041032
13	6	-5.256525	-1.153304	-0.907212
14	6	-4.053948	0.206473	0.751398
15	1	-5.36094	-2.106547	-1.420447
16	6	-6.139869	-0.11195	-1.218022
17	6	-4.958853	1.254825	0.428789
18	1	-4.852739	2.200534	0.952658
19	6	-5.962954	1.092741	-0.521366
20	1	-6.630272	1.926837	-0.726765
21	1	-3.583124	-1.844919	0.252235
22	6	-7.21312	-0.266128	-2.272187
23	1	-8.141869	0.231727	-1.977226
24	1	-6.909966	0.167001	-3.233333
25	1	-7.443083	-1.319746	-2.451978
26	8	-3.115265	0.36949	1.654094
27	1	-2.242907	-0.721091	2.021733
28	8	3.596745	-0.226062	-1.325325
29	6	3.501244	-1.534457	-1.404582
30	8	2.419622	-2.009502	-0.820384
31	8	4.346319	-2.256184	-1.972448

TS3a

E(B3LYP)= -1766.962707 Hartree

Zero-point correction= 0.183851 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.778857 Hartree

Sum of electronic and thermal Enthalpies = -1766.754097 Hartree

Sum of electronic and thermal Free Energies= -1766.814990 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	1.105086	-0.180765	0.027165
2	8	0.061885	4.185513	0.065289
3	8	0.109734	1.979477	0.484568
4	8	-0.247137	-2.117739	-0.517721
5	8	1.891017	-2.494825	-0.322048
6	6	-0.255379	3.010646	-0.192983
7	6	0.713921	-3.008345	-0.556377
8	8	0.516346	-4.224546	-0.794025
9	8	-1.058333	2.781297	-1.253719
10	8	0.809788	-0.53443	1.774107
11	8	1.393879	0.196692	-1.713353
12	6	-4.002593	0.929658	-0.930728
13	6	-5.267973	0.707655	-0.388159
14	6	-2.875366	0.159468	-0.53766
15	1	-6.097922	1.32603	-0.722652
16	6	-5.500387	-0.287643	0.56905
17	6	-3.124043	-0.853163	0.426512
18	1	-2.290364	-1.477483	0.724383
19	6	-4.395523	-1.061925	0.953684
20	1	-4.534537	-1.853434	1.687146
21	1	-3.864607	1.707086	-1.676515
22	6	-6.866994	-0.498919	1.181215
23	1	-7.656805	-0.108389	0.533753
24	1	-7.071413	-1.559915	1.353589
25	1	-6.964371	0.006502	2.149997
26	8	-1.676354	0.370203	-1.039907
27	1	-1.339721	1.777424	-1.230523
28	8	4.995771	1.095241	0.844191
29	6	3.821235	0.719178	0.611971
30	8	3.494573	-0.523416	0.362887
31	8	2.792639	1.525645	0.592548

INT3a

E(B3LYP)= -1766.967652 Hartree

Zero-point correction= 0.185219 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.782434 Hartree

Sum of electronic and thermal Enthalpies = -1766.756892 Hartree

Sum of electronic and thermal Free Energies= -1766.820870 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.97894	-0.204643	0.023852
2	8	-0.646122	4.534823	0.361492
3	8	-0.753355	2.376221	-0.257498
4	8	0.642899	-1.868289	0.879992
5	8	-1.337565	-2.616794	0.379413
6	6	-0.251844	3.351848	0.383895
7	6	-0.146189	-2.906978	0.828753
8	8	0.203236	-4.064325	1.175343
9	8	0.831233	3.078722	1.177381
10	8	-0.515302	-0.533063	-1.69388
11	8	-1.438941	0.157696	1.736213
12	6	3.596257	0.606212	1.000488
13	6	4.919794	0.337643	0.653545
14	6	2.53497	0.368456	0.097387
15	1	5.704149	0.535615	1.379817
16	6	5.262555	-0.184483	-0.599318
17	6	2.884009	-0.168032	-1.163425
18	1	2.088107	-0.377469	-1.869186
19	6	4.210647	-0.433744	-1.492573
20	1	4.434869	-0.848211	-2.472593
21	1	3.361734	1.003524	1.983466
22	6	6.701638	-0.445138	-0.982754
23	1	7.333861	-0.556955	-0.098068
24	1	6.799333	-1.355616	-1.581092
25	1	7.119232	0.376001	-1.577733
26	8	1.28644	0.667395	0.422927
27	1	1.079758	2.121705	0.984747
28	8	-4.984563	0.13365	-1.223138
29	6	-3.79029	0.033999	-0.839742
30	8	-3.267538	-1.073433	-0.389199
31	8	-2.943907	1.028631	-0.851703

TS4a

E(B3LYP)= -1766.966078 Hartree

Zero-point correction= 0.184992 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.781086 Hartree

Sum of electronic and thermal Enthalpies = -1766.756137 Hartree

Sum of electronic and thermal Free Energies= -1766.818110 Hartree

Center	Atomic	Coordinates(Angstroms)

Number	number	x	y	z
1	92	-0.996022	-0.243394	0.028753
2	8	0.051298	4.617124	-0.052697
3	8	-0.245105	2.460252	-0.638898
4	8	0.450223	-2.171962	0.505257
5	8	-1.637397	-2.603565	0.054268
6	6	0.192988	3.384205	0.098689
7	6	-0.464535	-3.094523	0.362089
8	8	-0.242415	-4.322078	0.50652
9	8	0.917061	2.995178	1.212987
10	8	-0.612301	-0.394354	-1.730523
11	8	-1.388518	-0.097242	1.7892
12	6	3.549237	0.381285	1.225352
13	6	4.875421	0.170829	0.849468
14	6	2.486101	0.187892	0.314697
15	1	5.661779	0.331201	1.582654
16	6	5.217948	-0.244863	-0.44251
17	6	2.835036	-0.237141	-0.987555
18	1	2.040023	-0.405361	-1.704968
19	6	4.16431	-0.44577	-1.345806
20	1	4.38902	-0.774958	-2.357488
21	1	3.313251	0.69915	2.236349
22	6	6.658578	-0.443454	-0.855966
23	1	6.777799	-1.329564	-1.486325
24	1	7.037888	0.410913	-1.42914
25	1	7.307783	-0.562897	0.015138
26	8	1.232795	0.42045	0.682323
27	1	1.049605	2.012218	1.126614
28	8	-4.943065	0.942366	-0.673789
29	6	-3.755933	0.573589	-0.492724
30	8	-3.386713	-0.677149	-0.431589
31	8	-2.758115	1.408385	-0.345869

INT4a

E(B3LYP)= -1766.983606 Hartree

Zero-point correction= 0.184236 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1766.79937 Hartree

Sum of electronic and thermal Enthalpies = -1766.772966 Hartree

Sum of electronic and thermal Free Energies= -1766.840810 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	1.183863	-0.159794	0.036767
2	8	-2.680378	4.632426	-1.615257

3	8	-2.167248	3.649208	0.352878
4	8	1.127509	-1.007869	-2.21235
5	8	3.072915	-1.049107	-1.192777
6	6	-2.271455	3.693115	-0.896472
7	6	2.403861	-1.326824	-2.288551
8	8	2.920297	-1.842163	-3.302275
9	8	-1.886732	2.553237	-1.602865
10	8	0.803815	-1.812295	0.666801
11	8	1.525474	1.500094	-0.599164
12	6	-2.819116	-1.175035	-0.998194
13	6	-3.985001	-1.900694	-0.757632
14	6	-2.186818	-0.459463	0.035753
15	1	-4.443576	-2.445838	-1.578092
16	6	-4.575408	-1.946974	0.51108
17	6	-2.777198	-0.504243	1.313191
18	1	-2.306152	0.037799	2.126021
19	6	-3.942328	-1.234577	1.537733
20	1	-4.367357	-1.251129	2.537671
21	1	-2.379581	-1.156921	-1.989972
22	6	-5.856719	-2.709755	0.758316
23	1	-5.876672	-3.141773	1.762461
24	1	-6.73569	-2.060749	0.668722
25	1	-5.980138	-3.523284	0.039065
26	8	-1.07373	0.252263	-0.193789
27	1	-1.58291	1.860003	-0.977731
28	8	2.738239	0.890563	3.707698
29	6	2.278274	0.571767	2.591128
30	8	3.00138	0.047003	1.628464
31	8	1.011973	0.729016	2.261531

1b

E(B3LYP)= -1502.325995 Hartree

Zero-point correction= 0.157016 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1502.168979 Hartree

Sum of electronic and thermal Enthalpies = -1502.14797 Hartree

Sum of electronic and thermal Free Energies= -1502.202610 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.952481	0.004478	0.096996
2	8	-0.728646	2.403809	0.115235
3	8	-2.66344	1.597775	-0.544077
4	8	-2.804679	-1.44419	-0.508871
5	8	-0.948696	-2.402063	0.173201

6	6	-1.942313	2.672586	-0.320823
7	6	-2.183542	-2.572676	-0.253499
8	8	-2.7064	-3.69807	-0.398979
9	8	-2.361554	3.83546	-0.503146
10	8	-1.541218	0.046381	1.811587
11	8	-0.348315	-0.038022	-1.609991
12	6	2.469923	-0.061276	0.48565
13	6	3.215965	1.135061	0.441628
14	6	3.144302	-1.255464	0.155197
15	6	4.564228	1.127929	0.090002
16	6	4.493277	-1.244178	-0.193818
17	6	5.237126	-0.057637	-0.231761
18	1	2.718649	2.067893	0.686121
19	1	2.59123	-2.188798	0.175775
20	1	5.105152	2.070117	0.064703
21	1	4.978271	-2.18388	-0.44449
22	8	1.188647	-0.062362	0.839427
23	6	6.709271	-0.060992	-0.574819
24	1	6.951389	-0.854352	-1.286962
25	1	7.017783	0.891222	-1.014037
26	1	7.330778	-0.224036	0.313653

COM1b

E(B3LYP)= -1849.233978 Hartree

Zero-point correction= 0.288962 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.945016 Hartree

Sum of electronic and thermal Enthalpies = -1848.914789 Hartree

Sum of electronic and thermal Free Energies= -1848.991710 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.172723	0.87747	0.19444
2	8	1.238581	0.96207	-0.241218
3	8	0.400385	-0.960401	0.418847
4	6	1.45861	-0.285335	0.060952
5	8	2.607632	-0.813224	0.014797
6	8	-1.466881	0.419146	-1.530221
7	8	-0.873754	1.316222	1.92552
8	6	7.072394	0.46934	-0.792685
9	6	8.274355	-0.188222	-0.544399
10	6	5.852503	-0.121947	-0.43588
11	1	9.205019	0.294303	-0.82835
12	6	8.310682	-1.450577	0.06295
13	6	5.871575	-1.38272	0.177365

