

## Supporting Information (SI)

---

# The environmental degradation of naphthalimide, rhodamine and bodipy fluorophores by hydroxyl radicals: A theoretical insight

Nguyen Linh Nam,<sup>1\*</sup> Mai Van Bay<sup>2\*</sup>, Nguyen Thi Hoa,<sup>1</sup> Nguyen Quang Trung,<sup>3</sup> Nguyen Minh Thong<sup>2</sup>, Adam Mechler<sup>4</sup>, Pham Cam Nam<sup>5</sup> Nguyen Khoa Hien,<sup>6</sup> Duong Tuan Quang<sup>7</sup> and Quan V. Vo<sup>1\*\*</sup>

<sup>1</sup>*The University of Danang - University of Technology and Education, Danang 550000, Vietnam.*

<sup>2</sup>*The University of Danang - University of Sciences and Education, Danang 550000, Vietnam.*

<sup>3</sup>*Quality assurance and Testing center 2, Da Nang 550000, Vietnam.*

<sup>4</sup>*Department of Biochemistry and Chemistry, La Trobe University, Victoria 3086, Australia.*

<sup>5</sup>*The University of Danang - University of Technology and Sciences, Danang 550000, Vietnam.*

<sup>6</sup>*Mien Trung Institute for Scientific Research, Vietnam National Museum of Nature, Vietnam Academy of Science and Technology, Hue 530000, Vietnam*

<sup>7</sup>*Department of Chemistry, Hue University, Hue 530000, Vietnam*

*\*: First authors have equal contributions.*

*\*\*Corresponding authors: [vvquan@ute.udn.vn](mailto:vvquan@ute.udn.vn);*

### Table of Contents

Table S1. The method to calculate rate constant following the conventional transition state theory .....	S2
Table S2. Bioconcentration (BCF) and biodegradability of FPHs and the main degradation products.....	S4
Table S3: The Cartesian coordinates, energies of TS of the reaction between FPHs with HO <sup>*</sup> in the studied media (M: methanol; P: pentyl ethanoate; H: water).....	S6
References .....	S92

**Table S1. The method to calculate rate constant following the conventional transition state theory**

The rate constant ( $k$ ) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):<sup>1-5</sup>

$$k = \sigma \kappa \frac{k_B T}{h} e^{-(\Delta G^\ddagger)/RT} \quad (1)$$

Where:  $\sigma$  is the reaction symmetry number,<sup>6-7</sup>

$\kappa$  contains the tunneling corrections calculated using the Eckart barrier,<sup>8</sup>

$k_B$  is the Boltzmann constant,

$h$  is the Planck constant,

$\Delta G^\ddagger$  is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.<sup>9-12</sup> The free energy of reaction  $\Delta G^\ddagger$  for the SET pathway was computed following the equations (2,3).

$$\Delta G_{\text{SET}}^\ddagger = \frac{\lambda}{4} \left( 1 + \frac{\Delta G_{\text{SET}}^0}{\lambda} \right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{\text{SET}} - \Delta G_{\text{SET}}^0 \quad (3)$$

where  $\Delta G_{\text{SET}}$  is the Gibbs energy of reaction,  $\Delta E_{\text{SET}}$  is the non-adiabatic energy difference between reactants and vertical products for SET.<sup>13-14</sup>

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results<sup>15</sup>. The apparent rate constants ( $k_{\text{app}}$ ) were calculated following the Collins–Kimball theory in the solvents at 298.15K;<sup>16</sup> the steady-state Smoluchowski rate constant ( $k_D$ ) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as according to equations (4,5).<sup>15,17</sup>

$$k_{\text{app}} = \frac{k_{\text{TST}} k_D}{k_{\text{TST}} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where  $R_{AB}$  is the reaction distance,  $N_A$  is the Avogadro constant, and  $D_{AB} = D_A + D_B$  ( $D_{AB}$  is the mutual diffusion coefficient of the reactants A and B),<sup>16,18</sup> where  $D_A$  or  $D_B$  is estimated using the

Stokes–Einstein formulation (6).<sup>19-20</sup>

$$D_{A \text{ or } B} = \frac{k_B T}{6\pi\eta a_{A \text{ or } B}} \quad (6)$$

$\eta$  is the viscosity of the solvents at 298.15 K (i.e.  $\eta(\text{H}_2\text{O}) = 8.91 \times 10^{-4}$  Pa s,  $\eta(\text{pentyl ethanoate}) = 8.62 \times 10^{-4}$  Pa s,  $\eta(\text{methanol}) = 5.43 \times 10^{-4}$  Pa s) and  $a$  is the radius of the solute.

All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex.

**Table S2. Bioconcentration (BCF) and biodegradability of FPHs and the main degradation products.**

Products	BCF	Biodegradability			
		BIOWIN3	BIOWIN4	BIOWIN5	Biodegradable
<b>BOD</b>	3.162	2.7727 (weeks)	3.5693 (days-weeks)	0.2192	NO
<b>B-P1</b>	3.162	2.8929 (weeks)	3.6728 (days-weeks)	0.3393	NO
<b>B-P1'</b>	3.162	2.5208 (weeks-months)	3.3899 (days-weeks)	0.2406	NO
<b>B-P2</b>	3.162	2.8929 (weeks)	3.6728 (days-weeks)	0.3404	NO
<b>B-P3</b>	3.162	2.8929 (weeks)	3.6728 (days-weeks)	0.3404	NO
<b>RDA-H2A</b>	59.110	2.5997 (weeks-months)	3.4701 (days-weeks)	-0.0078	NO
<b>R-H2A-P2</b>	15.400	2.7243 (weeks-months)	3.5765 (days-weeks)	0.0995	NO
<b>R-H2A-P4</b>	49.900	2.5730 (weeks-months)	3.4568 (days-weeks)	-0.0631	NO
<b>RDA-HA</b>	59.110	2.5997 (weeks-months)	2.5997 (weeks-months)	-0.0078	NO
<b>R-HA-P2</b>	47.360	2.7199 (weeks-months)	3.5736 (days-weeks)	0.1195	NO
<b>R-HA-P4</b>	3.162	2.7199 (weeks-months)	3.5736 (days-weeks)	0.1184	NO
<b>R-HA-P17</b>	353.600	2.5997 (weeks-months)	3.4701 (days-weeks)	-0.0078	NO
<b>RDA</b>	1419.000	2.3953 (weeks-months)	3.4083 (days-weeks)	-0.0179	NO
<b>R-P-SET</b>	1419.000	2.3953 (weeks-months)	3.4083 (days-weeks)	-0.0179	NO
<b>R-P1</b>	369.600	2.5200 (weeks-months)	3.5146 (days-weeks)	0.0895	NO
<b>R-P1'</b>	10.330	2.0686 (months)	3.1603 (weeks)	-0.0136	NO
<b>R-P2</b>	18.260	2.5200 (weeks-months)	3.5146 (days-weeks)	0.0895	NO
<b>R-P4</b>	156.000	2.5155 (weeks-months)	3.5117 (days-weeks)	0.1084	NO
<b>R-P4'</b>	23.750	2.1434 (months)	3.2288 (weeks)	0.0097	NO
<b>R-P5</b>	6.226	2.6559 (weeks-months)	3.5163 (days-weeks)	0.0631	NO
<b>R-P5'</b>	26.550	2.3523 (weeks-months)	3.2936 (days-weeks)	-0.0003	NO
<b>R-P6</b>	19.180	2.2090 (months)	3.1648 (weeks)	-0.0888	NO
<b>R-P7</b>	684.100	2.4164 (weeks-months)	3.4249 (days-weeks)	-0.0094	NO
<b>R-P8'</b>	9.101	2.3523 (weeks-months)	3.2936 (days-weeks)	-0.0003	NO
<b>R-P9</b>	22.620	2.1434 (months)	3.2288 (weeks)	0.0086	NO
<b>R-N17</b>	172.800	2.4159 (weeks-months)	3.3066 (days-weeks)	-0.2576	NO
<b>R-N18</b>	70.110	2.3953 (weeks-months)	3.4083 (days-weeks)	-0.0179	NO

<b>NPA</b>	9.588	2.7634 (weeks)	3.5632 (days-weeks)	0.1748	NO
<b>N-P4</b>	3.162	2.8836 (weeks)	3.6667 (days-weeks)	0.2801	NO
<b>N-P5</b>	3.162	2.8836 (weeks)	3.6667 (days-weeks)	0.2801	NO
<b>N-P6</b>	3.162	2.8836 (weeks)	3.6667 (days-weeks)	0.2889	NO
<b>N-P12</b>	3.162	2.5115 (weeks-months)	3.3838 (days-weeks)	0.1891	NO
<b>NPA - ANION</b>	9.588	2.7634 (weeks)	3.5632 (days-weeks)	0.1748	NO
<b>NA-P4</b>	3.162	2.8836 (weeks)	3.6667 (days-weeks)	0.2801	NO
<b>NA-P5</b>	3.162	2.8836 (weeks)	3.6667 (days-weeks)	0.2801	NO
<b>NA-P6</b>	4.623	2.7844 (weeks)	3.5798 (days-weeks)	0.1832	NO
<b>NA-P10</b>	3.162	2.5115 (weeks-months)	3.3838 (days-weeks)	0.1891	NO

**Table S3: The Cartesian coordinates, energies of TS of the reaction between FPHs with HO<sup>•</sup> in the studied media (M: methanol; P: pentyl ethanoate; H: water)**

Cartesian coordinates				Energies	
BOD-C1'-OH-TS-H					
Atom	X	Y	Z	Electronic Energy (EE)	-757.065
C	0.66169	-0.186783	-0.051727	Zero-point Energy Correction	0.164047
C	-0.110555	-1.270245	-0.384039	Thermal Correction to Energy	0.176206
C	0.730839	-2.411887	-0.31842	Thermal Correction to Enthalpy	0.17715
B	3.196636	-2.960632	0.281627	Thermal Correction to Free Energy	0.125256
C	5.700255	-2.426951	-0.113173		
C	6.543722	-1.288325	-0.186028		
C	5.732087	-0.18416	-0.074036		
C	3.208351	0.019295	0.180795		
C	4.394715	-0.657161	0.058756		
N	4.4337	-2.055767	0.023556		
C	1.9764	-0.676087	0.248647		
N	1.963483	-2.058038	0.025061		
F	3.191459	-4.059344	-0.562698		
F	3.199611	-3.373531	1.622823		
H	0.375628	0.85325	0.002634		
H	-1.155588	-1.283816	-0.650044		
H	0.480106	-3.446362	-0.50941		
H	5.974002	-3.472586	-0.154334		
H	7.61453	-1.315057	-0.311541		
H	6.014223	0.858166	-0.090439		
H	3.203105	1.102292	0.218824		
O	1.816589	-0.625941	2.342541		
H	2.396194	-1.392901	2.467389		
BOD-C1'-OH-TS-M					
Atom	X	Y	Z	Electronic Energy (EE)	-757.071
C	0.654759	-0.170912	-0.226671	Zero-point Energy Correction	0.163755
C	-0.15002	-1.280103	-0.342793	Thermal Correction to Energy	0.176092
C	0.69124	-2.413777	-0.202641	Thermal Correction to Enthalpy	0.177036
B	3.176552	-2.933835	0.301687	Thermal Correction to Free Energy	0.124322
C	5.668561	-2.390354	-0.166034		
C	6.510871	-1.248914	-0.224927		
C	5.721059	-0.157886	0.032054		
C	3.164487	0.046452	0.133935		
C	4.392915	-0.641465	0.279025		

N	4.419858	-2.029653	0.103451
C	1.985398	-0.636822	-0.023428
N	1.95011	-2.035171	-0.020747
F	3.22768	-4.032581	-0.54323
F	3.108154	-3.349015	1.638939
H	0.371354	0.870122	-0.283059
H	-1.214976	-1.312486	-0.512469
H	0.421444	-3.461277	-0.227082
H	5.930085	-3.429895	-0.311646
H	7.568902	-1.267806	-0.434962
H	6.003606	0.884164	0.070709
H	3.165925	1.130489	0.141344
O	4.460718	-0.503053	2.371193
H	3.865508	-1.253763	2.52193

BOD-C1'-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-757.063
C	0.666362	-0.186779	-0.030256	Zero-point Energy Correction	0.164112
C	-0.089042	-1.263409	-0.412082	Thermal Correction to Energy	0.176297
C	0.753615	-2.405559	-0.336597	Thermal Correction to Enthalpy	0.177241
B	3.205853	-2.958293	0.318867	Thermal Correction to Free Energy	0.125247
C	5.704127	-2.430976	-0.133809		
C	6.540668	-1.295201	-0.224558		
C	5.725812	-0.188542	-0.096113		
C	3.204469	0.012583	0.214606		
C	4.397733	-0.663559	0.064529		
N	4.437682	-2.056932	0.030042		
C	1.97572	-0.676487	0.310428		
N	1.968129	-2.058426	0.057585		
F	3.189545	-4.070215	-0.503966		
F	3.218734	-3.333559	1.668864		
H	0.370652	0.849569	0.040032		
H	-1.12466	-1.273446	-0.713022		
H	0.516117	-3.437118	-0.558224		
H	5.971498	-3.4777	-0.179515		
H	7.608979	-1.315704	-0.371724		
H	6.010058	0.853188	-0.118355		
H	3.200877	1.095353	0.256593		
O	1.805592	-0.602535	2.303692		
H	2.282662	-1.428825	2.479746		

BOD-C1-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.063
C	0.56907	-0.263944	-0.09421	Zero-point Energy Correction	0.162907

C	-0.229015	-1.414241	-0.230494	Thermal Correction to Energy	0.175579
C	0.627855	-2.502493	-0.193242	Thermal Correction to Enthalpy	0.176523
B	3.166726	-2.992232	0.019688	Thermal Correction to Free Energy	0.122224
C	5.676288	-2.385962	0.078787		
C	6.500773	-1.233441	0.117138		
C	5.660751	-0.143671	0.105936		
C	3.116963	0.009144	0.026306		
C	4.32799	-0.642574	0.059914		
N	4.393852	-2.036815	0.043597		
C	1.919554	-0.716487	-0.037138		
N	1.915322	-2.087665	-0.075517		
F	3.23884	-3.845137	-1.084186		
F	3.133808	-3.757981	1.189382		
H	0.27144	0.766878	-0.209239		
H	-1.302435	-1.454797	-0.323597		
H	0.396024	-3.557014	-0.245779		
H	5.971305	-3.426602	0.076416		
H	7.57882	-1.240476	0.147868		
H	5.922635	0.903842	0.125634		
H	3.084303	1.092375	0.047105		
O	0.581471	-0.008789	2.12181		
H	1.351111	0.5818	2.166281		

BOD-C1-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	
C	0.569879	-0.26032	-0.097003	Zero-point Energy Correction	0.163002
C	-0.228358	-1.41007	-0.232478	Thermal Correction to Energy	0.175599
C	0.628254	-2.498905	-0.192046	Thermal Correction to Enthalpy	0.176544
B	3.166375	-2.989487	0.022127	Thermal Correction to Free Energy	0.122715
C	5.676639	-2.386076	0.083223		
C	6.502236	-1.234201	0.116491		
C	5.663102	-0.143587	0.099273		
C	3.1186	0.010872	0.019157		
C	4.329991	-0.641723	0.055117		
N	4.394704	-2.035454	0.045761		
C	1.920791	-0.713504	-0.039936		
N	1.915251	-2.084782	-0.074314		
F	3.238756	-3.842053	-1.082184		
F	3.132533	-3.753411	1.192782		
H	0.271309	0.770671	-0.211846		
H	-1.302279	-1.450171	-0.324246		
H	0.395533	-3.55372	-0.241566		
H	5.970423	-3.427403	0.086006		
H	7.580658	-1.241746	0.148177		
H	5.926864	0.903936	0.114192		

H	3.087642	1.09458	0.033768
O	0.571232	-0.026944	2.115574
H	1.343317	0.557216	2.196429

BOD-C1-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-757.064
C	0.616895	-0.198733	-0.09974	Zero-point Energy Correction	0.163362
C	-0.196983	-1.348372	-0.159713	Thermal Correction to Energy	0.176016
C	0.650256	-2.445279	-0.106943	Thermal Correction to Enthalpy	0.17696
B	3.187934	-2.959037	0.058113	Thermal Correction to Free Energy	0.122712
C	5.704513	-2.378447	0.071793		
C	6.54164	-1.236371	0.069743		
C	5.712274	-0.136774	0.034492		
C	3.166644	0.041125	-0.031947		
C	4.37571	-0.621983	0.01309		
N	4.425916	-2.013709	0.037122		
C	1.964829	-0.669105	-0.071303		
N	1.943443	-2.040835	-0.050635		
F	3.237904	-3.840456	-1.019727		
F	3.158431	-3.678509	1.252946		
H	0.325939	0.820449	-0.29734		
H	-1.273322	-1.378727	-0.217561		
H	0.408227	-3.498701	-0.106026		
H	5.98268	-3.423225	0.098649		
H	7.619901	-1.252332	0.092128		
H	5.989068	0.907081	0.022545		
H	3.144385	1.124512	-0.03505		
O	0.616268	0.388258	1.96458		
H	0.5709	-0.517113	2.313244		

BOD-C2-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.063
C	0.704982	-0.097015	-0.094321	Zero-point Energy Correction	0.163627
C	-0.165803	-1.206463	-0.030963	Thermal Correction to Energy	0.176055
C	0.678787	-2.364556	-0.055444	Thermal Correction to Enthalpy	0.176999
B	3.176212	-2.951949	0.055541	Thermal Correction to Free Energy	0.123686
C	5.701876	-2.440942	0.062403		
C	6.568934	-1.322951	0.04694		
C	5.770119	-0.200451	0.010627		
C	3.240117	0.060527	-0.037344		
C	4.421207	-0.646156	0.002807		
N	4.432491	-2.042426	0.036704		
C	2.00258	-0.593609	-0.05124		
N	1.947406	-2.00049	-0.03298		

F	3.187613	-3.82471	-1.032501
F	3.125212	-3.687922	1.240643
H	0.434584	0.946988	-0.134455
H	-1.218026	-1.212141	-0.265355
H	0.384623	-3.405298	-0.050739
H	5.95539	-3.492036	0.091839
H	7.646315	-1.369976	0.061613
H	6.073092	0.835905	-0.010775
H	3.265021	1.143857	-0.061271
O	-0.502633	-1.442477	1.975954
H	-1.061188	-2.231183	1.907909

BOD-C2-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-757.07
C	0.621297	-0.198361	-0.138518	Zero-point Energy Correction	0.163594
C	-0.170516	-1.32606	-0.112046	Thermal Correction to Energy	0.176024
C	0.702698	-2.436114	-0.023799	Thermal Correction to Enthalpy	0.176968
B	3.229527	-2.924856	0.111518	Thermal Correction to Free Energy	0.123596
C	5.725871	-2.321397	0.088156		
C	6.560387	-1.15701	0.108728		
C	5.68659	-0.057074	-0.013497		
C	3.149549	0.081693	-0.069288		
C	4.390581	-0.562574	-0.007435		
N	4.454517	-1.966953	0.052938		
C	1.972143	-0.633211	-0.067428		
N	1.968699	-2.027592	0.002762		
F	3.276152	-3.829633	-0.949483		
F	3.226761	-3.623553	1.320031		
H	0.3117	0.834706	-0.202786		
H	-1.247327	-1.381405	-0.149844		
H	0.455504	-3.488506	0.021456		
H	6.026342	-3.359749	0.131924		
H	7.622866	-1.159339	-0.075568		
H	5.95196	0.987782	-0.071711		
H	3.118479	1.164039	-0.124517		
O	6.80772	-1.356367	2.147309		
H	7.399141	-2.124321	2.128154		

BOD-C2-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-757.061
C	0.69388	-0.107059	-0.102771	Zero-point Energy Correction	0.163523
C	-0.170164	-1.214665	-0.019364	Thermal Correction to Energy	0.176164
C	0.681441	-2.369568	-0.039205	Thermal Correction to Enthalpy	0.177109
B	3.180822	-2.95732	0.027479	Thermal Correction to Free Energy	0.122739

C	5.705519	-2.441885	0.079452
C	6.568975	-1.325142	0.067833
C	5.765916	-0.202056	0.017145
C	3.231402	0.053053	-0.049077
C	4.421673	-0.650983	-0.001579
N	4.434843	-2.042455	0.038705
C	1.999957	-0.598767	-0.059108
N	1.946934	-2.003429	-0.026279
F	3.189875	-3.778255	-1.098757
F	3.133999	-3.734918	1.179823
H	0.416473	0.934941	-0.146382
H	-1.221513	-1.223695	-0.25809
H	0.396537	-3.413074	-0.024841
H	5.954479	-3.49359	0.115652
H	7.646401	-1.366814	0.095429
H	6.071033	0.833757	-0.004011
H	3.2547	1.136486	-0.077839
O	-0.505759	-1.381625	1.963441
H	-1.028511	-2.198412	1.957936

#### BOD-C3-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.067
C	0.649486	-0.146304	-0.117597	Zero-point Energy Correction	0.16317
C	-0.188752	-1.244077	-0.157211	Thermal Correction to Energy	0.175552
C	0.636457	-2.395481	-0.138981	Thermal Correction to Enthalpy	0.176497
B	3.14862	-2.956827	0.034379	Thermal Correction to Free Energy	0.123473
C	5.678461	-2.444339	0.060725		
C	6.53834	-1.320921	0.084402		
C	5.732914	-0.202623	0.069633		
C	3.19701	0.038225	-0.013684		
C	4.386557	-0.656439	0.033357		
N	4.406145	-2.051781	0.030024		
C	1.974415	-0.639501	-0.084713		
N	1.931711	-2.018205	-0.124757		
F	3.208398	-3.890961	-0.996887		
F	3.045231	-3.639956	1.263418		
H	0.379957	0.899094	-0.105467		
H	-1.267162	-1.25519	-0.184842		
H	0.359954	-3.431425	-0.270964		
H	5.937803	-3.494319	0.06688		
H	7.615796	-1.361745	0.108608		
H	6.029833	0.835662	0.077028		
H	3.205856	1.121814	-0.002727		
O	0.338463	-2.772519	2.123965		
H	1.226679	-3.170799	2.087029		

## BOD-C3-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-757.073
C	0.646557	-0.201759	-0.065677	Zero-point Energy Correction	0.163118
C	-0.151781	-1.325445	-0.053679	Thermal Correction to Energy	0.175557
C	0.715735	-2.442679	-0.022366	Thermal Correction to Enthalpy	0.176501
B	3.248279	-2.938506	0.03635	Thermal Correction to Free Energy	0.123215
C	5.761864	-2.359266	-0.00178		
C	6.580239	-1.202092	-0.012748		
C	5.734533	-0.110694	-0.043268		
C	3.182889	0.055867	-0.059304		
C	4.411719	-0.613188	-0.059619		
N	4.465742	-1.99161	-0.057422		
C	1.99612	-0.646645	-0.043682		
N	1.985647	-2.041197	-0.015961		
F	3.241074	-3.857775	-1.011282		
F	3.299179	-3.636789	1.258024		
H	0.341938	0.834416	-0.091208		
H	-1.229559	-1.37322	-0.065713		
H	0.463398	-3.494558	-0.002923		
H	6.051373	-3.396703	-0.090374		
H	7.659087	-1.205842	0.014124		
H	5.997184	0.93693	-0.045358		
H	3.166119	1.139657	-0.075752		
O	5.951012	-2.655173	2.279407		
H	5.089292	-3.107137	2.231219		

## BOD-C3-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-757.068
C	0.643272	-0.145313	-0.122566	Zero-point Energy Correction	0.164062
C	-0.190552	-1.237317	-0.137846	Thermal Correction to Energy	0.176252
C	0.636823	-2.395314	-0.090882	Thermal Correction to Enthalpy	0.177197
B	3.152894	-2.958058	0.031696	Thermal Correction to Free Energy	0.12464
C	5.682012	-2.444475	0.074901		
C	6.541299	-1.323269	0.09159		
C	5.734758	-0.20327	0.063466		
C	3.194451	0.037448	-0.025482		
C	4.390414	-0.657371	0.028255		
N	4.409256	-2.048619	0.037782		
C	1.976273	-0.638506	-0.082265		
N	1.931631	-2.015197	-0.094152		
F	3.203622	-3.859116	-1.025575		
F	3.061854	-3.665604	1.243233		
H	0.371814	0.899784	-0.125763		

H	-1.269053	-1.250519	-0.150723
H	0.363061	-3.427649	-0.249533
H	5.935229	-3.495652	0.089274
H	7.618806	-1.361728	0.120684
H	6.035736	0.83392	0.063658
H	3.203345	1.121139	-0.030686
O	0.326166	-2.79002	2.042553
H	1.219063	-3.173911	2.089998