14	1	4.935929	-1.848212	0.464804
15	6	7.086109	-2.026238	0.417934
16	1	7.074596	-3.000942	0.896969
17	1	7.064644	1.447709	-1.26094
18	6	9.618944	-2.169323	0.299506
19	1	9.941741	-2.718773	-0.592234
20	1	10.418649	-1.468621	0.55358
21	1	9.533036	-2.893106	1.113516
22	8	4.706986	0.55448	-0.6944
23	1	3.887738	0.037603	-0.407907
24	8	-2.873716	2.562939	0.060626
25	6	-2.089557	3.543721	-0.340939
26	8	-0.833228	3.181008	-0.466965
27	8	-2.504159	4.69738	-0.576537
28	6	-4.938953	-1.113604	-0.04852
29	6	-5.852644	-2.077195	-0.470758
30	6	-3.658323	-1.481847	0.412667
31	1	-6.829418	-1.756011	-0.822497
32	6	-5.544746	-3.443714	-0.455841
33	6	-3.343868	-2.856131	0.422619
34	1	-2.361658	-3.162773	0.766786
35	6	-4.269716	-3.806366	-0.0034
36	1	-3.99104	-4.856505	0.015688
37	1	-5.201904	-0.061227	-0.071532
38	8	-2.784666	-0.571706	0.83558
39	6	-6.555734	-4.48401	-0.880703
40	1	-7.216489	-4.102416	-1.663618
41	1	-6.065067	-5.382978	-1.26267
42	1	-7.192473	-4.793565	-0.043521

TS1b

E(B3LYP)= -1849.219288 Hartree

Zero-point correction= 0.288184 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.931104 Hartree

Sum of electronic and thermal Enthalpies = -1848.901549 Hartree

Sum of electronic and thermal Free Energies= -1848.976440 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.755304	0.66169	0.100076
2	8	1.118813	-0.435147	-0.609916
3	8	0.256419	-2.443023	-1.080106
4	6	1.215083	-1.631095	-1.196152
5	8	2.29476	-1.887921	-1.83937

6	8	-1.481531	0.505797	-1.544412
7	8	-0.036209	0.787815	1.755578
8	6	6.453929	0.126618	-0.96268
9	6	7.403545	-0.055055	0.039971
10	6	5.24635	-0.586447	-0.938816
11	1	8.327814	0.513762	-0.003194
12	6	7.194273	-0.948028	1.098751
13	6	5.020765	-1.481005	0.119283
14	1	4.090561	-2.036079	0.154317
15	6	5.983621	-1.650059	1.113984
16	1	5.781847	-2.345954	1.923316
17	1	6.633934	0.825191	-1.772861
18	6	8.243799	-1.164886	2.164694
19	1	8.928845	-1.976914	1.894709
20	1	8.849261	-0.267609	2.315407
21	1	7.789515	-1.430484	3.122642
22	8	4.351484	-0.379128	-1.930375
23	1	3.508438	-0.951996	-1.826134
24	8	-1.778618	2.807957	0.376162
25	6	-0.775264	3.497894	-0.12463
26	8	0.231406	2.733541	-0.505704
27	8	-0.772884	4.737939	-0.22951
28	6	-4.904629	-0.005495	0.417792
29	6	-6.147827	-0.56634	0.1329
30	6	-3.787718	-0.821057	0.690101
31	1	-6.98597	0.093205	-0.075159
32	6	-6.343013	-1.953167	0.105517
33	6	-3.979573	-2.216702	0.657885
34	1	-3.131853	-2.863605	0.858357
35	6	-5.229689	-2.760924	0.370325
36	1	-5.33986	-3.841735	0.350458
37	1	-4.779596	1.072141	0.431586
38	8	-2.599689	-0.295025	0.983703
39	6	-7.703906	-2.551046	-0.168373
40	1	-8.290188	-1.917149	-0.838784
41	1	-7.619952	-3.539584	-0.627097
42	1	-8.284939	-2.670337	0.75371

INT1b

E(B3LYP)= -1849.219819 Hartree

Zero-point correction= 0.288106 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.931713 Hartree

Sum of electronic and thermal Enthalpies = -1848.901262 Hartree

Sum of electronic and thermal Free Energies= -1848.978390 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.617132	0.579956	-0.093199
2	8	-0.828709	-1.124124	0.242972
3	8	-0.223839	-3.042437	1.237406
4	6	-1.045487	-2.097099	1.143582
5	8	-2.114633	-1.999901	1.847348
6	8	1.325722	0.303731	1.543531
7	8	-0.103967	0.834365	-1.733108
8	6	-5.864855	0.572733	0.625784
9	6	-6.936709	0.340089	-0.231621
10	6	-4.839525	-0.375985	0.759999
11	1	-7.713688	1.094378	-0.316934
12	6	-7.035293	-0.837578	-0.984956
13	6	-4.922637	-1.557565	0.007627
14	1	-4.136301	-2.298284	0.095555
15	6	-6.004746	-1.773363	-0.846245
16	1	-6.041939	-2.695516	-1.419073
17	1	-5.805867	1.492225	1.198267
18	6	-8.219714	-1.094148	-1.888208
19	1	-9.076283	-1.484166	-1.326424
20	1	-8.55047	-0.177395	-2.383793
21	1	-7.977512	-1.826862	-2.661663
22	8	-3.817165	-0.110542	1.603009
23	1	-3.120671	-0.862011	1.626325
24	8	1.606592	2.76422	-0.186964
25	6	0.59456	3.397938	0.365665
26	8	-0.402144	2.594845	0.68227
27	8	0.577866	4.626529	0.569498
28	6	4.86905	0.264435	-0.665651
29	6	6.135825	-0.244942	-0.387305
30	6	3.751068	-0.58821	-0.758639
31	1	6.974525	0.442487	-0.318309
32	6	6.353981	-1.614725	-0.191966
33	6	3.966331	-1.9664	-0.559356
34	1	3.118292	-2.640272	-0.622897
35	6	5.239892	-2.458936	-0.281828
36	1	5.36813	-3.527166	-0.12966
37	1	4.726287	1.329883	-0.811319
38	8	2.539143	-0.110218	-1.039951
39	6	7.737539	-2.161888	0.074815
40	1	8.362908	-1.428923	0.590997
41	1	7.697493	-3.064025	0.690795
42	1	8.252317	-2.42821	-0.855817

TS2b

E(B3LYP)= -1849.215718 Hartree

Zero-point correction= 0.285312 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.930405 Hartree

Sum of electronic and thermal Enthalpies = -1848.900701 Hartree

Sum of electronic and thermal Free Energies= -1848.975550 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.343176	0.498017	0.181734
2	8	-0.288382	-3.794126	0.008969
3	8	0.335128	-1.684437	0.429102
4	8	1.038555	2.249658	-0.664426
5	8	-0.998113	2.783024	-0.046122
6	6	0.46168	-2.827965	-0.196734
7	6	0.148006	3.212801	-0.533139
8	8	0.366273	4.399594	-0.836013
9	8	1.458384	-2.928041	-1.063752
10	8	0.244385	0.822103	1.857159
11	8	-0.933921	0.128884	-1.480644
12	6	-3.646144	-0.165365	0.594418
13	6	-4.677563	0.793133	0.617031
14	6	-3.976696	-1.47094	0.183425
15	6	-5.976429	0.453027	0.24453
16	6	-5.280989	-1.793785	-0.185936
17	6	-6.310857	-0.844965	-0.162146
18	1	-4.442384	1.805812	0.927094
19	1	-3.195828	-2.223329	0.154533
20	1	-6.747508	1.218111	0.269285
21	1	-5.500662	-2.8097	-0.502574
22	8	-2.404619	0.156191	0.965909
23	6	-7.729438	-1.213733	-0.531183
24	1	-8.293101	-1.567684	0.33994
25	1	-8.270436	-0.356141	-0.939246
26	1	-7.752263	-2.012914	-1.276576
27	6	4.415433	-1.587624	0.242439
28	6	5.621906	-1.353935	0.89965
29	6	4.020979	-0.812576	-0.878761
30	1	5.881405	-1.976979	1.752381
31	6	6.506889	-0.345765	0.495567
32	6	4.925003	0.200937	-1.284692
33	1	4.660432	0.810096	-2.143982
34	6	6.125932	0.42057	-0.614375
35	1	6.786435	1.209383	-0.966421

36	1	3.7597	-2.380945	0.586765
37	6	7.795073	-0.077839	1.240696
38	1	8.231167	-1.001395	1.632147
39	1	8.538628	0.393979	0.592673
40	1	7.641215	0.591735	2.095759
41	8	2.888254	-1.008189	-1.525589
42	1	2.091136	-2.030801	-1.182838

INT2b

E(B3LYP)= -1849.215725 Hartree

Zero-point correction= 0.286031 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.929694 Hartree

Sum of electronic and thermal Enthalpies = -1848.899282 Hartree

Sum of electronic and thermal Free Energies= -1848.975350 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.347026	0.495884	0.184571
2	8	-0.307116	-3.789151	-0.054239
3	8	0.332719	-1.6922	0.406769
4	8	1.032909	2.249075	-0.659764
5	8	-0.99776	2.783242	-0.022698
6	6	0.447941	-2.823979	-0.238771
7	6	0.146122	3.213842	-0.514378
8	8	0.365697	4.402339	-0.808939
9	8	1.445465	-2.917191	-1.110145
10	8	0.251141	0.805959	1.858549
11	8	-0.950852	0.137295	-1.475205
12	6	-3.644159	-0.170161	0.611627
13	6	-4.64557	0.815812	0.511769
14	6	-4.007822	-1.500778	0.3331
15	6	-5.945116	0.477974	0.142343
16	6	-5.313547	-1.821217	-0.036352
17	6	-6.310415	-0.844455	-0.143824
18	1	-4.386955	1.846236	0.731421
19	1	-3.253952	-2.276602	0.412895
20	1	-6.693347	1.263179	0.07661
21	1	-5.560763	-2.858567	-0.2441
22	8	-2.401797	0.149265	0.982746
23	6	-7.716305	-1.194168	-0.574873
24	1	-7.925326	-2.255717	-0.422145
25	1	-8.461006	-0.620211	-0.016415
26	1	-7.875909	-0.980092	-1.637987
27	6	4.43044	-1.593648	0.223714
28	6	5.637011	-1.368952	0.883571

29	6	4.031635	-0.800639	-0.884636
30	1	5.898683	-2.006105	1.725238
31	6	6.519935	-0.352227	0.496054
32	6	4.934942	0.221612	-1.273264
33	1	4.668846	0.845138	-2.121804
34	6	6.136114	0.432038	-0.600297
35	1	6.794768	1.228149	-0.939384
36	1	3.776707	-2.394243	0.555306
37	6	7.808226	-0.094846	1.24479
38	1	8.253904	-1.025457	1.607954
39	1	8.545507	0.401934	0.60835
40	1	7.651802	0.548269	2.119518
41	8	2.899896	-0.988595	-1.531496
42	1	2.07437	-2.03475	-1.204057

TS3b

E(B3LYP)= -1849.214623 Hartree

Zero-point correction= 0.286778 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.927845 Hartree

Sum of electronic and thermal Enthalpies = -1848.898467 Hartree

Sum of electronic and thermal Free Energies= -1848.971370 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.255691	0.459014	0.170034
2	8	-0.405564	-3.93219	0.064645
3	8	0.157497	-1.803031	0.477323
4	8	1.106169	2.288438	-0.594546
5	8	-0.957606	2.73593	-0.003065
6	6	0.317381	-2.945447	-0.129544
7	6	0.184719	3.216751	-0.449377
8	8	0.370646	4.421239	-0.704942
9	8	1.336221	-3.026794	-0.985199
10	8	0.30096	0.748814	1.861291
11	8	-0.791004	0.131248	-1.518173
12	6	-3.597773	-0.114014	0.535215
13	6	-4.608071	0.864591	0.612785
14	6	-3.966786	-1.398791	0.091207
15	6	-5.922406	0.563897	0.26165
16	6	-5.286488	-1.682116	-0.255414
17	6	-6.294674	-0.713306	-0.1771
18	1	-4.344005	1.861151	0.950475
19	1	-3.205165	-2.167805	0.021863
20	1	-6.676006	1.34366	0.329903

21	1	-5.535892	-2.68304	-0.596883
22	8	-2.343363	0.169121	0.889029
23	6	-7.729452	-1.040675	-0.521786
24	1	-8.28311	-1.396626	0.354955
25	1	-8.257923	-0.163008	-0.902795
26	1	-7.787624	-1.825343	-1.280518
27	6	4.377244	-1.646061	0.181499
28	6	5.647446	-1.430074	0.714292
29	6	3.805706	-0.751636	-0.760396
30	1	6.04301	-2.146707	1.430268
31	6	6.426412	-0.322845	0.355396
32	6	4.604988	0.363659	-1.121964
33	1	4.205096	1.068134	-1.845224
34	6	5.870808	0.56378	-0.578084
35	1	6.444318	1.433524	-0.890122
36	1	3.806936	-2.518607	0.484896
37	6	7.787193	-0.076486	0.967101
38	1	7.729259	0.584818	1.840313
39	1	8.248698	-1.009905	1.300578
40	1	8.467592	0.395943	0.252721
41	8	2.610464	-0.932228	-1.285725
42	1	1.89556	-2.117173	-1.051527

INT3b

E(B3LYP)= -1849.229704 Hartree

Zero-point correction= 0.289615 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.940089 Hartree

Sum of electronic and thermal Enthalpies = -1848.91014 Hartree

Sum of electronic and thermal Free Energies= -1848.984300 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.047874	0.289103	-0.01628
2	8	-0.341379	-4.281737	-0.143751
3	8	-0.115473	-2.11776	0.415028
4	8	1.090952	2.252481	-0.895534
5	8	-0.918641	2.54818	-0.081083
6	6	0.200807	-3.173937	-0.240164
7	6	0.12386	3.105359	-0.654014
8	8	0.18665	4.321754	-0.93827
9	8	1.239373	-3.050247	-1.116884
10	8	0.632833	0.56604	1.636176
11	8	-0.689834	-0.045229	-1.672084
12	6	-3.431934	-0.048866	0.631136

13	6	-4.365781	0.846902	1.199569
14	6	-3.948953	-1.092696	-0.165701
15	6	-5.732274	0.701861	0.976201
16	6	-5.320831	-1.2238	-0.377807
17	6	-6.244777	-0.333376	0.181795
18	1	-3.995189	1.654412	1.822754
19	1	-3.258885	-1.801738	-0.609511
20	1	-6.417746	1.410449	1.433912
21	1	-5.680128	-2.044081	-0.993611
22	8	-2.133891	0.084356	0.865639
23	6	-7.728287	-0.466212	-0.076143
24	1	-7.979146	-1.467078	-0.435955
25	1	-8.31202	-0.279139	0.829855
26	1	-8.072704	0.248102	-0.833086
27	6	4.158939	-1.533475	-0.003722
28	6	5.486482	-1.370719	0.391716
29	6	3.345856	-0.419146	-0.298354
30	1	6.081075	-2.254362	0.607967
31	6	6.069696	-0.10455	0.516246
32	6	3.933524	0.857852	-0.179441
33	1	3.321828	1.722302	-0.40887
34	6	5.261022	1.000361	0.21787
35	1	5.680105	2.000472	0.295645
36	1	3.73962	-2.530152	-0.091142
37	6	7.498311	0.066944	0.979806
38	1	7.554484	0.234427	2.061973
39	1	8.098026	-0.819662	0.758571
40	1	7.974796	0.924749	0.497214
41	8	2.077117	-0.570736	-0.695897
42	1	1.614619	-2.127969	-1.018581

TS4b

E(B3LYP)= -1849.217865 Hartree

Zero-point correction= 0.288969 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.928896 Hartree

Sum of electronic and thermal Enthalpies = -1848.89919 Hartree

Sum of electronic and thermal Free Energies= -1848.974060 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.04183	0.663069	0.008198
2	8	0.086418	-4.669132	1.338544
3	8	0.32275	-2.825639	0.054835
4	8	-1.075631	2.517366	1.011574

5	8	0.912862	2.877712	0.164859
6	6	-0.206909	-3.513304	0.963285
7	6	-0.120598	3.39713	0.794956
8	8	-0.186614	4.589591	1.148076
9	8	-1.261918	-2.92386	1.656709
10	8	-0.701297	1.053495	-1.588924
11	8	0.767438	0.240576	1.602576
12	6	3.282357	-0.112872	-0.799731
13	6	4.339175	0.797112	-0.998033
14	6	3.613935	-1.421601	-0.391982
15	6	5.663484	0.409556	-0.797803
16	6	4.943123	-1.790188	-0.19801
17	6	5.998553	-0.889472	-0.397518
18	1	4.104727	1.810563	-1.306552
19	1	2.808613	-2.130082	-0.226827
20	1	6.45405	1.138166	-0.955583
21	1	5.164917	-2.805692	0.11988
22	8	2.016621	0.251604	-1.003519
23	6	7.437937	-1.313054	-0.213905
24	1	7.552056	-1.983739	0.642332
25	1	7.816957	-1.8469	-1.093228
26	1	8.088117	-0.449513	-0.053409
27	6	-3.467098	-1.302968	-0.98856
28	6	-4.776227	-1.390455	-1.459038
29	6	-3.152996	-0.50569	0.127885
30	1	-4.982589	-2.012007	-2.325973
31	6	-5.827298	-0.697802	-0.845768
32	6	-4.206462	0.19329	0.746512
33	1	-3.984059	0.816873	1.60557
34	6	-5.509778	0.096656	0.263431
35	1	-6.29797	0.654045	0.76211
36	1	-2.669589	-1.846008	-1.484366
37	6	-7.249761	-0.82464	-1.34085
38	1	-7.809185	0.102229	-1.189157
39	1	-7.280148	-1.066495	-2.406197
40	1	-7.790381	-1.618548	-0.812416
41	8	-1.901622	-0.426763	0.604208
42	1	-1.424541	-2.035013	1.268894

INT4b

E(B3LYP)= -1849.221040 Hartree

Zero-point correction= 0.288717 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1848.932323 Hartree

Sum of electronic and thermal Enthalpies = -1848.901635 Hartree

Sum of electronic and thermal Free Energies= -1848.979210 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.227221	-0.821436	0.038983
2	8	2.149527	3.955003	3.525483
3	8	1.458067	3.724936	1.387389
4	8	0.731346	-2.533684	1.382858
5	8	-1.303022	-2.85952	0.626638
6	6	1.888244	3.305733	2.488775
7	6	-0.307417	-3.344467	1.342819
8	8	-0.344694	-4.446104	1.918943
9	8	2.114236	1.932502	2.597393
10	8	0.438664	-1.58079	-1.457075
11	8	-0.872373	-0.012862	1.515687
12	6	-3.275163	0.370163	-0.981242
13	6	-4.45282	-0.33487	-0.660732
14	6	-3.389105	1.753425	-1.220453
15	6	-5.680164	0.319513	-0.589112
16	6	-4.625666	2.392358	-1.144338
17	6	-5.798698	1.694504	-0.831797
18	1	-4.386149	-1.40041	-0.467449
19	1	-2.494168	2.316402	-1.464566
20	1	-6.567213	-0.254753	-0.335858
21	1	-4.676614	3.461359	-1.331871
22	8	-2.101481	-0.254424	-1.06874
23	6	-7.141177	2.387403	-0.78572
24	1	-7.030513	3.454924	-0.57987
25	1	-7.675937	2.293736	-1.738139
26	1	-7.78492	1.959965	-0.01221
27	6	2.989946	1.230873	-1.532752
28	6	4.176838	1.305292	-2.259085
29	6	2.883602	0.389475	-0.410379
30	1	4.223419	1.960805	-3.124326
31	6	5.305995	0.556752	-1.90339
32	6	4.01429	-0.365105	-0.049133
33	1	3.951008	-1.021812	0.812022
34	6	5.194747	-0.279004	-0.78522
35	1	6.04801	-0.879502	-0.482414
36	1	2.128148	1.820659	-1.826873
37	6	6.599207	0.667923	-2.677977
38	1	7.183625	-0.253113	-2.610409
39	1	6.413905	0.87331	-3.735507
40	1	7.228436	1.480155	-2.295869
41	8	1.748252	0.320732	0.303777

42	1	1.899145	1.494266	1.746514

1c

E(B3LYP)= -1661.0335938 Hartree

Zero-point correction= 0.286151 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1660.747443 Hartree

Sum of electronic and thermal Enthalpies = -1660.72011 Hartree

Sum of electronic and thermal Free Energies= -1660.811334 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.04984	-1.04788	0.06724
2	8	1.939957	-2.289495	-0.779828
3	8	0.347918	-3.481992	0.133723
4	6	1.5248	-3.492903	-0.458257
5	8	2.170255	-4.533686	-0.687618
6	8	-0.797068	-1.203676	-1.52185
7	8	0.841614	-0.921989	1.687464
8	6	2.254832	1.524591	-0.40634
9	6	2.080393	2.556913	0.538549
10	6	3.508208	1.436456	-1.045011
11	6	3.111	3.450259	0.821952
12	6	4.528741	2.3381	-0.74887
13	6	4.356658	3.366496	0.186034
14	1	1.125723	2.643011	1.046539
15	1	3.667787	0.647174	-1.772004
16	1	2.940998	4.231469	1.558038
17	1	5.483337	2.236484	-1.257932
18	8	1.274371	0.673654	-0.700588
19	6	5.456943	4.361192	0.477269
20	1	5.334614	5.280664	-0.107101
21	1	5.466739	4.649724	1.531936
22	1	6.439081	3.949557	0.23187
23	8	-1.542692	0.399355	0.75594
24	6	-2.656463	1.021964	0.377052
25	6	-2.625036	2.356932	-0.077495
26	1	-1.667946	2.864675	-0.135381
27	1	-3.961777	-0.642784	0.771246
28	1	-6.025896	0.539723	0.113994
29	1	-6.149173	3.816564	-1.583215
30	1	-6.696098	3.717717	0.088074
31	1	-7.106069	2.430896	-1.04424
32	1	-3.731486	4.044578	-0.792843
33	6	-3.794963	3.016513	-0.446338