BOD-C5-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.067
C	0.646693	-0.201915	-0.067054	Zero-point Energy Correction	0.163059
C	-0.150773	-1.325923	-0.06124	Thermal Correction to Energy	0.175506
C	0.717265	-2.442869	-0.028442	Thermal Correction to Enthalpy	0.176451
B	3.249603	-2.936846	0.050396	Thermal Correction to Free Energy	0.123208
C	5.763018	-2.358	-0.009807		
C	6.580026	-1.200536	-0.014817		
C	5.73309	-0.109085	-0.039095		
C	3.182216	0.057111	-0.053371		
C	4.411536	-0.612262	-0.057669		
N	4.465913	-1.991022	-0.065718		
C	1.996636	-0.645779	-0.040671		
N	1.98697	-2.04106	-0.016179		
F	3.239339	-3.879797	-0.974827		
F	3.30524	-3.609038	1.288013		
H	0.342429	0.83396	-0.092366		
H	-1.228024	-1.374735	-0.078628		
H	0.465223	-3.494524	-0.011705		
H	6.052924	-3.394194	-0.106714		
H	7.65857	-1.20347	0.009598		
H	5.994247	0.938505	-0.03654		
H	3.165364	1.140581	-0.0655		
O	5.953354	-2.68202	2.272967		
H	5.076782	-3.100491	2.200376		

BOD-C6-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.063
C	0.621147	-0.198472	-0.140903	Zero-point Energy Correction	0.163656
C	-0.1705	-1.326281	-0.115094	Thermal Correction to Energy	0.176081
C	0.702591	-2.436113	-0.025484	Thermal Correction to Enthalpy	0.177025
B	3.229057	-2.925146	0.114259	Thermal Correction to Free Energy	0.12371
C	5.72496	-2.320535	0.092117		
C	6.559668	-1.155735	0.116402		
C	5.684725	-0.055535	-0.008794		

C	3.148306	0.082725	-0.068716
C	4.389671	-0.56113	-0.005076
N	4.453736	-1.96634	0.054701
C	1.971895	-0.63281	-0.068071
N	1.968807	-2.027705	0.002563
F	3.276904	-3.833325	-0.94332
F	3.226429	-3.621539	1.324279
H	0.312365	0.834386	-0.205907
H	-1.246837	-1.382058	-0.154284
H	0.455348	-3.48816	0.019608
H	6.026055	-3.358399	0.136178
H	7.62043	-1.159058	-0.075557
H	5.949207	0.989102	-0.067871
H	3.116679	1.164677	-0.124253
O	6.825478	-1.352542	2.144034
H	7.394523	-2.135861	2.106246

#### BOD-C7-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
C	0.73891	-0.13113	-0.014158	Zero-point Energy Correction	-757.063
C	-0.103315	-1.219114	-0.025831	Thermal Correction to Energy	0.163023
C	0.719409	-2.373569	-0.018206	Thermal Correction to Enthalpy	0.176612
B	3.227643	-2.985248	0.03645	Thermal Correction to Free Energy	0.12243
C	5.773991	-2.503099	-0.091749		
C	6.634139	-1.417215	-0.107049		
C	5.834451	-0.263946	-0.007239		
C	3.284419	0.015843	0.010415		
C	4.481497	-0.713212	0.003384		
N	4.483936	-2.084595	-0.02343		
C	2.071372	-0.632976	0.000025		
N	2.00296	-2.027253	-0.004704		
F	3.197996	-3.856918	-1.05445		
F	3.210925	-3.73078	1.219649		
H	0.478833	0.917006	-0.016478		
H	-1.181741	-1.223855	-0.039341		
H	0.42238	-3.413631	-0.021133		
H	6.004969	-3.5585	-0.127241		
H	7.710133	-1.460793	-0.160764		
H	6.138279	0.765196	-0.120853		
H	3.319082	1.099127	0.021486		
O	5.748039	0.002529	2.202697		
H	4.961913	0.572041	2.228922		

#### BOD-C8-OH-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-757.062
C	0.619527	-0.199821	-0.20261	Zero-point Energy Correction	0.16459
C	-0.186079	-1.324599	-0.318435	Thermal Correction to Energy	0.176563
C	0.658141	-2.442319	-0.209125	Thermal Correction to Enthalpy	0.177507
B	3.154146	-2.948342	0.219736	Thermal Correction to Free Energy	0.126021
C	5.678217	-2.403115	-0.050257		
C	6.521457	-1.262945	-0.103811		
C	5.709444	-0.161462	0.004911		
C	3.132465	0.045459	0.119011		
C	4.369823	-0.643793	0.129782		
N	4.401977	-2.027313	0.078627		
C	1.941444	-0.655909	-0.034278		
N	1.925956	-2.046912	-0.043436		
F	3.220177	-3.989455	-0.702271		
F	3.102425	-3.473249	1.517315		
H	0.324286	0.83829	-0.241992		
H	-1.253485	-1.358116	-0.469841		
H	0.404784	-3.492706	-0.245469		
H	5.948735	-3.448413	-0.106539		
H	7.594063	-1.288631	-0.212571		
H	5.984018	0.882613	0.007702		
H	3.13423	1.125575	0.05815		
O	3.805972	0.061947	2.172321		
H	3.484938	-0.819064	2.424778		

BOD-C8-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-757.069
C	0.616627	-0.20028	-0.203931	Zero-point Energy Correction	0.164391
C	-0.189254	-1.325169	-0.311969	Thermal Correction to Energy	0.176423
C	0.655722	-2.442723	-0.201216	Thermal Correction to Enthalpy	0.177367
B	3.153705	-2.949649	0.208044	Thermal Correction to Free Energy	0.125623
C	5.678055	-2.403235	-0.03968		
C	6.521582	-1.26366	-0.093517		
C	5.708819	-0.161462	0.005492		
C	3.130921	0.045377	0.110042		
C	4.368551	-0.643233	0.124618		
N	4.40126	-2.02673	0.08079		
C	1.939635	-0.656003	-0.038846		
N	1.923632	-2.046737	-0.041149		
F	3.220107	-3.975674	-0.731493		
F	3.102409	-3.49554	1.496786		
H	0.320553	0.837913	-0.24553		
H	-1.257701	-1.35918	-0.45864		
H	0.402107	-3.493569	-0.232426		
H	5.94858	-3.449206	-0.08942		

H	7.595355	-1.289464	-0.194389
H	5.984226	0.882778	0.00762
H	3.132451	1.125843	0.048602
O	3.815039	0.068946	2.161848
H	3.504281	-0.811624	2.430063

BOD-C8-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-757.063
C	0.622231	-0.19893	-0.209331	Zero-point Energy Correction	0.164482
C	-0.17343	-1.325458	-0.393064	Thermal Correction to Energy	0.17657
C	0.669626	-2.441173	-0.283744	Thermal Correction to Enthalpy	0.177515
B	3.151065	-2.906392	0.31506	Thermal Correction to Free Energy	0.12551
C	5.669195	-2.396608	-0.130917		
C	6.513506	-1.257724	-0.17566		
C	5.707363	-0.155827	-0.010251		
C	3.134124	0.040428	0.185215		
C	4.372051	-0.63667	0.121021		
N	4.40114	-2.019495	0.034294		
C	1.936634	-0.654921	-0.009123		
N	1.929046	-2.041281	-0.062575		
F	3.201281	-4.080114	-0.414045		
F	3.117847	-3.17402	1.695041		
H	0.319336	0.837523	-0.230609		
H	-1.234034	-1.355846	-0.587359		
H	0.427557	-3.492182	-0.352081		
H	5.931472	-3.442429	-0.209624		
H	7.583081	-1.280076	-0.312606		
H	5.991554	0.885273	0.017871		
H	3.128879	1.122451	0.179933		
O	3.754731	-0.065454	2.220865		
H	3.522406	-0.993356	2.403386		

NPA-ANION-C10-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-741.949
O	2.415756	2.263422	0.069141	Zero-point Energy Correction	0.1616
O	2.408447	-2.247215	-0.103193	Thermal Correction to Energy	0.173834
N	2.455498	0.010361	-0.038308	Thermal Correction to Enthalpy	0.174778
C	-0.415586	0.021683	0.043197	Thermal Correction to Free Energy	0.122217
C	0.296859	1.23192	0.025367		
C	0.303384	-1.209984	0.130328		
C	-1.827117	0.017146	0.011403		
C	1.794258	1.187181	0.026261		
C	1.800809	-1.16704	-0.018611		
C	-0.394558	2.427318	-0.020455		

C	-0.402767	-2.414416	0.023682
C	-2.509212	1.255389	-0.031421
C	-2.505912	-1.233235	-0.008433
C	-1.801713	2.436781	-0.043275
C	-1.803819	-2.418923	-0.01573
H	0.153205	3.361568	-0.04294
H	0.149223	-3.346474	0.005588
H	-3.593484	1.257855	-0.058389
H	-3.590347	-1.235885	-0.035536
H	-2.327471	3.383158	-0.07814
H	-2.333112	-3.362528	-0.059139
O	0.463593	-1.295317	2.238736
H	0.835061	-2.190893	2.288514

#### NPA-ANION-C4-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-741.948
O	2.410078	2.200256	0.144402	Zero-point Energy Correction	0.161856
O	2.388486	-2.308598	-0.086131	Thermal Correction to Energy	0.173997
N	2.442527	-0.052835	0.026369	Thermal Correction to Enthalpy	0.174941
C	-0.427579	-0.041145	0.005692	Thermal Correction to Free Energy	0.122482
C	0.28905	1.176607	0.045216		
C	0.283009	-1.259411	-0.022701		
C	-1.844778	-0.041325	-0.020351		
C	1.784921	1.127052	0.076		
C	1.778578	-1.22602	-0.028785		
C	-0.399036	2.369666	0.059669		
C	-0.413279	-2.470486	0.00219		
C	-2.519475	1.198162	-0.005218		
C	-2.532375	-1.293437	-0.066562		
C	-1.808299	2.37783	0.032509		
C	-1.840844	-2.467921	-0.068451		
H	0.146956	3.30454	0.091385		
H	0.128175	-3.395211	-0.141937		
H	-3.603825	1.207401	-0.025283		
H	-3.616264	-1.287723	-0.106518		
H	-2.333956	3.325024	0.0426		
H	-2.363348	-3.415894	-0.101115		
O	-0.063076	-2.673393	2.08545		
H	-0.650339	-1.946947	2.352043		

#### NPA-ANION-C5-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-741.945
O	2.426987	2.288799	0.022448	Zero-point Energy Correction	0.161537
O	2.493184	-2.220571	-0.131118	Thermal Correction to Energy	0.173815

N	2.497762	0.034894	-0.055028	Thermal Correction to Enthalpy	0.174759
C	-0.370983	0.002079	0.006876	Thermal Correction to Free Energy	0.12176
C	0.323709	1.225881	0.000383		
C	0.36113	-1.21903	-0.012982		
C	-1.791107	-0.00979	0.019221		
C	1.820338	1.203095	-0.008558		
C	1.856706	-1.152946	-0.071602		
C	-0.381812	2.412695	-0.001396		
C	-0.303685	-2.411252	0.008564		
C	-2.486488	1.227632	0.010177		
C	-2.457091	-1.249944	0.029281		
C	-1.791863	2.412751	0.000907		
C	-1.732029	-2.445425	0.099825		
H	0.157207	3.352351	-0.007058		
H	0.24735	-3.343714	-0.013521		
H	-3.571013	1.217565	0.014227		
H	-3.54111	-1.274253	0.025473		
H	-2.324322	3.355823	-0.003552		
H	-2.244371	-3.384974	-0.058436		
O	-1.930084	-2.686319	2.156077		
H	-1.320423	-3.440866	2.175006		

NPA-ANION-C6-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	
O	2.434606	2.248802	-0.026186	Zero-point Energy Correction	-741.949
O	2.398538	-2.263106	0.04947	Thermal Correction to Energy	0.161232
N	2.455001	-0.006805	0.013137	Thermal Correction to Enthalpy	0.173612
C	-0.41514	0.020514	0.012742	Thermal Correction to Free Energy	0.174556
C	0.307357	1.23274	-0.008535		0.121107
C	0.289106	-1.21224	0.021232		
C	-1.827571	0.034691	0.003256		
C	1.80303	1.177176	-0.007155		
C	1.787344	-1.179147	0.029101		
C	-0.37375	2.431398	-0.030111		
C	-0.403276	-2.403753	0.010172		
C	-2.498693	1.274499	-0.018275		
C	-2.52453	-1.21398	0.047088		
C	-1.781812	2.451114	-0.035531		
C	-1.808276	-2.408286	-0.00026		
H	0.180232	3.362062	-0.044982		
H	0.139904	-3.340335	-0.000422		
H	-3.583349	1.286546	-0.020451		
H	-3.600524	-1.215804	-0.074845		
H	-2.301052	3.40165	-0.053108		
H	-2.34335	-3.350182	-0.022332		