34	6	-5.046673	2.389687	-0.383753
35	6	-5.074434	1.06184	0.059742
36	6	-3.913392	0.386572	0.433006
37	6	-6.314594	3.125612	-0.752084
38	8	-1.823667	-2.588471	1.171876
39	1	-2.080854	-2.437286	2.088461
40	1	-1.285908	-3.39816	1.15082

Asp*

E(B3LYP)= -228.707038 Hartree

Zero-point correction= 0.048202 (Hartree/Particle)

Sum of electronic and zero-point Energies= -228.658837 Hartree

Sum of electronic and thermal Enthalpies = -228.653531 Hartree

Sum of electronic and thermal Free Energies= -228.669780 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	8	-0.761565	1.124142	0.001889
2	8	-0.761477	-1.124192	0.00189
3	6	-0.187706	0.000011	-0.010352
4	6	1.3516	0.000038	-0.004442
5	1	1.698135	-0.000151	1.034792
6	1	1.751421	-0.893055	-0.488293
7	1	1.75141	0.893312	-0.487965

TS1c

E(B3LYP)= -1889.7381101 Hartree

Zero-point correction= 0.334980 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1889.403130Hartree

Sum of electronic and thermal Enthalpies = -1889.370207 Hartree

Sum of electronic and thermal Free Energies= -1889.476014 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.059711	-0.750724	-0.352492
2	8	1.495959	-2.377568	-1.409326
3	8	-0.459515	-3.111684	-0.739301
4	6	0.6849	-3.403497	-1.338468
5	8	0.953248	-4.53594	-1.780223
6	8	-0.565532	-0.300955	-1.985158
7	8	0.681087	-1.21908	1.282895
8	6	3.032026	0.915174	-0.146909
9	6	3.060579	1.597058	1.086567
10	6	4.260829	0.7283	-0.812643

11	6	4.261404	2.0622	1.619653
12	6	5.452115	1.19822	-0.264363
13	6	5.483815	1.872907	0.963239
14	1	2.12804	1.762264	1.614706
15	1	4.261672	0.213953	-1.767976
16	1	4.244017	2.588464	2.570249
17	1	6.379522	1.038119	-0.807583
18	8	1.894228	0.48546	-0.688281
19	6	6.784781	2.350597	1.566487
20	1	7.506656	2.625097	0.792801
21	1	6.630116	3.222419	2.207349
22	1	7.251969	1.574019	2.183447
23	8	-0.918116	1.090232	0.500046
24	6	-1.678449	2.122713	0.136226
25	6	-1.160955	3.433713	0.121727
26	1	-0.125156	3.588585	0.405097
27	1	-3.445782	0.950145	-0.198001
28	1	-4.85549	2.878896	-0.853321
29	1	-3.84393	6.443922	-0.541341
30	1	-5.208847	5.353273	-0.813852
31	1	-4.078332	5.698302	-2.120221
32	1	-1.529221	5.512233	-0.241176
33	6	-1.960869	4.514904	-0.243139
34	6	-3.302705	4.348727	-0.609413
35	6	-3.815504	3.045155	-0.584793
36	6	-3.031065	1.952001	-0.221925
37	6	-4.152881	5.521815	-1.040646
38	8	-0.47572	-4.105101	1.853141
39	1	-0.086335	-3.302453	2.221897
40	1	-0.55503	-3.875538	0.902007
41	8	-3.372964	-1.249995	2.739946
42	6	-3.83203	-1.51218	1.59428
43	8	-3.170158	-1.570373	0.521724
44	6	-5.340483	-1.808585	1.507624
45	1	-5.693469	-1.822005	0.475379
46	1	-5.908461	-1.070458	2.079511
47	1	-5.538569	-2.787901	1.955578

INT1c

E(B3LYP)= -1889.7525328 Hartree

Zero-point correction= 0.335372 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1889.417161Hartree

Sum of electronic and thermal Enthalpies = -1889.383747 Hartree

Sum of electronic and thermal Free Energies= -1889.489937 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.003078	-0.760266	-0.267073
2	8	1.834289	-1.975184	-1.34877
3	8	0.16427	-3.20949	-0.655927
4	6	1.339266	-3.179948	-1.257368
5	8	1.911125	-4.205522	-1.686799
6	8	-0.726356	-0.487304	-1.904594
7	8	0.714698	-1.070123	1.370008
8	6	2.715077	1.375703	-0.237907
9	6	2.823307	1.929801	1.057916
10	6	3.862244	1.451318	-1.060369
11	6	4.010334	2.513741	1.495991
12	6	5.041358	2.037611	-0.605829
13	6	5.148123	2.579953	0.681532
14	1	1.959418	1.897679	1.712669
15	1	3.805946	1.043738	-2.064439
16	1	4.050236	2.931149	2.498902
17	1	5.899684	2.075963	-1.271611
18	8	1.592717	0.832252	-0.683518
19	6	6.441541	3.183326	1.179882
20	1	7.026896	3.605765	0.358826
21	1	6.256787	3.980153	1.905317
22	1	7.072567	2.435778	1.675278
23	8	-1.158423	1.035421	0.547513
24	6	-2.077741	1.936445	0.23152
25	6	-1.819721	3.318296	0.373085
26	1	-0.845736	3.629775	0.736955
27	1	-3.585962	0.512747	-0.336844
28	1	-5.294395	2.20875	-0.891074
29	1	-4.980236	5.847971	-0.176933
30	1	-6.108278	4.563393	-0.627427
31	1	-5.010531	5.237484	-1.829184
32	1	-2.55248	5.32194	0.185062
33	6	-2.789471	4.268481	0.060383
34	6	-4.058842	3.902482	-0.406406
35	6	-4.317613	2.532196	-0.540458
36	6	-3.359841	1.567992	-0.233021
37	6	-5.093177	4.940911	-0.776726
38	8	0.446248	-4.154103	1.913613
39	1	0.582413	-3.269648	2.276656
40	1	0.298445	-3.955072	0.960911
41	8	-2.694966	-1.811001	2.529637
42	6	-2.881452	-2.108967	1.335761

43	8	-2.110249	-1.802692	0.358873
44	6	-4.120323	-2.914018	0.943141
45	1	-4.669377	-2.394309	0.15384
46	1	-4.776184	-3.076719	1.798345
47	1	-3.811269	-3.882058	0.538403

Prod

E(B3LYP)= -1813.2754851 Hartree

Zero-point correction= 0.311099 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1812.964386Hartree

Sum of electronic and thermal Enthalpies = -1812.934028 Hartree

Sum of electronic and thermal Free Energies= -1813.033092 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.074883	-0.939343	-0.158287
2	8	1.699341	-2.332892	-1.105553
3	8	-0.124488	-3.373621	-0.489465
4	6	1.077496	-3.482369	-0.99925
5	8	1.583884	-4.574713	-1.35043
6	8	-0.775153	-0.681255	-1.810539
7	8	0.61767	-1.199768	1.493736
8	6	2.773755	1.025685	-0.234849
9	6	2.965246	1.428362	1.106649
10	6	3.866468	1.206898	-1.11487
11	6	4.176975	1.970819	1.531471
12	6	5.070572	1.749523	-0.673044
13	6	5.259065	2.142506	0.659004
14	1	2.147359	1.305077	1.807718
15	1	3.746567	0.913563	-2.153045
16	1	4.281634	2.270218	2.571245
17	1	5.884103	1.872015	-1.383618
18	8	1.630514	0.522808	-0.670479
19	6	6.580999	2.698455	1.137447
20	1	7.065443	3.301054	0.364046
21	1	6.450949	3.328285	2.021358
22	1	7.282052	1.900178	1.409185
23	8	-1.086677	0.986806	0.571035
24	6	-1.879321	1.979243	0.197312
25	6	-1.427241	3.318368	0.214932
26	1	-0.407062	3.515879	0.528282
27	1	-3.590133	0.743023	-0.219158
28	1	-5.065418	2.614978	-0.866419
29	1	-4.25884	6.205774	-0.419909
30	1	-5.538564	5.054169	-0.821174

31	1	-4.361104	5.529159	-2.04291
32	1	-1.880834	5.384292	-0.119122
33	6	-2.266247	4.368381	-0.150709
34	6	-3.590658	4.150161	-0.55332
35	6	-4.041262	2.823884	-0.567838
36	6	-3.215548	1.760754	-0.206194
37	6	-4.483651	5.293337	-0.979048
38	8	-2.774157	-1.852021	2.704746
39	6	-3.022504	-2.077105	1.50519
40	8	-2.269317	-1.773107	0.515709
41	6	-4.331863	-2.769499	1.12383
42	1	-4.905798	-2.127849	0.449654
43	1	-4.932693	-2.998389	2.004017
44	1	-4.115035	-3.694146	0.581932

H2O

E(B3LYP)= -76.4664776 Hartree

Zero-point correction= 0.021194 (Hartree/Particle)

Sum of electronic and zero-point Energies= -76.445283 Hartree

Sum of electronic and thermal Enthalpies = -76.441503 Hartree

Sum of electronic and thermal Free Energies= -76.449620 Hartree

Center	Atomic		Coordinates(Angstroms)		
Number	number		x	y	z
1	8	0	0		0.117999
2	1	0	0.762134		-0.471997
3	1	0	-0.762134		-0.471997

COM1

E(B3LYP)= -1496.560233 Hartree

Zero-point correction= 0.078042 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.482191 Hartree

Sum of electronic and thermal Enthalpies = -1496.462993 Hartree

Sum of electronic and thermal Free Energies= -1496.509630 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.012349	-0.028811	0.042993
2	8	0.624622	2.3469	-0.053995
3	8	-1.961357	1.458608	0.035344
4	8	2.276674	0.916448	-0.047447
5	8	-2.38815	-0.682111	0.103711
6	8	1.767356	-1.770958	0.076046
7	8	-0.292641	-2.489722	0.154585

8	6	-2.881851	0.535317	0.085749
9	6	1.921945	2.175712	-0.089926
10	6	0.981896	-2.810394	0.144459
11	8	1.389859	-3.995163	0.196009
12	8	2.74254	3.123956	-0.159523
13	8	-4.112668	0.775308	0.11408
14	8	-0.029161	-0.100244	-1.769702
15	8	0.045582	0.031839	1.85591
16	8	-2.86022	-3.34271	0.428124
17	1	-3.007099	-2.37767	0.336587
18	1	-1.881899	-3.338144	0.357722

TS1

E(B3LYP)= -1496.547534 Hartree

Zero-point correction= 0.077604 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.469929 Hartree

Sum of electronic and thermal Enthalpies = -1496.451385 Hartree

Sum of electronic and thermal Free Energies= -1496.497270 Hartree

Center	Atomic		Coordinates(Angstroms)	
Number	number	x	y	z
1	92	0.126156	-0.059826	-0.178858
2	8	0.630482	2.296347	-0.129298
3	8	-2.409023	1.458421	0.379123
4	8	2.343927	0.957046	0.134562
5	8	-2.121164	-0.485461	-0.637811
6	8	1.782057	-1.837344	-0.006543
7	8	-0.297355	-2.496028	-0.175879
8	6	-2.885005	0.303885	0.11028
9	6	1.930205	2.194951	0.049627
10	6	0.958063	-2.855525	-0.031095
11	8	1.326609	-4.048092	0.070014
12	8	2.688242	3.188822	0.129824
13	8	-3.998995	-0.14765	0.527464
14	8	0.383006	-0.037769	-1.97275
15	8	-0.085703	-0.11229	1.618253
16	8	-2.95347	-2.879892	0.909
17	1	-3.362592	-2.008301	0.734531
18	1	-2.062708	-2.788237	0.518535

INT1

E(B3LYP)= -1496.558202 Hartree

Zero-point correction= 0.077395 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.480807 Hartree

Sum of electronic and thermal Enthalpies = -1496.461451 Hartree

Sum of electronic and thermal Free Energies= -1496.506470 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.281744	-0.08724	0.252092
2	8	0.527491	2.304272	0.161081
3	8	-1.908681	0.221309	0.62926
4	8	2.351935	1.119394	-0.151741
5	8	-3.802639	-0.644477	-0.192974
6	8	1.914441	-1.885757	-0.001478
7	8	-0.16219	-2.46611	0.405704
8	6	-3.11867	0.401361	0.065773
9	6	1.822344	2.318802	-0.081962
10	6	1.07477	-2.873999	0.179047
11	8	1.396318	-4.079533	0.145326
12	8	2.476609	3.373119	-0.23106
13	8	-3.503789	1.582484	-0.153271
14	8	-0.041055	-0.1323	-1.53065
15	8	0.598228	-0.04507	2.037845
16	8	-2.850582	-3.166387	0.182423
17	1	-3.180244	-2.239577	0.065999
18	1	-1.883297	-3.057237	0.267563

TS2

E(B3LYP)= -1496.539118 Hartree

Zero-point correction= 0.077302 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.461815 Hartree

Sum of electronic and thermal Enthalpies = -1496.443417 Hartree

Sum of electronic and thermal Free Energies= -1496.48802 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.004149	-0.371734	0.242914
2	8	0.333356	2.064684	0.325379
3	8	-2.08309	0.655324	0.394686
4	8	2.117912	0.856166	-0.012793
5	8	-3.752567	-0.571027	-0.456385
6	8	2.005807	-1.829509	-0.020067
7	8	0.079598	-2.850499	-0.046381
8	6	-3.255143	0.599313	-0.223937
9	6	1.627404	2.060026	0.127897
10	6	1.384892	-2.969916	-0.125812
11	8	1.963733	-4.071451	-0.286162
12	8	2.323236	3.104152	0.076835

13	8	-3.842809	1.672102	-0.543692
14	8	-0.221655	-0.328041	-1.55122
15	8	0.237336	-0.42246	2.037473
16	8	-2.141814	-2.033701	0.929779
17	1	-2.826047	-1.57875	0.340557
18	1	-1.738436	-2.774101	0.456707

INT2

E(B3LYP)= -1496.53925997 Hartree

Zero-point correction= 0.077536 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.461724 Hartree

Sum of electronic and thermal Enthalpies = -1496.442809 Hartree

Sum of electronic and thermal Free Energies= -1496.488500 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.150933	0.022567	0.097946
2	8	-0.776308	2.315141	0.11637
3	8	-2.200423	-0.049549	0.311545
4	8	1.366062	2.134151	-0.241663
5	8	-3.107167	-1.95333	-0.448666
6	8	2.604671	-0.197832	-0.228057
7	8	1.50485	-2.075459	-0.103339
8	6	-3.237558	-0.6864	-0.202809
9	6	0.348676	2.943619	-0.106724
10	6	2.671112	-1.49898	-0.268468
11	8	3.735844	-2.140323	-0.445853
12	8	0.442045	4.194586	-0.183247
13	8	-4.314902	-0.060556	-0.422442
14	8	-0.106688	-0.133315	-1.686505
15	8	0.409581	0.15042	1.886367
16	8	-0.880057	-2.357083	0.698501
17	1	-1.766805	-2.332269	0.191286
18	1	-0.232524	-2.908161	0.241647

TS3

E(B3LYP)= -1496.53695 Hartree

Zero-point correction= 0.073538 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.463412 Hartree

Sum of electronic and thermal Enthalpies = -1496.444783 Hartree

Sum of electronic and thermal Free Energies= -1496.490610 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z

1	92	0.014393	-0.444024	0.218363
2	8	0.311962	2.001801	0.204965
3	8	-2.112578	0.845524	0.355681
4	8	2.143218	0.834039	0.021379
5	8	-3.788787	-0.465214	-0.357298
6	8	2.065279	-1.814535	-0.015714
7	8	0.20955	-2.949708	0.092856
8	6	-3.323868	0.751695	-0.094606
9	6	1.613213	2.025355	0.075559
10	6	1.510503	-2.995083	-0.036992
11	8	2.155196	-4.065972	-0.167641
12	8	2.281055	3.089226	0.008076
13	8	-4.061012	1.753383	-0.279539
14	8	-0.178558	-0.443367	-1.582186
15	8	0.200346	-0.446016	2.021111
16	8	-2.025297	-1.811787	0.525172
17	1	-2.956905	-1.223631	0.02963
18	1	-1.80717	-2.678555	0.167387

INT3

E(B3LYP)= -1496.53807764 Hartree

Zero-point correction= 0.077078 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.461 Hartree

Sum of electronic and thermal Enthalpies = -1496.442044 Hartree

Sum of electronic and thermal Free Energies= -1496.488470 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.014656	-0.482699	0.204648
2	8	0.28871	1.969079	0.180943
3	8	-2.161074	0.910397	0.352298
4	8	2.139302	0.825457	0.034336
5	8	-3.853834	-0.382522	-0.373443
6	8	2.079722	-1.825007	-0.032103
7	8	0.248664	-2.995223	0.113665
8	6	-3.362211	0.848253	-0.077147
9	6	1.591137	2.008283	0.073089
10	6	1.549125	-3.017	-0.022644
11	8	2.215554	-4.077255	-0.132617
12	8	2.24551	3.081993	0.011233
13	8	-4.123022	1.826833	-0.243366
14	8	-0.162229	-0.466433	-1.599538
15	8	0.199377	-0.472076	2.008957
16	8	-1.981437	-1.774588	0.460855

17	1	-3.126153	-1.06577	-0.084647
18	1	-1.733011	-2.678292	0.241778

TS4

E(B3LYP)= -1496.536516 Hartree

Zero-point correction= 0.077229 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.459287 Hartree

Sum of electronic and thermal Enthalpies = -1496.441138 Hartree

Sum of electronic and thermal Free Energies= -1496.487450 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.19888	-0.548676	0.22252
2	8	0.363498	1.864056	0.434906
3	8	-2.385491	1.096152	-0.03636
4	8	2.233929	0.833709	-0.029414
5	8	-3.979309	-0.488582	-0.13668
6	8	2.192169	-1.898913	-0.143093
7	8	0.334552	-3.029696	0.053792
8	6	-3.599265	0.825699	-0.259271
9	6	1.651682	1.977105	0.215813
10	6	1.628945	-3.080592	-0.139853
11	8	2.262644	-4.150312	-0.305413
12	8	2.258301	3.075882	0.239519
13	8	-4.506073	1.632086	-0.582742
14	8	-0.050838	-0.464103	-1.56981
15	8	0.50003	-0.622299	2.009534
16	8	-1.835455	-1.639058	0.6122
17	1	-3.153087	-1.011519	0.147151
18	1	-1.67346	-2.586073	0.545211

INT4

E(B3LYP)= -1496.551553 Hartree

Zero-point correction= 0.076689 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1496.474864 Hartree

Sum of electronic and thermal Enthalpies = -1496.455225 Hartree

Sum of electronic and thermal Free Energies= -1496.505290 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.693069	-0.679686	0.264408
2	8	0.86536	1.695026	0.612038
3	8	-4.82787	0.505785	0.813731
4	8	2.733162	0.645701	0.12416
5	8	-3.574968	0.061891	-1.011704

6	8	2.403209	-2.323805	-0.288546
7	8	0.3393	-3.040985	-0.051878
8	6	-4.779258	0.443048	-0.441356
9	6	2.162434	1.79455	0.400875
10	6	1.593245	-3.356176	-0.306836
11	8	1.968856	-4.52543	-0.540982
12	8	2.781091	2.879244	0.459682
13	8	-5.696114	0.684575	-1.262271
14	8	0.362472	-0.392816	-1.495506
15	8	0.974141	-0.961604	2.033791
16	8	-1.538231	-0.48332	0.660231
17	1	-2.893145	-0.113441	-0.307417
18	1	-1.848518	-0.570234	1.567364

COM2

E(B3LYP)= -1578.798386 Hartree

Zero-point correction= 0.181518 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1578.616868 Hartree

Sum of electronic and thermal Enthalpies = -1578.593285 Hartree

Sum of electronic and thermal Free Energies= -1578.65452 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.800997	-0.021088	0.232144
2	8	-0.73766	1.754727	1.453894
3	8	-2.890931	1.977565	1.079898
4	8	-4.11237	-0.32847	-0.448959
5	8	-2.671037	-1.890913	-1.00294
6	6	-1.813491	2.498342	1.619765
7	6	-3.923158	-1.481912	-1.047191
8	8	-4.833765	-2.131363	-1.603492
9	8	-1.801986	3.587851	2.230912
10	8	-2.125955	-0.894263	1.785941
11	8	-1.418568	0.825244	-1.323458
12	8	0.250707	-1.049868	0.123166
13	1	0.446728	-1.69062	0.814739
14	6	4.558709	-0.471177	-1.802293
15	6	3.44551	-0.599114	-0.958921
16	6	5.836532	-0.329131	-1.268849
17	1	6.679813	-0.229085	-1.945994
18	6	3.651104	-0.573934	0.427556
19	6	6.058989	-0.311643	0.114848
20	1	2.802524	-0.658371	1.096456
21	6	4.939684	-0.432911	0.944391

22	1	5.070339	-0.41506	2.02239
23	1	4.406513	-0.481654	-2.876187
24	6	7.454141	-0.191981	0.683405
25	1	7.432558	0.169467	1.714167
26	1	7.96952	-1.159198	0.687139
27	1	8.067318	0.497278	0.096637
28	8	2.222292	-0.737295	-1.523671
29	1	1.487922	-0.856307	-0.835374