O	-2.787346	-1.340405	2.207896
H	-3.056517	-2.272811	2.249082

NPA-C10-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-742.421
O	2.450308	2.255798	0.02794	Zero-point Energy Correction	0.175157
O	2.449387	-2.250375	-0.105671	Thermal Correction to Energy	0.187479
N	2.389547	0.004485	-0.043293	Thermal Correction to Enthalpy	0.188423
C	-0.396636	0.01524	0.039253	Thermal Correction to Free Energy	0.136117
C	0.29678	1.239092	0.029711		
C	0.306496	-1.23121	0.138321		
C	-1.807881	0.00985	0.008151		
C	1.776171	1.242996	0.014847		
C	1.787291	-1.235758	-0.016591		
C	-0.397182	2.434206	-0.002383		
C	-0.40227	-2.435219	0.015655		
C	-2.495503	1.245634	-0.022616		
C	-2.491486	-1.237398	-0.015587		
C	-1.801187	2.435027	-0.022718		
C	-1.798826	-2.430516	-0.026347		
H	0.151697	3.368599	-0.017107		
H	0.150704	-3.367223	-0.008595		
H	-3.580048	1.239454	-0.047361		
H	-3.576003	-1.233005	-0.043757		
H	3.405554	0.009456	-0.100633		
H	-2.334836	3.377166	-0.045833		
H	-2.3352	-3.36975	-0.077137		
O	0.563854	-1.197465	2.177864		
H	0.663239	-2.148158	2.352126		

NPA-C10-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-742.415
O	2.446415	2.259411	0.045213	Zero-point Energy Correction	0.175695
O	2.443972	-2.254314	-0.122144	Thermal Correction to Energy	0.187942
N	2.392122	0.004509	-0.045476	Thermal Correction to Enthalpy	0.188886
C	-0.398297	0.014948	0.045043	Thermal Correction to Free Energy	0.136779
C	0.295758	1.238168	0.032407		
C	0.307305	-1.230684	0.1492		
C	-1.809753	0.009106	0.011539		
C	1.780942	1.248578	0.023874		
C	1.791918	-1.241075	-0.020428		
C	-0.39654	2.43223	-0.004896		
C	-0.400671	-2.432758	0.020903		
C	-2.495976	1.245479	-0.025142		

C	-2.492944	-1.238915	-0.008778
C	-1.801211	2.433827	-0.028699
C	-1.799328	-2.429592	-0.019325
H	0.158266	3.362877	-0.019833
H	0.157447	-3.361509	-0.011891
H	-3.580493	1.241238	-0.050559
H	-3.577395	-1.236268	-0.036638
H	3.40679	0.009621	-0.095995
H	-2.334672	3.375972	-0.055579
H	-2.334545	-3.369562	-0.07036
O	0.553373	-1.195276	2.16234
H	0.661486	-2.145084	2.333461

#### NPA-C12-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-742.418
O	2.449548	2.256984	0.02453	Zero-point Energy Correction	0.175055
O	2.446964	-2.250882	-0.088688	Thermal Correction to Energy	0.187425
N	2.387447	0.004857	-0.042243	Thermal Correction to Enthalpy	0.188369
C	-0.398112	0.017013	0.043931	Thermal Correction to Free Energy	0.135888
C	0.295566	1.240506	0.031589		
C	0.303813	-1.229762	0.146031		
C	-1.809092	0.012102	0.009884		
C	1.7739	1.243699	0.014403		
C	1.784012	-1.234775	-0.007		
C	-0.398329	2.43575	-0.004383		
C	-0.405573	-2.433513	0.019005		
C	-2.496591	1.247592	-0.024079		
C	-2.493564	-1.23465	-0.016713		
C	-1.802075	2.436963	-0.025594		
C	-1.801675	-2.428236	-0.027564		
H	0.150342	3.369733	-0.02221		
H	0.146804	-3.365466	-0.003056		
H	-3.580702	1.24048	-0.051099		
H	-3.577622	-1.228357	-0.047928		
H	3.402973	0.009055	-0.100409		
H	-2.335179	3.378826	-0.05179		
H	-2.338086	-3.366761	-0.081298		
O	0.544751	-1.217818	2.187889		
H	0.724447	-2.162412	2.32503		

#### NPA-C4-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-742.42
O	2.444499	2.208374	0.093461	Zero-point Energy Correction	0.174769
O	2.421942	-2.300567	-0.016163	Thermal Correction to Energy	0.187257

N	2.37202	-0.044008	0.029225	Thermal Correction to Enthalpy	0.188201
C	-0.41027	-0.035186	0.00669	Thermal Correction to Free Energy	0.135132
C	0.287495	1.198362	0.039803		
C	0.280943	-1.266748	-0.017136		
C	-1.828537	-0.034827	-0.019014		
C	1.765313	1.198506	0.05813		
C	1.757392	-1.281014	-0.003196		
C	-0.403265	2.389607	0.052001		
C	-0.417293	-2.478256	0.006983		
C	-2.508491	1.202759	-0.004132		
C	-2.521853	-1.282912	-0.062903		
C	-1.810533	2.389543	0.030388		
C	-1.842876	-2.465042	-0.065257		
H	0.143633	3.324845	0.076438		
H	0.122858	-3.401134	-0.157724		
H	-3.593139	1.203012	-0.022176		
H	-3.605845	-1.268452	-0.102453		
H	3.389688	-0.047918	0.042992		
H	-2.343204	3.332628	0.040036		
H	-2.372915	-3.408738	-0.098531		
O	-0.060833	-2.739891	2.042201		
H	-0.640334	-2.03453	2.377667		

NPA-C4-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	
O	2.440926	2.216224	0.128724	Zero-point Energy Correction	-742.414
O	2.426829	-2.296492	-0.113401	Thermal Correction to Energy	0.175437
N	2.378579	-0.039877	0.029942	Thermal Correction to Enthalpy	0.188758
C	-0.407207	-0.034758	0.009383	Thermal Correction to Free Energy	0.135989
C	0.289352	1.198969	0.045601		
C	0.286529	-1.266678	-0.013504		
C	-1.825945	-0.034888	-0.018679		
C	1.773228	1.207177	0.075438		
C	1.767599	-1.284907	-0.036486		
C	-0.401597	2.389354	0.052931		
C	-0.408098	-2.477921	0.035362		
C	-2.505759	1.202194	-0.0112		
C	-2.517069	-1.285662	-0.056539		
C	-1.808503	2.389482	0.022476		
C	-1.836412	-2.465592	-0.044592		
H	0.151035	3.320917	0.080973		
H	0.138457	-3.397114	-0.124397		
H	-3.59034	1.202925	-0.03379		
H	-3.600893	-1.274798	-0.100254		
H	3.394819	-0.042181	0.029301		

H	-2.342115	3.332026	0.026267
H	-2.365395	-3.410153	-0.065065
O	-0.084849	-2.722126	2.043272
H	-0.726775	-2.06771	2.365567

NPA-C4-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-742.417
O	2.445623	2.208617	0.092016	Zero-point Energy Correction	0.174911
O	2.425003	-2.30138	-0.020409	Thermal Correction to Energy	0.187316
N	2.373859	-0.044367	0.025337	Thermal Correction to Enthalpy	0.18826
C	-0.408084	-0.036906	0.007642	Thermal Correction to Free Energy	0.135446
C	0.288921	1.19698	0.041083		
C	0.283396	-1.267832	-0.017486		
C	-1.826211	-0.037319	-0.016947		
C	1.765676	1.19775	0.056857		
C	1.758897	-1.281154	-0.005897		
C	-0.402835	2.38762	0.055353		
C	-0.414884	-2.479643	0.00899		
C	-2.507177	1.1995	-0.000238		
C	-2.519456	-1.285169	-0.062942		
C	-1.810059	2.386697	0.03517		
C	-1.840273	-2.467065	-0.06584		
H	0.142853	3.323076	0.080106		
H	0.125503	-3.402404	-0.153218		
H	-3.591458	1.197976	-0.01766		
H	-3.603032	-1.269729	-0.103191		
H	3.391088	-0.047782	0.036858		
H	-2.342991	3.329116	0.046297		
H	-2.369699	-3.410587	-0.099786		
O	-0.077286	-2.726716	2.050859		
H	-0.660977	-2.010867	2.354376		

NPA-C5-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-742.418
O	2.462114	2.291091	-0.025387	Zero-point Energy Correction	0.174669
O	2.529158	-2.214397	-0.089529	Thermal Correction to Energy	0.187275
N	2.427936	0.037677	-0.063226	Thermal Correction to Enthalpy	0.18822
C	-0.352799	0.005461	0.009484	Thermal Correction to Free Energy	0.134542
C	0.32266	1.244018	-0.000365		
C	0.360979	-1.229017	-0.007417		
C	-1.773315	-0.007795	0.021268		
C	1.800196	1.269486	-0.027072		
C	1.838871	-1.212207	-0.057137		
C	-0.385801	2.429551	0.000967		

C	-0.30612	-2.4211	0.013411
C	-2.473833	1.226742	0.014242
C	-2.444805	-1.245491	0.028252
C	-1.792536	2.419909	0.007802
C	-1.732288	-2.448097	0.105038
H	0.153472	3.369717	-0.007258
H	0.247096	-3.352962	-0.008989
H	-3.558486	1.207955	0.01846
H	-3.529113	-1.261419	0.019709
H	3.445201	0.054419	-0.090451
H	-2.3332	3.35817	0.006707
H	-2.251007	-3.383507	-0.058656
O	-1.887639	-2.679524	2.138675
H	-1.384108	-3.509657	2.165651

NPA-C5-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-742.414
O	2.45682	2.258259	0.009941	Zero-point Energy Correction	0.175541
O	2.545616	-2.252499	-0.176959	Thermal Correction to Energy	0.187912
N	2.439268	0.001701	-0.07804	Thermal Correction to Enthalpy	0.188856
C	-0.34467	-0.045062	0.006076	Thermal Correction to Free Energy	0.135981
C	0.325402	1.196175	0.028552		
C	0.3748	-1.27779	-0.04968		
C	-1.763725	-0.067463	0.032891		
C	1.808413	1.236039	-0.010063		
C	1.858678	-1.25829	-0.108644		
C	-0.387395	2.377065	0.072162		
C	-0.285601	-2.472196	-0.060577		
C	-2.46895	1.161498	0.072806		
C	-2.429471	-1.314675	0.000533		
C	-1.793499	2.358683	0.093894		
C	-1.713543	-2.513331	0.027086		
H	0.152763	3.316341	0.086695		
H	0.277956	-3.396316	-0.104931		
H	-3.553418	1.138903	0.088721		
H	-3.513356	-1.33562	-0.005409		
H	3.454638	0.024808	-0.115818		
H	-2.340424	3.292798	0.126108		
H	-2.222958	-3.444986	-0.174869		
O	-1.969811	-2.907817	1.993032		
H	-1.524903	-2.1272	2.360671		

NPA-C5-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-742.415
------	---	---	---	------------------------	----------

O	2.462572	2.292105	-0.028029	Zero-point Energy Correction	0.174606
O	2.528798	-2.214847	-0.08488	Thermal Correction to Energy	0.187218
N	2.42784	0.037988	-0.063665	Thermal Correction to Enthalpy	0.188162
C	-0.352589	0.006659	0.010929	Thermal Correction to Free Energy	0.134484
C	0.322934	1.244846	-0.001099		
C	0.360783	-1.228196	-0.004421		
C	-1.772897	-0.006158	0.023368		
C	1.799481	1.269752	-0.028492		
C	1.837785	-1.2116	-0.05454		
C	-0.385674	2.4305	-0.001426		
C	-0.306882	-2.419774	0.017627		
C	-2.473527	1.228069	0.014434		
C	-2.445209	-1.243309	0.031665		
C	-1.79219	2.421236	0.005863		
C	-1.733325	-2.446372	0.109182		
H	0.153235	3.370378	-0.011504		
H	0.244884	-3.352075	-0.002915		
H	-3.557799	1.208213	0.018623		
H	-3.529181	-1.257582	0.02158		
H	3.444637	0.054543	-0.091032		
H	-2.332418	3.359238	0.003143		
H	-2.251364	-3.38113	-0.057614		
O	-1.887608	-2.693032	2.140892		
H	-1.379657	-3.520429	2.14649		

NPA-C6-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-742.421
O	2.465733	2.245448	-0.017005	Zero-point Energy Correction	0.174649
O	2.43324	-2.260948	0.042679	Thermal Correction to Energy	0.187141
N	2.382782	-0.006667	0.01768	Thermal Correction to Enthalpy	0.188086
C	-0.399603	0.018249	0.014589	Thermal Correction to Free Energy	0.134863
C	0.303589	1.245065	-0.008002		
C	0.286861	-1.228843	0.022912		
C	-1.811739	0.032179	0.00631		
C	1.781078	1.23883	-0.003349		
C	1.765953	-1.242599	0.029244		
C	-0.380612	2.442831	-0.031049		
C	-0.407129	-2.418933	0.008677		
C	-2.488556	1.268091	-0.015454		
C	-2.515336	-1.214827	0.057109		
C	-1.78526	2.453371	-0.035692		
C	-1.810146	-2.416721	-0.000765		
H	0.174363	3.373572	-0.046423		
H	0.137416	-3.355449	-0.006633		
H	-3.573498	1.270853	-0.014886		

H	-3.590768	-1.207469	-0.071518
H	3.400499	-0.013122	0.021884
H	-2.312762	3.399152	-0.053492
H	-2.351172	-3.354878	-0.027478
O	-2.743459	-1.326607	2.173221
H	-3.070312	-2.238749	2.254693

NPA-C6-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-742.416
O	2.441228	2.215956	0.068756	Zero-point Energy Correction	0.175331
O	2.389459	-2.299942	0.051248	Thermal Correction to Energy	0.187764
N	2.354402	-0.040964	0.066221	Thermal Correction to Enthalpy	0.188708
C	-0.430756	-0.004704	0.016478	Thermal Correction to Free Energy	0.13573
C	0.278053	1.220022	0.023081		
C	0.251333	-1.253822	0.013148		
C	-1.844032	0.014582	-0.011119		
C	1.760992	1.214449	0.053845		
C	1.734399	-1.281042	0.043802		
C	-0.400354	2.419164	0.002247		
C	-0.449476	-2.440385	-0.028624		
C	-2.514019	1.254909	-0.029875		
C	-2.555775	-1.229748	0.013444		
C	-1.805744	2.436058	-0.027459		
C	-1.851823	-2.433487	-0.057898		
H	0.163972	3.344184	0.007385		
H	0.097348	-3.375386	-0.050407		
H	-3.598648	1.262933	-0.042528		
H	-3.624581	-1.216247	-0.156238		
H	3.370292	-0.052957	0.088959		
H	-2.32908	3.384107	-0.043661		
H	-2.39714	-3.367657	-0.10077		
O	-3.022048	-1.457264	2.036337		
H	-2.126839	-1.61093	2.380882		

NPA-C6-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-742.418
O	2.467439	2.24698	-0.02194	Zero-point Energy Correction	0.174547
O	2.433934	-2.260747	0.042779	Thermal Correction to Energy	0.187076
N	2.383975	-0.00579	0.014536	Thermal Correction to Enthalpy	0.188021
C	-0.398156	0.019826	0.017461	Thermal Correction to Free Energy	0.134695
C	0.305127	1.246367	-0.008208		
C	0.287828	-1.227399	0.025678		
C	-1.810216	0.034115	0.010908		
C	1.781658	1.239613	-0.006257		

C	1.766004	-1.241334	0.029111
C	-0.379154	2.444143	-0.03276
C	-0.406822	-2.417281	0.013371
C	-2.487032	1.269902	-0.013564
C	-2.514507	-1.212242	0.062687
C	-1.783681	2.455053	-0.036511
C	-1.809632	-2.414639	0.005727
H	0.17542	3.374597	-0.050674
H	0.136764	-3.353861	-0.002146
H	-3.571624	1.271839	-0.01338
H	-3.589343	-1.203792	-0.067766
H	3.401231	-0.012512	0.016267
H	-2.310727	3.400546	-0.056349
H	-2.351202	-3.352097	-0.018261
O	-2.754833	-1.342684	2.178237
H	-3.081288	-2.256776	2.228307

NPA-N2-OH-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-742.395
O	2.234524	2.412098	0.258712	Zero-point Energy Correction	0.170465
O	2.398797	-2.095882	0.031735	Thermal Correction to Energy	0.183522
N	2.315465	0.159111	0.126166	Thermal Correction to Enthalpy	0.184466
C	-0.500288	0.061554	0.021718	Thermal Correction to Free Energy	0.127088
C	0.151525	1.301663	0.12321		
C	0.241607	-1.129995	-0.025734		
C	-1.917554	0.012751	-0.035082		
C	1.64607	1.350354	0.176832		
C	1.734919	-1.076046	0.046498		
C	-0.590967	2.491372	0.172841		
C	-0.410214	-2.36833	-0.130352		
C	-2.642233	1.216627	0.015968		
C	-2.550151	-1.238518	-0.139299		
C	-1.972956	2.447453	0.120504		
C	-1.791598	-2.41997	-0.186927		
H	-0.067478	3.436506	0.250391		
H	0.182234	-3.274494	-0.164657		
H	-3.725641	1.186203	-0.026859		
H	-3.632876	-1.284344	-0.183383		
H	3.41306	0.183157	0.169692		
H	-2.546963	3.364554	0.158636		
H	-2.296608	-3.374147	-0.267801		
O	4.943125	0.144152	0.139045		
H	5.240825	-0.769495	0.097076		

## NPA-N2-OH-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-742.359
O	2.234524	2.412098	0.258712	Zero-point Energy Correction	0.171326
O	2.398797	-2.095882	0.031735	Thermal Correction to Energy	0.184013
N	2.315465	0.159111	0.126166	Thermal Correction to Enthalpy	0.184957
C	-0.500288	0.061554	0.021718	Thermal Correction to Free Energy	0.131428
C	0.151525	1.301663	0.12321		
C	0.241607	-1.129995	-0.025734		
C	-1.917554	0.012751	-0.035082		
C	1.64607	1.350354	0.176832		
C	1.734919	-1.076046	0.046498		
C	-0.590967	2.491372	0.172841		
C	-0.410214	-2.36833	-0.130352		
C	-2.642233	1.216627	0.015968		
C	-2.550151	-1.238518	-0.139299		
C	-1.972956	2.447453	0.120504		
C	-1.791598	-2.41997	-0.186927		
H	-0.067478	3.436506	0.250391		
H	0.182234	-3.274494	-0.164657		
H	-3.725641	1.186203	-0.026859		
H	-3.632876	-1.284344	-0.183383		
H	3.41306	0.183157	0.169692		
H	-2.546963	3.364554	0.158636		
H	-2.296608	-3.374147	-0.267801		
O	4.943125	0.144152	0.139045		
H	5.240825	-0.769495	0.097076		

## NPA-N2-OH-TS

Atom	X	Y	Z	Electronic Energy (EE)	-742.384
O	2.443916	2.230046	-0.036142	Zero-point Energy Correction	0.170685
O	2.413633	-2.281181	-0.066971	Thermal Correction to Energy	0.183839
N	2.381441	-0.025277	-0.066749	Thermal Correction to Enthalpy	0.184783
C	-0.407542	-0.006562	-0.025251	Thermal Correction to Free Energy	0.129363
C	0.29367	1.217634	-0.029407		
C	0.276938	-1.240078	-0.040493		
C	-1.825257	0.00291	0.001162		
C	1.777878	1.211631	-0.046226		
C	1.761255	-1.254102	-0.059167		
C	-0.394824	2.426267	-0.010843		
C	-0.428275	-2.439269	-0.033431		
C	-2.49968	1.242253	0.021082		
C	-2.517102	-1.22718	0.009618		
C	-1.788581	2.437294	0.014808		
C	-1.822089	-2.43165	-0.007267		
H	0.163623	3.354288	-0.015042		

H	0.117378	-3.374819	-0.04561
H	-3.583894	1.249245	0.042535
H	-3.601345	-1.219025	0.03107
H	3.444038	-0.039031	-0.002045
H	-2.319258	3.380471	0.029904
H	-2.365339	-3.367736	0.000554
O	4.691945	-0.297275	0.900836
H	5.011059	-1.175557	1.149493

RDA-C'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.796
O	-0.09375	1.857266	0.059123	Zero-point Energy Correction	0.294949
N	4.616787	2.121147	-0.498093	Thermal Correction to Energy	0.314118
N	-4.796302	1.784372	0.109625	Thermal Correction to Enthalpy	0.315062
C	0.055048	-0.919547	0.454656	Thermal Correction to Free Energy	0.246874
C	1.23584	-0.145057	0.38883		
C	-1.186574	-0.283048	0.326284		
C	1.132721	1.251863	0.050263		
C	-1.23223	1.131618	0.16125		
C	3.537641	1.453134	-0.234337		
C	-3.629936	1.133342	0.170131		
C	0.130937	-2.380106	0.702076		
C	2.204867	2.022776	-0.237873		
C	-2.410273	1.83233	0.093404		
C	2.564985	-0.712793	0.385681		
C	-2.441009	-0.964337	0.370917		
C	3.647182	0.035046	0.097355		
C	-3.619562	-0.291049	0.298411		
C	0.698821	-3.230978	-0.248961		
C	-0.372553	-2.90828	1.893804		
C	0.755112	-4.600161	-0.011067		
C	-0.298863	-4.276222	2.13378		
C	0.261046	-5.123426	1.181038		
H	2.073161	3.073384	-0.471254		
H	-2.395152	2.908578	-0.02747		
H	2.676118	-1.758836	0.641079		
H	-2.446289	-2.043186	0.461279		
H	4.641407	-0.396088	0.107319		
H	-4.566749	-0.816292	0.331989		
H	-0.811159	-2.243044	2.629848		
H	1.187701	-5.256996	-0.756385		
H	-0.681751	-4.67935	3.06379		
H	0.312146	-6.189781	1.367219		
H	4.375113	3.092709	-0.703499		
H	-4.825271	2.788824	0.008567		

H	-5.669854	1.279652	0.156338
H	1.086158	-2.819307	-1.174572
O	1.045579	0.221067	2.682243
H	1.316539	-0.678744	2.902761

RDA-C1-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.791
O	-0.141417	1.834681	0.020769	Zero-point Energy Correction	0.295328
N	4.599299	2.14421	-0.275655	Thermal Correction to Energy	0.314321
N	-4.871805	1.821118	0.116741	Thermal Correction to Enthalpy	0.315266
C	0.025577	-0.934728	0.446741	Thermal Correction to Free Energy	0.247425
C	1.169938	-0.190735	0.298036		
C	-1.252554	-0.282384	0.358242		
C	1.086081	1.235486	0.065423		
C	-1.290089	1.108467	0.151905		
C	3.504731	1.474411	-0.085103		
C	-3.690104	1.139382	0.15968		
C	0.084475	-2.395911	0.705968		
C	2.167741	2.029723	-0.111372		
C	-2.470122	1.819378	0.057469		
C	2.503166	-0.730473	0.430497		
C	-2.495517	-0.946497	0.438219		
C	3.611537	0.045198	0.181197		
C	-3.683165	-0.263444	0.345847		
C	0.607961	-3.264677	-0.253982		
C	-0.388018	-2.90857	1.917124		
C	0.658067	-4.632633	-0.004178		
C	-0.32412	-4.274838	2.168235		
C	0.195756	-5.13888	1.207384		
H	2.036308	3.092273	-0.280604		
H	-2.440769	2.89067	-0.102824		
H	2.620447	-1.796328	0.570141		
H	-2.511256	-2.021624	0.568684		
H	4.603389	-0.389831	0.211057		
H	-4.628345	-0.790265	0.407795		
H	-0.796394	-2.2337	2.661682		
H	1.059961	-5.301374	-0.756209		
H	-0.682725	-4.664216	3.113763		
H	0.239346	-6.20398	1.402557		
H	4.370486	3.124698	-0.448908		
H	-4.862012	2.759452	-0.257261		
H	-5.712081	1.289672	-0.061662		
H	0.969346	-2.866168	-1.195801		
O	2.946341	-0.257106	2.497049		
H	3.735892	-0.81254	2.589902		