TS5

E(B3LYP)= -1578.777819 Hartree

Zero-point correction= 0.181126 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1578.596693 Hartree

Sum of electronic and thermal Enthalpies = -1578.574274 Hartree

Sum of electronic and thermal Free Energies= -1578.63192 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.110956	-0.002913	0.015358
2	8	0.225093	1.983608	-0.086399
3	8	-1.938902	2.26818	0.022864
4	8	-3.506851	0.004054	0.184948
5	8	-2.556857	-1.959765	0.097054
6	6	-0.765038	2.848711	-0.03456
7	6	-3.686858	-1.296484	0.17002
8	8	-4.808412	-1.842883	0.22033
9	8	-0.59922	4.08622	-0.040096
10	8	-0.96463	0.027191	1.813331
11	8	-1.23786	-0.071516	-1.779236
12	8	0.083419	-2.290707	0.165292
13	1	-0.399833	-2.920424	-0.380123
14	6	3.475331	0.724027	-0.334013
15	6	2.906384	-0.563757	-0.499323
16	6	4.813689	0.88606	0.01638
17	1	5.206296	1.893482	0.134341
18	6	3.771988	-1.664178	-0.276043
19	6	5.666903	-0.206859	0.226435
20	1	3.373518	-2.66872	-0.386906
21	6	5.108649	-1.482257	0.07564
22	1	5.733069	-2.357765	0.237037
23	1	2.831912	1.585629	-0.472906
24	6	7.127154	-0.016591	0.569939
25	1	7.524092	-0.879961	1.110804
26	1	7.744579	0.113738	-0.327297

27	1	7.280023	0.868243	1.194488
28	8	1.644752	-0.730567	-0.853184
29	1	0.879592	-1.887285	-0.352064

TS1b'

E(B3LYP)= -1731.007361 Hartree

Zero-point correction= 0.206514 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1730.800847 Hartree

Sum of electronic and thermal Enthalpies = -1730.774601 Hartree

Sum of electronic and thermal Free Energies= -1730.840420 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.787659	-0.401115	-0.020459
2	8	2.373804	1.173784	1.014468
3	8	3.074885	-0.882738	0.814228
4	8	1.422029	-2.780726	-0.015341
5	8	-0.553819	-2.330216	-0.82004
6	6	3.343429	0.324055	1.232931
7	6	0.324759	-3.256543	-0.541705
8	8	0.133729	-4.481229	-0.757753
9	8	4.426619	0.640389	1.79
10	8	1.475102	-0.223538	-1.687839
11	8	0.116673	-0.615383	1.647439
12	6	-2.579483	0.326982	-0.305042
13	6	-2.956136	0.70928	1.007302
14	6	-3.637423	0.028999	-1.199408
15	6	-4.293983	0.779619	1.386731
16	6	-4.971007	0.104314	-0.801471
17	6	-5.335635	0.477008	0.498676
18	1	-2.173381	0.944733	1.719461
19	1	-3.386748	-0.260558	-2.21541
20	1	-4.535193	1.08109	2.403401
21	1	-5.748963	-0.13259	-1.523212
22	8	-1.325188	0.272825	-0.694688
23	6	-6.782434	0.521439	0.935409
24	1	-7.45072	0.672177	0.083463
25	1	-7.088771	-0.41072	1.425613
26	1	-6.961206	1.331325	1.648535
27	8	0.377264	2.46909	-0.369168
28	6	1.082871	3.469688	-0.669438
29	8	1.039113	4.594482	-0.093846
30	6	2.055974	3.3446	-1.851701
31	1	1.741686	4.025403	-2.649506

32	1	2.093005	2.327688	-2.24099
33	1	3.058378	3.653471	-1.542489

INT1b'

E(B3LYP)= -1731.009280 Hartree

Zero-point correction= 0.206322 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1730.802958 Hartree

Sum of electronic and thermal Enthalpies = -1730.775633 Hartree

Sum of electronic and thermal Free Energies= -1730.844120 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	0.872737	-0.290844	-0.029366
2	8	2.622121	1.357286	0.655449
3	8	3.240778	-0.730695	0.624173
4	8	1.639728	-2.657829	-0.057124
5	8	-0.431789	-2.33866	-0.6484
6	6	3.588462	0.504267	0.857996
7	6	0.524941	-3.204513	-0.458862
8	8	0.387646	-4.443549	-0.645965
9	8	4.741121	0.83964	1.242929
10	8	1.396281	-0.101557	-1.754602
11	8	0.366675	-0.480413	1.700529
12	6	-2.595731	0.135494	-0.334871
13	6	-2.987025	-0.06132	1.016861
14	6	-3.652424	0.329677	-1.264547
15	6	-4.327479	-0.061783	1.393907
16	6	-4.987701	0.324823	-0.86727
17	6	-5.363598	0.126988	0.468067
18	1	-2.208196	-0.21049	1.756798
19	1	-3.395125	0.490156	-2.307522
20	1	-4.576111	-0.212922	2.442088
21	1	-5.75928	0.480969	-1.617655
22	8	-1.347051	0.154819	-0.72448
23	6	-6.815918	0.086875	0.887004
24	1	-7.45069	0.614267	0.169846
25	1	-7.193582	-0.940662	0.957854
26	1	-6.964479	0.549406	1.86733
27	8	0.174668	2.189613	0.16283
28	6	0.443922	3.341438	-0.287041
29	8	0.16116	4.419353	0.299688
30	6	1.131266	3.449207	-1.651691
31	1	0.474567	3.987008	-2.342658
32	1	1.370358	2.471345	-2.065931

33	1	2.047746	4.037586	-1.556008

COM1c'

E(B3LYP)= -2077.919358 Hartree

Zero-point correction= 0.338954 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.580404 Hartree

Sum of electronic and thermal Enthalpies = -2077.54452 Hartree

Sum of electronic and thermal Free Energies= -2077.632630 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.481529	-0.898458	-0.049526
2	8	-3.56492	-2.213507	-0.39268
3	8	-1.699105	-3.298028	-0.686947
4	8	0.645343	-2.212613	-0.324059
5	8	0.926116	-0.100521	0.143481
6	6	-3.002617	-3.354192	-0.688887
7	6	1.47399	-1.244739	-0.103685
8	8	2.741108	-1.415993	-0.128047
9	8	-3.652471	-4.400792	-0.949604
10	8	-1.516635	-1.367836	1.698193
11	8	-1.431843	-0.454074	-1.802786
12	6	-1.114883	2.562599	0.258205
13	6	-1.096241	2.906494	-1.117608
14	6	-0.98596	3.644155	1.17167
15	6	-0.958015	4.229212	-1.535364
16	6	-0.849275	4.958379	0.734998
17	6	-0.829366	5.288558	-0.628291
18	1	-1.198202	2.109495	-1.84583
19	1	-1.000904	3.421707	2.234624
20	1	-0.952158	4.443009	-2.601751
21	1	-0.756979	5.750412	1.474697
22	8	-1.249512	1.334203	0.692371
23	6	-0.651256	6.716607	-1.092448
24	1	-1.264794	7.410728	-0.509658
25	1	0.3886	7.051627	-0.996038
26	1	-0.930742	6.82786	-2.143371
27	8	-3.688036	0.385337	0.037024
28	6	-4.743863	0.570538	0.710712
29	8	-5.759649	1.17954	0.28548
30	6	-4.800049	0.032581	2.143861
31	1	-5.063976	0.843669	2.828119
32	1	-3.855391	-0.413822	2.450453
33	1	-5.590848	-0.719848	2.215412

34	6	6.624765	1.093061	0.642921
35	1	6.323748	2.07795	0.9837
36	6	5.633151	0.152432	0.327686
37	8	4.336124	0.511138	0.458069
38	6	6.033981	-1.121575	-0.103622
39	1	5.27922	-1.861433	-0.343729
40	6	7.38973	-1.430728	-0.214805
41	1	7.672798	-2.425353	-0.547319
42	6	7.973343	0.766003	0.525471
43	6	8.388604	-0.499882	0.091908
44	1	8.718886	1.513856	0.779896
45	6	9.853914	-0.835765	-0.064284
46	1	10.034524	-1.904255	0.07715
47	1	10.466524	-0.291148	0.658763
48	1	10.221751	-0.57386	-1.063124
49	1	3.693529	-0.246754	0.218828

TS1c'

E(B3LYP)= -2077.914944 Hartree

Zero-point correction= 0.338045 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.576899 Hartree

Sum of electronic and thermal Enthalpies = -2077.541621 Hartree

Sum of electronic and thermal Free Energies= -2077.629320 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.784436	-0.48746	0.028938
2	8	-4.115685	-0.686847	-0.840028
3	8	-3.010163	-2.5343	-0.4894
4	8	-0.178488	-2.937428	-0.616261
5	8	0.33918	-1.365043	0.847
6	6	-4.141954	-1.990676	-0.862537
7	6	0.655666	-2.472176	0.22105
8	8	1.786585	-3.042347	0.472792
9	8	-5.146901	-2.663749	-1.20637
10	8	-2.395831	-0.704145	1.716555
11	8	-1.202152	-0.238029	-1.66232
12	6	0.442465	2.167866	0.401716
13	6	0.982291	2.204501	-0.908189
14	6	0.903639	3.164954	1.29871
15	6	1.917665	3.167808	-1.27981
16	6	1.839791	4.119639	0.908531
17	6	2.374784	4.145844	-0.386598
18	1	0.641758	1.465412	-1.624332

19	1	0.505135	3.173077	2.308833
20	1	2.301747	3.159036	-2.297231
21	1	2.161012	4.866305	1.630797
22	8	-0.440844	1.273217	0.789142
23	6	3.4181	5.162112	-0.792136
24	1	3.29999	6.098183	-0.239289
25	1	4.435784	4.800802	-0.600029
26	1	3.356021	5.393375	-1.85914
27	8	-2.978599	1.668755	-0.187222
28	6	-4.027454	2.317218	0.132118
29	8	-4.43013	3.336852	-0.474447
30	6	-4.829738	1.806962	1.327012
31	1	-5.605031	2.51805	1.613414
32	1	-4.171115	1.612435	2.175968
33	1	-5.290225	0.854785	1.052471
34	6	5.837635	-0.982814	1.541655
35	1	5.843451	-0.819531	2.614198
36	6	4.706643	-1.569569	0.95179
37	8	3.668168	-1.916604	1.741228
38	6	4.709121	-1.766173	-0.438581
39	1	3.841685	-2.214881	-0.908643
40	6	5.814098	-1.387389	-1.201404
41	1	5.787176	-1.548412	-2.275404
42	6	6.931381	-0.611833	0.76386
43	6	6.948461	-0.806782	-0.623841
44	1	7.790446	-0.15719	1.249045
45	6	8.152645	-0.428843	-1.455686
46	1	7.878556	-0.273767	-2.502037
47	1	8.919631	-1.211592	-1.432481
48	1	8.619064	0.489876	-1.089785
49	1	2.88051	-2.326201	1.210044