## RDA-C1-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.122837	1.79939	-0.042968	Zero-point Energy Correction	-993.272 0.308033
N	4.560891	2.225656	-0.215057	Thermal Correction to Energy	0.327478
N	-4.833247	1.806658	0.043678	Thermal Correction to Enthalpy	0.328422
C	0.005967	-0.94482	0.422842	Thermal Correction to Free Energy	0.259849
C	1.174722	-0.193555	0.263834		
C	-1.242672	-0.298439	0.331132		
C	1.080095	1.200293	0.03363		
C	-1.275323	1.100497	0.099836		
C	3.463969	1.474838	-0.055233		
C	-3.668847	1.145466	0.126007		
C	0.079444	-2.39976	0.701252		
C	2.179502	2.025585	-0.122153		
C	-2.443724	1.820246	0.001049		
C	2.501563	-0.727323	0.426075		
C	-2.500874	-0.957889	0.430593		
C	3.610827	0.070571	0.185273		
C	-3.670896	-0.268357	0.335307		
C	0.604378	-3.272846	-0.254493		
C	-0.376559	-2.897674	1.924339		
C	0.664132	-4.63674	0.010929		
C	-0.297723	-4.260359	2.190518		
C	0.217696	-5.130927	1.233809		
H	2.034411	3.085406	-0.292618		
H	-2.408097	2.888753	-0.174229		
H	2.631511	-1.798549	0.48966		
H	-2.522085	-2.030784	0.576442		
H	4.60736	-0.354217	0.224813		
H	-4.623311	-0.780596	0.409082		
H	-0.78043	-2.215942	2.665299		
H	1.061624	-5.312392	-0.737679		
H	-0.642854	-4.641358	3.144758		
H	0.271084	-6.193695	1.440929		
H	5.481562	1.813842	-0.160619		
H	4.489228	3.215314	-0.405137		
H	-4.855693	2.802824	-0.119381		
H	-5.71228	1.31674	0.12411		
H	0.953152	-2.883101	-1.205044		
O	2.719248	-0.470233	2.443821		
H	3.619865	-0.806268	2.587721		

## RDA-C1-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.255
O	-0.119691	1.799641	-0.038915	Zero-point Energy Correction	0.308192
N	4.56388	2.22634	-0.220262	Thermal Correction to Energy	0.327858
N	-4.832584	1.802751	0.044827	Thermal Correction to Enthalpy	0.328803
C	0.011203	-0.943926	0.429624	Thermal Correction to Free Energy	0.25957
C	1.178148	-0.19117	0.273062		
C	-1.238209	-0.297166	0.332479		
C	1.082379	1.201247	0.040106		
C	-1.270527	1.10144	0.10194		
C	3.467175	1.47205	-0.054498		
C	-3.664839	1.143741	0.124502		
C	0.082558	-2.399168	0.70601		
C	2.183613	2.024309	-0.119513		
C	-2.440925	1.819815	0.001655		
C	2.506099	-0.72501	0.442677		
C	-2.49501	-0.95875	0.425495		
C	3.613802	0.069932	0.185149		
C	-3.665183	-0.270095	0.328503		
C	0.597483	-3.272067	-0.255107		
C	-0.367833	-2.898293	1.930536		
C	0.653954	-4.63661	0.006721		
C	-0.292052	-4.261365	2.192891		
C	0.213995	-5.13138	1.231187		
H	2.040212	3.083749	-0.291168		
H	-2.405923	2.888265	-0.17289		
H	2.627423	-1.797555	0.495706		
H	-2.513253	-2.031878	0.567634		
H	4.609559	-0.357429	0.214548		
H	-4.615857	-0.785753	0.396596		
H	-0.760073	-2.215907	2.676789		
H	1.042075	-5.312863	-0.74591		
H	-0.630646	-4.643168	3.148801		
H	0.264669	-6.194484	1.435654		
H	5.486	1.819652	-0.172973		
H	4.49226	3.214738	-0.411481		
H	-4.861018	2.799053	-0.110534		
H	-5.710547	1.312001	0.121262		
H	0.937921	-2.882549	-1.208645		
O	2.676984	-0.480959	2.430063		
H	3.587559	-0.77492	2.599607		

RDA-C11-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.776
O	-0.15167	1.708457	-0.337288	Zero-point Energy Correction	0.296039
N	4.569436	2.024125	-0.377876	Thermal Correction to Energy	0.314569

N	-4.847415	1.972011	0.307676	Thermal Correction to Enthalpy	0.315513
C	-0.151407	-1.023611	0.298045	Thermal Correction to Free Energy	0.249593
C	1.094498	-0.295853	0.153812		
C	-1.333935	-0.323689	0.300873		
C	1.041873	1.069755	-0.174509		
C	-1.325283	1.096552	0.001734		
C	3.432911	1.289833	-0.160003		
C	-3.736515	1.304756	0.2908		
C	-0.087714	-2.508789	0.499297		
C	2.168413	1.851718	-0.353688		
C	-2.437587	1.866507	-0.016136		
C	2.384374	-0.821696	0.390508		
C	-2.643574	-0.880142	0.593126		
C	3.520154	-0.061919	0.239524		
C	-3.75649	-0.123609	0.602048		
C	0.873624	-3.282554	-0.234911		
C	-0.528932	-3.03301	1.756186		
C	1.219395	-4.555101	0.175424		
C	-0.163707	-4.298545	2.154319		
C	0.69841	-5.072376	1.362231		
H	2.055583	2.895903	-0.620978		
H	-2.357331	2.917837	-0.269281		
H	2.494596	-1.844285	0.727206		
H	-2.714614	-1.932144	0.821998		
H	4.495582	-0.49212	0.435677		
H	-4.718068	-0.563187	0.842485		
H	-1.150664	-2.416573	2.394003		
H	1.904208	-5.144045	-0.421872		
H	-0.52491	-4.690444	3.09743		
H	0.97848	-6.067307	1.68702		
H	5.418619	1.684438	0.052232		
H	4.471061	3.029959	-0.382146		
H	-4.660091	2.94702	0.06916		
H	1.275029	-2.868967	-1.151971		
O	-1.468889	-3.051192	-0.785422		
H	-1.357691	-4.014182	-0.755745		

RDA-C11-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.157187	1.714863	-0.211428	Zero-point Energy Correction	-993.263
N	4.531441	2.026507	-0.315157	Thermal Correction to Energy	0.308667
N	-4.825718	1.992376	0.243068	Thermal Correction to Enthalpy	0.327637
C	-0.114206	-1.022754	0.331179	Thermal Correction to Free Energy	0.328581
C	1.09205	-0.300529	0.205205		0.262261
C	-1.335109	-0.317742	0.328323		

C	1.031995	1.08949	-0.092344
C	-1.318178	1.078256	0.054566
C	3.41842	1.302557	-0.134104
C	-3.696607	1.270121	0.268386
C	-0.063542	-2.509791	0.512417
C	2.146695	1.873932	-0.284895
C	-2.451148	1.859182	0.008899
C	2.403961	-0.832952	0.406349
C	-2.623413	-0.882857	0.587018
C	3.519105	-0.071569	0.248019
C	-3.752674	-0.125965	0.571082
C	0.900146	-3.285965	-0.214897
C	-0.531815	-3.035217	1.75831
C	1.22645	-4.564005	0.192697
C	-0.18088	-4.305594	2.154301
C	0.684899	-5.082065	1.370029
H	2.029007	2.922273	-0.531437
H	-2.366856	2.914049	-0.22287
H	2.520875	-1.858431	0.730146
H	-2.703421	-1.936819	0.802845
H	4.503151	-0.491984	0.421613
H	-4.717675	-0.572887	0.781379
H	-1.155789	-2.418021	2.393392
H	1.911652	-5.15751	-0.400197
H	-0.559176	-4.699359	3.090238
H	0.950794	-6.081958	1.692722
H	5.443084	1.610033	-0.193027
H	4.481774	3.000925	-0.575665
H	-4.80929	2.975473	0.012824
H	-5.720302	1.556662	0.4138
H	1.311904	-2.872811	-1.12789
O	-1.425456	-2.973613	-0.812525
H	-1.338294	-3.940171	-0.82886

RDA-C11-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.248
O	-0.157254	1.717058	-0.20449	Zero-point Energy Correction	0.309124
N	4.533862	2.020992	-0.305757	Thermal Correction to Energy	0.328131
N	-4.826626	1.993065	0.238745	Thermal Correction to Enthalpy	0.329075
C	-0.120138	-1.023514	0.328935	Thermal Correction to Free Energy	0.262493
C	1.087891	-0.300513	0.20522		
C	-1.338158	-0.316434	0.326552		
C	1.029336	1.089634	-0.087918		
C	-1.318024	1.080624	0.05511		
C	3.417055	1.298498	-0.127582		

C	-3.697065	1.270025	0.264421
C	-0.06807	-2.510492	0.512293
C	2.147522	1.872435	-0.276661
C	-2.45191	1.860539	0.009077
C	2.397708	-0.835992	0.404862
C	-2.627044	-0.883516	0.578158
C	3.514558	-0.076249	0.24926
C	-3.75511	-0.126129	0.563559
C	0.886917	-3.286568	-0.224934
C	-0.513607	-3.030329	1.767877
C	1.218655	-4.56377	0.181791
C	-0.154115	-4.299091	2.165261
C	0.697951	-5.078106	1.370924
H	2.031805	2.921412	-0.519633
H	-2.36879	2.915287	-0.221521
H	2.510533	-1.86323	0.723577
H	-2.7023	-1.940757	0.777523
H	4.496894	-0.500801	0.421289
H	-4.721081	-0.573847	0.766117
H	-1.13228	-2.41167	2.406807
H	1.892049	-5.160523	-0.421079
H	-0.518103	-4.688824	3.108279
H	0.969434	-6.076785	1.69191
H	5.444462	1.603614	-0.186599
H	4.490565	2.994851	-0.566034
H	-4.813497	2.973892	0.002232
H	-5.722729	1.558729	0.400003
H	1.282534	-2.875511	-1.14587
O	-1.448391	-2.969934	-0.771579
H	-1.33477	-3.931939	-0.826617

RDA-C12-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.788
O	-0.098716	1.816664	-0.10608	Zero-point Energy Correction	0.295869
N	4.615914	2.207956	-0.327955	Thermal Correction to Energy	0.314651
N	-4.85066	1.760724	0.084649	Thermal Correction to Enthalpy	0.315595
C	-0.005672	-0.929709	0.449838	Thermal Correction to Free Energy	0.24852
C	1.210114	-0.177432	0.261906		
C	-1.217261	-0.293394	0.356954		
C	1.114271	1.196326	-0.016763		
C	-1.26465	1.126827	0.077725		
C	3.500378	1.445166	-0.101471		
C	-3.70068	1.166074	0.145431		
C	0.071715	-2.379804	0.747284		
C	2.221894	2.002885	-0.202038		

C	-2.419647	1.824733	-0.018919
C	2.510835	-0.711298	0.37653
C	-2.500788	-0.954967	0.478979
C	3.627696	0.06918	0.19664
C	-3.659522	-0.277754	0.383292
C	0.641045	-3.266343	-0.156935
C	-0.400687	-2.862815	1.996493
C	0.6857	-4.630863	0.131979
C	-0.391467	-4.253555	2.250059
C	0.165062	-5.124217	1.332542
H	2.088781	3.057549	-0.412927
H	-2.391234	2.888705	-0.226236
H	2.63344	-1.759966	0.618553
H	-2.514368	-2.026335	0.640344
H	4.618989	-0.359162	0.290232
H	-4.610224	-0.790842	0.473671
H	-0.984761	-2.206278	2.628822
H	1.119708	-5.313793	-0.588667
H	-0.80192	-4.61928	3.183357
H	0.192949	-6.187466	1.537268
H	5.490657	1.850261	0.030352
H	4.508544	3.210465	-0.258758
H	-4.707098	2.756522	-0.089456
H	1.033841	-2.896465	-1.097331
O	1.245286	-2.328397	3.140617
H	1.901576	-2.814539	2.615268

RDA-C12-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.273
O	-0.10385	1.812015	-0.05297	Zero-point Energy Correction	0.307503
N	4.580728	2.226876	-0.249732	Thermal Correction to Energy	0.326393
N	-4.811387	1.794365	0.072617	Thermal Correction to Enthalpy	0.327338
C	0.039259	-0.930553	0.42599	Thermal Correction to Free Energy	0.260158
C	1.214209	-0.181232	0.255307		
C	-1.208601	-0.287648	0.351562		
C	1.107714	1.215592	0.009926		
C	-1.248563	1.110936	0.107982		
C	3.487245	1.470389	-0.086283		
C	-3.64331	1.141746	0.152599		
C	0.111128	-2.384748	0.695613		
C	2.201696	2.030836	-0.164438		
C	-2.422886	1.822026	0.013068		
C	2.5342	-0.716063	0.349225		
C	-2.464589	-0.953483	0.464225		
C	3.629306	0.071955	0.182514		

C	-3.637751	-0.271647	0.373876
C	0.637095	-3.260551	-0.236361
C	-0.314	-2.870808	1.963471
C	0.686036	-4.631475	0.041033
C	-0.310205	-4.264491	2.19963
C	0.208562	-5.130727	1.253055
H	2.064037	3.089296	-0.349841
H	-2.395429	2.888912	-0.173197
H	2.659857	-1.768849	0.568258
H	-2.481786	-2.026232	0.615066
H	4.628155	-0.341909	0.259329
H	-4.587216	-0.787606	0.457973
H	-0.8796	-2.218009	2.617046
H	1.089495	-5.309537	-0.70199
H	-0.69401	-4.638239	3.14188
H	0.234029	-6.196398	1.447013
H	5.50298	1.820399	-0.187133
H	4.505642	3.216827	-0.435064
H	-4.841371	2.788865	-0.100154
H	-5.686918	1.299284	0.16094
H	0.992307	-2.885842	-1.190003
O	1.41087	-2.387036	2.956873
H	1.20208	-2.85	3.784717

#### RDA-C12-TS

Atom	X	Y	Z	Electronic Energy (EE)	-993.257
O	-0.109966	1.813304	-0.061242	Zero-point Energy Correction	0.308484
N	4.576347	2.22475	-0.235507	Thermal Correction to Energy	0.327947
N	-4.819764	1.795735	0.036965	Thermal Correction to Enthalpy	0.328891
C	0.032265	-0.92301	0.457266	Thermal Correction to Free Energy	0.260777
C	1.206069	-0.172545	0.290282		
C	-1.216003	-0.281131	0.359024		
C	1.099817	1.219664	0.020515		
C	-1.253667	1.114326	0.099651		
C	3.48023	1.471672	-0.063919		
C	-3.649512	1.144879	0.127568		
C	0.100931	-2.374726	0.740315		
C	2.196465	2.031103	-0.161385		
C	-2.428963	1.823548	-0.01134		
C	2.524417	-0.704267	0.410307		
C	-2.471924	-0.946554	0.465301		
C	3.620383	0.079636	0.235034		
C	-3.644423	-0.26607	0.359365		
C	0.630452	-3.258886	-0.186299		
C	-0.338018	-2.849252	2.007079		

C	0.665573	-4.62713	0.093965
C	-0.348911	-4.243871	2.24486
C	0.171758	-5.11657	1.305396
H	2.060688	3.085787	-0.365989
H	-2.399777	2.888303	-0.208142
H	2.642959	-1.749716	0.662111
H	-2.48817	-2.017991	0.623304
H	4.617776	-0.33208	0.334566
H	-4.592834	-0.783985	0.438813
H	-0.913559	-2.193885	2.647953
H	1.067518	-5.312801	-0.642513
H	-0.739552	-4.6109	3.186352
H	0.185909	-6.181563	1.503647
H	5.498034	1.820972	-0.16147
H	4.506876	3.210327	-0.440456
H	-4.853374	2.788262	-0.141086
H	-5.695292	1.301925	0.122473
H	0.996394	-2.888341	-1.13735
O	1.28724	-2.322823	3.059673
H	1.790767	-3.148853	2.978539

RDA-C13-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.761
O	-0.106635	1.846613	-0.087783	Zero-point Energy Correction	0.294316
N	4.622598	2.207194	-0.228014	Thermal Correction to Energy	0.313028
N	-4.802594	1.750274	0.006405	Thermal Correction to Enthalpy	0.313972
C	0.044322	-0.90876	0.442706	Thermal Correction to Free Energy	0.246781
C	1.22878	-0.136186	0.27241		
C	-1.187225	-0.27046	0.338765		
C	1.113845	1.249497	0.000999		
C	-1.242672	1.138181	0.073272		
C	3.52188	1.500102	-0.071945		
C	-3.634761	1.12338	0.10417		
C	0.139176	-2.357448	0.733693		
C	2.208545	2.057935	-0.174453		
C	-2.421307	1.825948	-0.036894		
C	2.541464	-0.684814	0.397772		
C	-2.441876	-0.956823	0.450855		
C	3.642423	0.092807	0.230819		
C	-3.617086	-0.294763	0.343273		
C	0.575418	-3.233364	-0.272305		
C	-0.233077	-2.810421	1.990512		
C	0.508602	-4.608918	-0.002312		
C	0.019064	-4.179745	2.361397		
C	0.159427	-5.085041	1.246159		

H	2.078339	3.113747	-0.382956
H	-2.416539	2.890238	-0.236521
H	2.638714	-1.737072	0.633066
H	-2.429041	-2.025865	0.619941
H	4.639896	-0.318159	0.327746
H	-4.564151	-0.815001	0.423326
H	-0.616242	-2.11198	2.72688
H	0.699276	-5.313367	-0.806653
H	-0.537103	-4.550678	3.21677
H	0.070146	-6.152198	1.418608
H	4.375185	3.179998	-0.428238
H	-4.84537	2.744202	-0.174682
H	-5.670635	1.24099	0.102801
H	0.848575	-2.858529	-1.251207
O	1.592528	-4.130778	3.220623
H	1.753478	-5.054293	3.453876

#### RDA-C13-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.271
O	-0.108128	1.818928	-0.098298	Zero-point Energy Correction	0.307736
N	4.579619	2.219062	-0.285319	Thermal Correction to Energy	0.327228
N	-4.814238	1.81621	0.024872	Thermal Correction to Enthalpy	0.328172
C	0.028226	-0.909999	0.456768	Thermal Correction to Free Energy	0.259487
C	1.204707	-0.164503	0.276076		
C	-1.217596	-0.269421	0.358198		
C	1.102487	1.22342	-0.01156		
C	-1.253993	1.124149	0.080238		
C	3.483081	1.470425	-0.10342		
C	-3.64875	1.162238	0.122707		
C	0.105685	-2.36323	0.748816		
C	2.199398	2.030983	-0.205023		
C	-2.426062	1.835517	-0.032682		
C	2.522175	-0.698539	0.396105		
C	-2.47639	-0.92827	0.487084		
C	3.620666	0.081275	0.211337		
C	-3.647209	-0.245338	0.379173		
C	0.619108	-3.244567	-0.219984		
C	-0.326441	-2.852485	1.966797		
C	0.666109	-4.614914	0.025826		
C	-0.188315	-4.231113	2.264111		
C	0.242808	-5.114554	1.245621		
H	2.065004	3.083721	-0.422625		
H	-2.3956	2.897506	-0.244713		
H	2.645293	-1.744236	0.651011		
H	-2.495248	-1.995862	0.667599		

H	4.618061	-0.331827	0.308762
H	-4.598269	-0.755953	0.476725
H	-0.724877	-2.18026	2.718765
H	1.027281	-5.28573	-0.744383
H	-0.680517	-4.629189	3.141897
H	0.268683	-6.17989	1.444286
H	5.500414	1.812383	-0.2057
H	4.508199	3.202913	-0.50154
H	-4.840657	2.806621	-0.170707
H	-5.691521	1.326855	0.126797
H	0.955092	-2.850277	-1.173089
O	1.577839	-4.094969	3.273122
H	1.74992	-5.048834	3.328211

RDA-C13-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.255
O	-0.097271	1.795585	-0.081743	Zero-point Energy Correction	0.308055
N	4.591259	2.183343	-0.266542	Thermal Correction to Energy	0.327697
N	-4.803381	1.81395	0.046634	Thermal Correction to Enthalpy	0.328641
C	0.028552	-0.938645	0.461039	Thermal Correction to Free Energy	0.258964
C	1.207302	-0.193987	0.281613		
C	-1.214548	-0.289983	0.36394		
C	1.109257	1.195711	0.001428		
C	-1.244021	1.105132	0.092425		
C	3.491412	1.436618	-0.089444		
C	-3.639178	1.154444	0.137198		
C	0.097622	-2.391966	0.752067		
C	2.21004	2.000492	-0.188206		
C	-2.413821	1.822123	-0.016369		
C	2.523367	-0.730608	0.399094		
C	-2.476546	-0.943407	0.487503		
C	3.624275	0.046086	0.218258		
C	-3.643718	-0.254181	0.384549		
C	0.63607	-3.274227	-0.198089		
C	-0.372383	-2.882013	1.961084		
C	0.675193	-4.645464	0.057018		
C	-0.252545	-4.258991	2.267432		
C	0.213044	-5.142647	1.263272		
H	2.078417	3.054335	-0.39994		
H	-2.377638	2.884838	-0.222734		
H	2.642713	-1.777657	0.647019		
H	-2.499136	-2.012053	0.659642		
H	4.619274	-0.371772	0.316404		
H	-4.595782	-0.762863	0.477954		
H	-0.788338	-2.206505	2.699984		

H	1.059245	-5.319956	-0.69873
H	-0.790619	-4.656073	3.117137
H	0.236091	-6.206573	1.465858
H	5.511023	1.774252	-0.197816
H	4.526384	3.166576	-0.483803
H	-4.829425	2.80422	-0.145371
H	-5.682942	1.328849	0.14113
H	0.996507	-2.886157	-1.144493
O	1.361909	-4.17272	3.441808
H	2.03838	-4.069862	2.753649

RDA-C14-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.785
O	-0.109862	1.826479	-0.023302	Zero-point Energy Correction	0.295166
N	4.627782	2.12565	-0.301583	Thermal Correction to Energy	0.314299
N	-4.842914	1.849008	0.131327	Thermal Correction to Enthalpy	0.315243
C	0.053009	-0.928465	0.471517	Thermal Correction to Free Energy	0.246832
C	1.201546	-0.199863	0.29262		
C	-1.227837	-0.271467	0.387769		
C	1.115452	1.221724	0.02641		
C	-1.260852	1.111357	0.14238		
C	3.538124	1.450286	-0.11202		
C	-3.660895	1.158666	0.174492		
C	0.106827	-2.382192	0.75845		
C	2.200187	2.00551	-0.171386		
C	-2.43924	1.826851	0.040815		
C	2.542101	-0.741834	0.392796		
C	-2.47294	-0.925722	0.493658		
C	3.632216	0.023419	0.200938		
C	-3.658763	-0.237486	0.395842		
C	0.652342	-3.266922	-0.18014		
C	-0.40348	-2.874011	1.974548		
C	0.71191	-4.620452	0.09517		
C	-0.33072	-4.217833	2.263981		
C	0.288235	-5.110717	1.353341		
H	2.071491	3.063845	-0.369257		
H	-2.404125	2.893159	-0.149368		
H	2.655555	-1.790869	0.637941		
H	-2.49725	-1.997563	0.648196		
H	4.627166	-0.399239	0.283059		
H	-4.605396	-0.758753	0.479544		
H	-0.848703	-2.18344	2.682009		
H	1.11581	-5.310157	-0.636636		
H	-0.713246	-4.597471	3.203576		
H	0.181398	-6.177184	1.499882		

H	4.392798	3.098826	-0.502145
H	-4.8265	2.767033	-0.290733
H	-5.679815	1.312736	-0.05042
H	1.011898	-2.883428	-1.128202
O	2.147082	-5.158976	2.245936
H	2.611853	-5.539356	1.484067

RDA-C14-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.271
O	-0.101183	1.795444	-0.077941	Zero-point Energy Correction	0.307731
N	4.587262	2.175802	-0.260247	Thermal Correction to Energy	0.327276
N	-4.80751	1.816233	0.029004	Thermal Correction to Enthalpy	0.32822
C	0.02054	-0.93642	0.464508	Thermal Correction to Free Energy	0.259329
C	1.201896	-0.197027	0.286677		
C	-1.222549	-0.288812	0.365883		
C	1.106158	1.193347	0.006274		
C	-1.251066	1.105647	0.09362		
C	3.487885	1.430946	-0.082374		
C	-3.645742	1.155658	0.126765		
C	0.087913	-2.38737	0.758825		
C	2.206501	1.99701	-0.182538		
C	-2.419154	1.823489	-0.019959		
C	2.517585	-0.736343	0.407023		
C	-2.484948	-0.942688	0.483324		
C	3.619224	0.039879	0.226934		
C	-3.65205	-0.253616	0.373821		
C	0.62502	-3.267362	-0.188301		
C	-0.398185	-2.873392	1.986059		
C	0.693718	-4.619862	0.090056		
C	-0.312408	-4.2163	2.277162		
C	0.297307	-5.107388	1.358426		
H	2.076369	3.051188	-0.395706		
H	-2.382289	2.886331	-0.226601		
H	2.637205	-1.783434	0.657091		
H	-2.511076	-2.01171	0.65481		
H	4.61476	-0.377819	0.323857		
H	-4.605869	-0.760653	0.462604		
H	-0.833642	-2.182069	2.69912		
H	1.086558	-5.310028	-0.647661		
H	-0.675882	-4.595499	3.224767		
H	0.198909	-6.174392	1.510808		
H	5.506482	1.765167	-0.182166		
H	4.519801	3.160579	-0.47372		
H	-4.828014	2.808064	-0.159999		
H	-5.687772	1.330705	0.12339		