INT1c'

E(B3LYP)= -2077.930342 Hartree

Zero-point correction= 0.338126 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.592216 Hartree

Sum of electronic and thermal Enthalpies = -2077.556212 Hartree

Sum of electronic and thermal Free Energies= -2077.644200 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.819057	-0.349301	-0.04271
2	8	-4.215463	-0.869843	0.043583
3	8	-2.895256	-2.420139	-0.761843

4	8	0.222136	-2.236378	-2.976521
5	8	-0.074038	-1.596131	-0.842917
6	6	-4.124974	-2.07514	-0.461311
7	6	0.707949	-1.983725	-1.840609
8	8	1.970235	-2.096381	-1.58244
9	8	-5.113579	-2.826512	-0.638172
10	8	-1.590702	-1.07444	1.603748
11	8	-2.07978	0.391626	-1.674523
12	6	0.664497	2.088715	-0.107051
13	6	0.652883	2.432781	-1.478757
14	6	1.541011	2.824487	0.724585
15	6	1.471569	3.445117	-1.97519
16	6	2.352205	3.833765	0.210839
17	6	2.342628	4.168108	-1.149689
18	1	-0.017421	1.894789	-2.13946
19	1	1.568196	2.587749	1.783685
20	1	1.429616	3.680034	-3.03592
21	1	3.008711	4.375717	0.886885
22	8	-0.097453	1.132097	0.397636
23	6	3.252998	5.23876	-1.706775
24	1	3.47464	6.003379	-0.957386
25	1	4.212706	4.823801	-2.037623
26	1	2.803052	5.735705	-2.570578
27	8	-2.962675	1.56547	0.933795
28	6	-3.788613	1.957624	1.832714
29	8	-4.231966	3.12142	1.902606
30	6	-4.228366	0.920754	2.860183
31	1	-4.961715	1.336799	3.551023
32	1	-3.358533	0.569271	3.421621
33	1	-4.643408	0.056678	2.337594
34	6	4.866194	-1.579966	2.032139
35	1	4.287704	-1.72067	2.939082
36	6	4.209496	-1.647956	0.792705
37	8	2.882882	-1.890131	0.77511
38	6	4.969176	-1.454234	-0.372558
39	1	4.47664	-1.496113	-1.337078
40	6	6.339552	-1.206157	-0.286511
41	1	6.901605	-1.056769	-1.204077
42	6	6.23451	-1.331309	2.097861
43	6	7.004953	-1.142184	0.942652
44	1	6.712817	-1.281366	3.071978
45	6	8.495739	-0.906015	1.022847
46	1	8.862758	-0.380381	0.137882
47	1	9.049408	-1.849446	1.093744
48	1	8.759182	-0.311198	1.901545

49	1	2.492076	-1.938056	-0.182594

TS2c'

E(B3LYP)= -2077.928341 Hartree

Zero-point correction= 0.334298 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.594043 Hartree

Sum of electronic and thermal Enthalpies = -2077.558423 Hartree

Sum of electronic and thermal Free Energies= -2077.644680 Hartree

Center	Atomic		Coordinates(Angstroms)	
Number	number	x	y	z
1	92	-1.72798	-0.447256	-0.042654
2	8	-4.093165	-1.08732	0.015658
3	8	-2.67674	-2.575078	-0.737473
4	8	0.427622	-2.326539	-2.906826
5	8	0.115515	-1.695728	-0.77069
6	6	-3.930358	-2.292609	-0.470825
7	6	0.865068	-2.103594	-1.755796
8	8	2.145748	-2.293048	-1.489431
9	8	-4.87276	-3.095818	-0.662094
10	8	-1.47549	-1.124372	1.616723
11	8	-1.986838	0.242565	-1.694055
12	6	0.44967	2.229136	-0.143138
13	6	1.144083	2.24458	-1.373128
14	6	0.380893	3.450508	0.565514
15	6	1.729614	3.413574	-1.85637
16	6	0.970122	4.6098	0.067115
17	6	1.660278	4.622242	-1.152359
18	1	1.214428	1.324958	-1.943887
19	1	-0.14988	3.470701	1.511802
20	1	2.253069	3.382883	-2.808467
21	1	0.888609	5.529127	0.641389
22	8	-0.103374	1.127028	0.341837
23	6	2.326686	5.877359	-1.667927
24	1	2.416035	5.861789	-2.757267
25	1	1.762974	6.772096	-1.389754
26	1	3.338445	5.994888	-1.261769
27	8	-2.993526	1.399582	0.875081
28	6	-3.814922	1.766498	1.789825
29	8	-4.292414	2.915523	1.865705
30	6	-4.20321	0.717809	2.825258
31	1	-4.947177	1.107597	3.519962
32	1	-3.314579	0.405818	3.380526
33	1	-4.585849	-0.166022	2.311081

34	6	4.939648	-1.360676	2.027451
35	1	4.343	-1.449481	2.930162
36	6	4.309129	-1.58413	0.780864
37	8	3.022016	-1.898513	0.728689
38	6	5.120142	-1.44779	-0.371368
39	1	4.673388	-1.604406	-1.347064
40	6	6.469885	-1.113153	-0.268
41	1	7.054778	-1.01554	-1.1793
42	6	6.289143	-1.027934	2.110349
43	6	7.091212	-0.897787	0.968141
44	1	6.729416	-0.861908	3.090439
45	6	8.563637	-0.56914	1.069005
46	1	8.770645	0.079793	1.924575
47	1	8.920268	-0.060449	0.169348
48	1	9.175456	-1.470795	1.194079
49	1	2.534068	-2.067917	-0.394339

INT2c'

E(B3LYP)= -2077.92973 Hartree

Zero-point correction= 0.337425 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.592305 Hartree

Sum of electronic and thermal Enthalpies = -2077.556085 Hartree

Sum of electronic and thermal Free Energies= -2077.645180 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-1.728878	-0.513042	-0.060594
2	8	-3.917186	-1.58833	-0.031668
3	8	-2.290448	-2.687034	-0.99715
4	8	0.597054	-1.543704	-3.16906
5	8	0.332144	-1.355421	-0.938971
6	6	-3.561871	-2.67607	-0.671439
7	6	1.033332	-1.511512	-2.006235
8	8	2.363058	-1.662401	-1.83075
9	8	-4.351925	-3.608232	-0.943148
10	8	-1.295989	-1.302187	1.506669
11	8	-2.157504	0.288443	-1.621081
12	6	0.080487	2.409787	-0.00966
13	6	0.816308	2.53382	-1.208441
14	6	-0.165499	3.59525	0.71775
15	6	1.279679	3.774473	-1.642279
16	6	0.305017	4.827207	0.269228
17	6	1.040548	4.948788	-0.917023
18	1	1.015578	1.6412	-1.791344

19	1	-0.73678	3.528611	1.637908
20	1	1.84188	3.829425	-2.570844
21	1	0.091998	5.716821	0.856166
22	8	-0.352317	1.236752	0.432238
23	6	1.57991	6.284117	-1.376707
24	1	1.662096	6.327249	-2.465971
25	1	0.93553	7.106687	-1.055101
26	1	2.579215	6.478741	-0.969378
27	8	-3.244185	0.980646	1.071862
28	6	-4.075466	1.120694	2.041032
29	8	-4.73668	2.158224	2.233924
30	6	-4.2309	-0.061798	2.989692
31	1	-5.003371	0.131625	3.733832
32	1	-3.28026	-0.252385	3.495036
33	1	-4.473534	-0.95684	2.413883
34	6	5.227412	-1.315963	1.946881
35	1	4.598933	-1.459045	2.821567
36	6	4.607901	-1.345284	0.665816
37	8	3.320723	-1.540953	0.529912
38	6	5.482453	-1.141173	-0.440237
39	1	5.060321	-1.145509	-1.440525
40	6	6.848722	-0.930633	-0.26669
41	1	7.469922	-0.775771	-1.146317
42	6	6.595583	-1.104003	2.099261
43	6	7.445525	-0.908749	1.001431
44	1	7.0152	-1.087918	3.102784
45	6	8.935576	-0.715695	1.173999
46	1	9.169792	-0.268449	2.14418
47	1	9.34719	-0.062872	0.398677
48	1	9.483407	-1.664728	1.117306
49	1	2.677426	-1.592972	-0.847742

TS3c'

E(B3LYP)= -2077.913914 Hartree

Zero-point correction= 0.338081 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.575834 Hartree

Sum of electronic and thermal Enthalpies = -2077.540232 Hartree

Sum of electronic and thermal Free Energies= -2077.628100 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.525441	-1.099695	0.261625
2	8	0.322228	-3.214562	1.386345
3	8	-1.388527	-1.855588	1.503354

4	8	-1.47545	4.41747	3.026569
5	8	-2.254953	2.300486	3.051893
6	6	-0.894824	-3.024543	1.846809
7	6	-1.765735	3.316392	2.493573
8	8	-1.506106	3.242808	1.13978
9	8	-1.51236	-3.86183	2.533684
10	8	-0.134969	-1.84081	-1.240981
11	8	1.195672	-0.359367	1.759245
12	6	2.195177	1.664843	-0.882554
13	6	1.775238	2.885912	-0.315982
14	6	3.487516	1.614344	-1.441384
15	6	2.618354	3.99532	-0.316155
16	6	4.31651	2.734954	-1.430393
17	6	3.905656	3.949537	-0.867966
18	1	0.782268	2.954818	0.116053
19	1	3.825592	0.685678	-1.888447
20	1	2.2619	4.923064	0.123838
21	1	5.30567	2.661226	-1.874118
22	8	1.394718	0.599147	-0.918577
23	6	4.819544	5.153125	-0.831092
24	1	5.587507	5.091856	-1.606043
25	1	4.263569	6.082863	-0.980039
26	1	5.335812	5.238334	0.132436
27	8	2.597866	-2.123449	-0.095911
28	6	3.355744	-2.695191	-0.973752
29	8	3.298601	-2.502394	-2.194572
30	6	4.38347	-3.656079	-0.388618
31	1	5.023328	-3.124226	0.320351
32	1	4.998036	-4.099637	-1.171405
33	1	3.872867	-4.44707	0.166964
34	6	-3.406924	-0.275874	-1.670182
35	1	-2.559776	-0.907803	-1.917977
36	6	-3.191606	0.801876	-0.763933
37	8	-2.018704	1.051054	-0.24203
38	6	-4.341366	1.59451	-0.477019
39	1	-4.232287	2.435019	0.201675
40	6	-5.58376	1.32359	-1.046205
41	1	-6.426226	1.963653	-0.792313
42	6	-4.657619	-0.529562	-2.228134
43	6	-5.781133	0.256026	-1.932765
44	1	-4.764084	-1.366678	-2.915093
45	6	-7.143923	-0.055959	-2.509453
46	1	-7.744922	0.850263	-2.629301
47	1	-7.716782	-0.73714	-1.867498
48	1	-7.063256	-0.533621	-3.490188

49	1	-1.775782	2.358241	0.742444

INT3c'

E(B3LYP)= -2077.933304 Hartree

Zero-point correction= 0.338958 (Hartree/Particle)

Sum of electronic and zero-point Energies= -2077.594346 Hartree

Sum of electronic and thermal Enthalpies = -2077.55802 Hartree

Sum of electronic and thermal Free Energies= -2077.646820 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	0.198032	-1.088876	0.069984
2	8	0.248061	-3.433029	0.788896
3	8	-1.652834	-2.372588	1.013436
4	8	-1.78729	3.243202	4.105098
5	8	-2.30993	1.093028	3.650343
6	6	-1.002872	-3.500316	1.173772
7	6	-1.880201	2.236923	3.364832
8	8	-1.443468	2.440145	2.0585
9	8	-1.525671	-4.536351	1.648044
10	8	-0.307544	-1.627985	-1.579753
11	8	0.678819	-0.540338	1.725132
12	6	2.105979	1.720626	-0.665611
13	6	1.769362	2.792076	0.192564
14	6	3.343529	1.806437	-1.342338
15	6	2.628591	3.877194	0.355787
16	6	4.190321	2.898528	-1.164451
17	6	3.85794	3.958655	-0.311239
18	1	0.823218	2.763223	0.722619
19	1	3.622659	1.001351	-2.014442
20	1	2.331978	4.684298	1.020986
21	1	5.132124	2.927347	-1.706393
22	8	1.295316	0.690876	-0.858738
23	6	4.796036	5.124822	-0.097255
24	1	5.425735	5.29595	-0.97438
25	1	4.246	6.047568	0.106601
26	1	5.4663	4.954609	0.753778
27	8	2.477312	-1.935515	-0.165006
28	6	3.331325	-2.446098	-0.971069
29	8	3.138755	-2.688249	-2.177383
30	6	4.685442	-2.78175	-0.344441
31	1	5.059035	-1.931267	0.230508
32	1	5.41527	-3.062834	-1.103893
33	1	4.561587	-3.615636	0.353141

34	6	-2.416703	1.161436	-1.974705
35	1	-1.403097	1.229976	-2.353314
36	6	-2.614333	0.7234	-0.647969
37	8	-1.595166	0.413702	0.15442
38	6	-3.945878	0.657282	-0.186322
39	1	-4.126521	0.330598	0.832356
40	6	-5.013956	1.003138	-1.012478
41	1	-6.024987	0.939646	-0.618672
42	6	-3.495262	1.503066	-2.787906
43	6	-4.817866	1.430354	-2.331546
44	1	-3.301519	1.838636	-3.803464
45	6	-5.982547	1.770113	-3.233425
46	1	-6.840652	2.127853	-2.658434
47	1	-6.318097	0.897542	-3.806417
48	1	-5.714569	2.545811	-3.955771
49	1	-1.537708	1.61142	1.535563

Prod'

E(B3LYP)= -1813.27556 Hartree

Zero-point correction= 0.310917 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1812.964644 Hartree

Sum of electronic and thermal Enthalpies = -1812.933234 Hartree

Sum of electronic and thermal Free Energies= -1813.012270 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.061494	-0.957344	-0.166336
2	8	-0.011163	-3.389718	-0.503225
3	8	1.780872	-2.277568	-1.087342
4	6	1.199204	-3.449766	-1.000508
5	8	1.748062	-4.519002	-1.358849
6	8	0.610911	-1.198238	1.497364
7	8	-0.738083	-0.727886	-1.832352
8	6	-1.939412	1.931435	0.177777
9	6	-1.59706	2.743941	-0.927454
10	6	-3.111747	2.280543	0.886578
11	6	-2.385484	3.832989	-1.293163
12	6	-3.889156	3.372103	0.505412
13	6	-3.549882	4.173756	-0.592397
14	1	-0.697819	2.507528	-1.485412
15	1	-3.394982	1.680612	1.745592
16	1	-2.083501	4.435801	-2.145929
17	1	-4.781451	3.607471	1.079871
18	8	-1.19406	0.907071	0.559907

19	6	-4.415737	5.337197	-1.019276
20	1	-4.961901	5.7594	-0.171643
21	1	-3.818219	6.136766	-1.465613
22	1	-5.160239	5.036264	-1.766033
23	8	-2.243721	-1.882109	0.446854
24	6	-3.01301	-2.22756	1.410469
25	8	-2.776051	-2.072	2.623276
26	6	-4.326293	-2.88187	0.978417
27	1	-4.874535	-2.209029	0.313595
28	1	-4.949153	-3.129452	1.837984
29	1	-4.113476	-3.792623	0.411793
30	6	2.809004	1.687354	1.123497
31	1	1.932606	1.685681	1.762202
32	6	2.712812	1.106066	-0.161547
33	8	1.590477	0.573042	-0.615821
34	6	3.876976	1.14149	-0.963746
35	1	3.83072	0.713246	-1.959976
36	6	5.060148	1.710876	-0.498753
37	1	5.931693	1.715761	-1.148343
38	6	4.000396	2.254321	1.572172
39	6	5.155016	2.277328	0.77932
40	1	4.030683	2.691854	2.566845
41	6	6.453186	2.859112	1.290905
42	1	7.051898	3.276862	0.476968
43	1	7.06925	2.099893	1.787524
44	1	6.274187	3.654952	2.018765

U-3CO_3-Asp*

E(B3LYP)= -1648.761224 Hartree

Zero-point correction= 0.101943 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1648.659281 Hartree

Sum of electronic and thermal Enthalpies = -1648.63647 Hartree

Sum of electronic and thermal Free Energies= -1648.692640 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.286215	-0.127578	0.084094
2	8	1.202608	-1.833627	0.023007
3	8	-2.156632	3.207063	-1.344767
4	8	1.410615	-3.757213	-1.113714
5	8	-0.883655	2.059972	0.105981
6	8	-1.723937	-2.11759	0.293338
7	8	-2.748529	-0.183229	0.314171
8	6	-1.186606	3.205961	-0.522388

9	6	1.97073	-2.726922	-0.62071
10	6	-2.867482	-1.48489	0.377365
11	8	-3.971228	-2.072841	0.505962
12	8	3.220037	-2.494123	-0.682052
13	8	-0.48546	4.231153	-0.242464
14	8	-0.444048	-0.190613	-1.724924
15	8	-0.127243	-0.074127	1.896209
16	8	1.849819	1.066136	-0.255083
17	6	2.956694	1.461038	0.243331
18	8	3.81865	2.106771	-0.391052
19	6	3.241935	1.085777	1.696564
20	1	3.625889	0.060417	1.71825
21	1	2.329951	1.105598	2.293998
22	1	3.996347	1.743552	2.129228

U-3CO_3-Asp*(hexa-coor)

E(B3LYP)= -1648.74935 Hartree

Zero-point correction= 0.102279 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1648.647071 Hartree

Sum of electronic and thermal Enthalpies = -1648.624257 Hartree

Sum of electronic and thermal Free Energies= -1648.68009 Hartree

Center	Atomic	Coordinates(Angstroms)		
Number	number	x	y	z
1	92	-0.234224	-0.358958	-0.001024
2	8	0.397799	-2.788118	-0.152319
3	8	-1.147444	3.298156	-1.505325
4	8	2.483309	-3.575834	-0.513541
5	8	-0.777023	1.883451	0.202598
6	8	-2.053726	-2.044642	0.27561
7	8	-2.690292	0.034412	0.399943
8	6	-0.962321	3.111656	-0.253232
9	6	1.67221	-2.620121	-0.363213
10	6	-3.050357	-1.217975	0.43299
11	8	-4.243111	-1.594832	0.600817
12	8	2.029779	-1.366328	-0.402436
13	8	-0.955388	4.071558	0.597212
14	8	-0.527531	-0.365605	-1.791714
15	8	0.075291	-0.428388	1.786121
16	8	1.773386	1.256971	-0.38531
17	6	2.835117	1.698449	0.138045
18	8	3.746039	2.301533	-0.491567
19	6	3.048711	1.487185	1.641426
20	1	3.767329	0.672993	1.782119

21	1	2.124539	1.217272	2.151423
22	1	3.480265	2.384365	2.090944

U-2CO_3-Asp*

E(B3LYP)= -1460.581062 Hartree

Zero-point correction= 0.098772 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1460.48229 Hartree

Sum of electronic and thermal Enthalpies = -1460.461705 Hartree

Sum of electronic and thermal Free Energies= -1460.50834 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.378206	-0.370963	-0.068669
2	8	-2.791513	-0.714043	0.332621
3	8	-2.166622	1.341038	-0.092871
4	8	1.006131	3.331719	0.80412
5	8	0.713094	1.567968	-0.556234
6	6	-3.161574	0.531063	0.166955
7	6	1.400758	2.663905	-0.204231
8	8	2.410385	2.975508	-0.91598
9	8	-4.35756	0.910935	0.248385
10	8	-0.656721	-0.674592	-1.842321
11	8	-0.115969	-0.132665	1.713418
12	8	-0.555101	-2.598143	0.330648
13	1	-0.761972	-3.157471	-0.424249
14	8	1.959097	-1.128553	-0.367015
15	6	3.155741	-1.067117	0.07843
16	8	4.128531	-1.640232	-0.456817
17	6	3.385882	-0.227822	1.333427
18	1	3.198824	0.823297	1.09776
19	1	4.406872	-0.338192	1.699122
20	1	2.676416	-0.51075	2.113781

U-2CO_3-Asp*(hexa-coor)

E(B3LYP)= -1460.573942 Hartree

Zero-point correction= 0.099696 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1460.474246 Hartree

Sum of electronic and thermal Enthalpies = -1460.453974 Hartree

Sum of electronic and thermal Free Energies= -1460.50212 Hartree

Center Number	Atomic number	Coordinates(Angstroms) x	y	z
1	92	-0.352679	-0.032207	-0.156685
2	8	-2.659164	-1.061305	0.262521

3	8	-2.576372	1.093327	-0.06336
4	8	-0.370848	2.439134	-0.590607
5	8	1.589007	1.480872	-0.602522
6	6	-3.328321	0.058193	0.182956
7	6	0.915897	2.589346	-0.742156
8	8	1.457822	3.699847	-0.999001
9	8	-4.578586	0.128145	0.330595
10	8	-0.563283	-0.287943	-1.946413
11	8	-0.162708	0.295321	1.62174
12	8	-0.385165	-2.32467	0.23228
13	1	-1.319752	-2.509622	0.377574
14	8	1.932611	-1.145417	-0.350184
15	6	3.134346	-1.147118	0.052857
16	8	4.098786	-1.633084	-0.5915
17	6	3.414178	-0.519928	1.419696
18	1	3.15935	0.540883	1.374509
19	1	4.460414	-0.63561	1.705299
20	1	2.776894	-0.975813	2.181589