H	0.965745	-2.884766	-1.143973
O	2.157235	-5.122563	2.214945
H	2.614329	-5.580807	1.491321

RDA-C14-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.255
O	-0.086602	1.778458	-0.062273	Zero-point Energy Correction	0.308256
N	4.599082	2.161969	-0.29357	Thermal Correction to Energy	0.327793
N	-4.791163	1.808876	0.110267	Thermal Correction to Enthalpy	0.328737
C	0.03757	-0.964321	0.437707	Thermal Correction to Free Energy	0.259924
C	1.217315	-0.220269	0.254504		
C	-1.205531	-0.310328	0.361584		
C	1.118994	1.174139	-0.002816		
C	-1.233597	1.088477	0.111443		
C	3.500523	1.413707	-0.116584		
C	-3.628157	1.144298	0.175574		
C	0.103833	-2.417796	0.7142		
C	2.21878	1.980161	-0.192372		
C	-2.402036	1.810884	0.024627		
C	2.534538	-0.759632	0.349484		
C	-2.468672	-0.962931	0.477476		
C	3.634382	0.018497	0.168381		
C	-3.634635	-0.269089	0.393113		
C	0.671749	-3.287978	-0.229387		
C	-0.41122	-2.924971	1.917331		
C	0.729823	-4.643574	0.026797		
C	-0.34001	-4.27852	2.18555		
C	0.284993	-5.158209	1.268839		
H	2.086027	3.037084	-0.387472		
H	-2.363753	2.876724	-0.164583		
H	2.657265	-1.810594	0.578101		
H	-2.494682	-2.034932	0.626034		
H	4.629485	-0.402948	0.247913		
H	-4.587412	-0.778068	0.478007		
H	-0.860369	-2.247452	2.634882		
H	1.14975	-5.320518	-0.706867		
H	-0.731837	-4.671572	3.115615		
H	0.157043	-6.225485	1.38669		
H	5.518948	1.749945	-0.246669		
H	4.53269	3.147467	-0.500043		
H	-4.816143	2.802531	-0.063635		
H	-5.671398	1.323528	0.197334		
H	1.042151	-2.891409	-1.168121		
O	2.063038	-5.37302	2.182872		
H	2.248304	-4.437966	2.365955		

## RDA-C2-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.794
O	-0.096364	1.837489	-0.043233	Zero-point Energy Correction	0.29506
N	4.61859	2.102548	-0.519737	Thermal Correction to Energy	0.314164
N	-4.790804	1.784237	0.142573	Thermal Correction to Enthalpy	0.315108
C	0.053481	-0.930969	0.421048	Thermal Correction to Free Energy	0.246952
C	1.239514	-0.176013	0.257494		
C	-1.184883	-0.284844	0.351465		
C	1.13396	1.23909	-0.001392		
C	-1.232073	1.12595	0.124244		
C	3.540086	1.463394	-0.190092		
C	-3.627398	1.136111	0.200259		
C	0.129257	-2.390653	0.674886		
C	2.210523	2.031566	-0.216455		
C	-2.407974	1.826391	0.054266		
C	2.534368	-0.722065	0.366947		
C	-2.443273	-0.957783	0.466924		
C	3.651059	0.074071	0.246728		
C	-3.618144	-0.283149	0.400323		
C	0.672779	-3.243734	-0.288998		
C	-0.343586	-2.9171	1.879471		
C	0.732765	-4.612431	-0.051323		
C	-0.265975	-4.284817	2.11907		
C	0.267847	-5.133895	1.153412		
H	2.078176	3.083066	-0.444463		
H	-2.394125	2.895497	-0.118231		
H	2.649812	-1.77103	0.605555		
H	-2.450414	-2.031533	0.602308		
H	4.641725	-0.358172	0.273933		
H	-4.566449	-0.800318	0.485434		
H	-0.761591	-2.252357	2.627598		
H	1.145358	-5.27064	-0.806682		
H	-0.625256	-4.685922	3.059292		
H	0.321753	-6.20015	1.339275		
H	4.378773	3.058802	-0.79078		
H	-4.821802	2.782521	-0.011931		
H	-5.663831	1.284961	0.240698		
H	1.037703	-2.833486	-1.224223		
O	3.950504	0.753361	2.502282		
H	3.659065	-0.113791	2.802351		

## RDA-C2-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.277
------	---	---	---	------------------------	----------

O	-0.093657	1.806803	-0.080694	Zero-point Energy Correction	0.308079
N	4.581309	2.222823	-0.350407	Thermal Correction to Energy	0.327472
N	-4.791453	1.796431	0.125618	Thermal Correction to Enthalpy	0.328416
C	0.045739	-0.939945	0.42294	Thermal Correction to Free Energy	0.259944
C	1.22693	-0.182886	0.239837		
C	-1.194167	-0.295353	0.354411		
C	1.118447	1.214269	-0.026607		
C	-1.235973	1.106748	0.104461		
C	3.492784	1.481354	-0.15204		
C	-3.628863	1.141039	0.187738		
C	0.126737	-2.395695	0.689807		
C	2.204178	2.031028	-0.232428		
C	-2.406656	1.819007	0.025825		
C	2.531157	-0.714272	0.329816		
C	-2.45454	-0.95767	0.484215		
C	3.645032	0.091173	0.197085		
C	-3.625169	-0.273837	0.409967		
C	0.672916	-3.254656	-0.267751		
C	-0.344557	-2.912324	1.89959		
C	0.736121	-4.621083	-0.018219		
C	-0.260737	-4.277356	2.150925		
C	0.274292	-5.133009	1.191643		
H	2.058292	3.082727	-0.446719		
H	-2.380877	2.885075	-0.164989		
H	2.667709	-1.766418	0.54591		
H	-2.470535	-2.029462	0.63651		
H	4.635799	-0.343634	0.166679		
H	-4.575564	-0.785768	0.506433		
H	-0.763567	-2.24263	2.643059		
H	1.148771	-5.28511	-0.768965		
H	-0.617324	-4.671663	3.095465		
H	0.331311	-6.197855	1.386691		
H	5.503575	1.817408	-0.269719		
H	4.508801	3.209236	-0.55876		
H	-4.820259	2.791835	-0.04542		
H	-5.668119	1.306001	0.232716		
H	1.033388	-2.852199	-1.20844		
O	3.914009	0.623762	2.299926		
H	3.732192	-0.260633	2.658284		

RDA-C2-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.092846	1.802221	-0.081984	Zero-point Energy Correction	0.308633
N	4.581939	2.220719	-0.333651	Thermal Correction to Energy	0.328081
N	-4.794126	1.797758	0.129523	Thermal Correction to Enthalpy	0.329025

C	0.048166	-0.942727	0.419492	Thermal Correction to Free Energy	0.26034
C	1.226963	-0.186307	0.242134		
C	-1.194759	-0.296635	0.349663		
C	1.117322	1.211754	-0.025636		
C	-1.234855	1.103635	0.101424		
C	3.491624	1.483174	-0.138167		
C	-3.628221	1.141375	0.18651		
C	0.1274	-2.398221	0.68855		
C	2.204276	2.028341	-0.23261		
C	-2.406628	1.817763	0.024432		
C	2.532753	-0.720443	0.324701		
C	-2.453567	-0.958096	0.479006		
C	3.649451	0.090085	0.219153		
C	-3.624132	-0.272331	0.405893		
C	0.663382	-3.261532	-0.270602		
C	-0.334188	-2.909952	1.904156		
C	0.726863	-4.626845	-0.016393		
C	-0.249892	-4.273851	2.15992		
C	0.275499	-5.133299	1.199294		
H	2.057376	3.079248	-0.447782		
H	-2.378105	2.883974	-0.16472		
H	2.666273	-1.776955	0.519798		
H	-2.468579	-2.029821	0.631251		
H	4.632566	-0.352532	0.131614		
H	-4.573143	-0.786339	0.501726		
H	-0.745103	-2.236555	2.648732		
H	1.130402	-5.295049	-0.767997		
H	-0.597726	-4.664228	3.108998		
H	0.332662	-6.19718	1.397694		
H	5.501091	1.829618	-0.183427		
H	4.515385	3.213409	-0.508263		
H	-4.827061	2.792404	-0.038716		
H	-5.670398	1.307739	0.23182		
H	1.014127	-2.863914	-1.216812		
O	4.028912	0.584845	2.189505		
H	3.606366	-0.171986	2.626164		

RDA-C3-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.008976	1.777417	-0.030678	Zero-point Energy Correction	-992.799
N	4.69389	2.021817	-0.5094	Thermal Correction to Energy	0.294802
N	-4.708526	1.850659	0.200441	Thermal Correction to Enthalpy	0.314059
C	0.090011	-0.975274	0.420571	Thermal Correction to Free Energy	0.315003
C	1.278085	-0.239677	0.22795		0.245942
C	-1.142657	-0.305801	0.373131		

C	1.185458	1.144157	-0.00779
C	-1.164048	1.101501	0.146742
C	3.613758	1.3548	-0.228141
C	-3.552942	1.178254	0.244364
C	0.143178	-2.435275	0.672536
C	2.301217	1.953036	-0.174667
C	-2.324074	1.836984	0.087047
C	2.605382	-0.81238	0.296937
C	-2.412212	-0.948021	0.501225
C	3.70643	-0.065595	0.08127
C	-3.570369	-0.240909	0.443317
C	0.683511	-3.293209	-0.289089
C	-0.346667	-2.957302	1.872342
C	0.722933	-4.662865	-0.054033
C	-0.288131	-4.326227	2.109688
C	0.241822	-5.180147	1.146212
H	2.17406	3.000788	-0.412351
H	-2.280051	2.905093	-0.085684
H	2.699848	-1.86436	0.532222
H	-2.446857	-2.021234	0.635916
H	4.696442	-0.503549	0.124235
H	-4.529443	-0.737061	0.535801
H	-0.761173	-2.288669	2.618869
H	1.132678	-5.325034	-0.807406
H	-0.659446	-4.72454	3.046358
H	0.280498	-6.247333	1.33043
H	4.45397	2.999166	-0.690946
H	-4.721447	2.847846	0.041383
H	-5.589144	1.367012	0.300591
H	1.061097	-2.885858	-1.220662
O	2.417307	2.648393	2.2168
H	1.647398	2.103272	2.409473

RDA-C3-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.269
O	-0.107787	1.804836	-0.0153	Zero-point Energy Correction	0.308287
N	4.564677	2.124348	-0.526998	Thermal Correction to Energy	0.327466
N	-4.80972	1.778667	0.077563	Thermal Correction to Enthalpy	0.32841
C	0.032759	-0.944045	0.45322	Thermal Correction to Free Energy	0.260689
C	1.212407	-0.183282	0.293998		
C	-1.208281	-0.299816	0.368807		
C	1.097549	1.199819	0.052693		
C	-1.251473	1.10733	0.131331		
C	3.513221	1.468556	-0.011601		
C	-3.643536	1.133369	0.160217		

C	0.108128	-2.404161	0.70243
C	2.196066	2.023385	-0.124741
C	-2.423217	1.817392	0.031798
C	2.544593	-0.729677	0.393942
C	-2.468371	-0.967865	0.467057
C	3.639078	0.041622	0.24098
C	-3.637631	-0.285656	0.371891
C	0.657229	-3.250761	-0.264044
C	-0.373666	-2.936417	1.900815
C	0.713131	-4.621	-0.034758
C	-0.298927	-4.305797	2.131659
C	0.239554	-5.149153	1.163644
H	2.063622	3.07325	-0.355413
H	-2.396056	2.885218	-0.148124
H	2.657065	-1.786321	0.599529
H	-2.484432	-2.040726	0.610108
H	4.638281	-0.372161	0.31169
H	-4.588483	-0.801166	0.442834
H	-0.796017	-2.276333	2.651039
H	1.128802	-5.27534	-0.792307
H	-0.665208	-4.712859	3.067022
H	0.289971	-6.217124	1.342729
H	5.490602	1.757136	-0.35029
H	4.497422	3.125675	-0.656043
H	-4.843684	2.775337	-0.085895
H	-5.684348	1.28001	0.162486
H	1.027164	-2.835702	-1.195694
O	3.395637	2.183082	1.842497
H	2.788037	1.623555	2.350446

RDA-C3-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.251
O	-0.108989	1.803694	-0.00945	Zero-point Energy Correction	0.309031
N	4.563948	2.126251	-0.535848	Thermal Correction to Energy	0.32803
N	-4.81559	1.781646	0.080613	Thermal Correction to Enthalpy	0.328974
C	0.032762	-0.946446	0.448773	Thermal Correction to Free Energy	0.261859
C	1.208966	-0.187164	0.289318		
C	-1.211816	-0.299932	0.364737		
C	1.095404	1.200224	0.056403		
C	-1.252969	1.104829	0.131376		
C	3.511514	1.469104	-0.00988		
C	-3.646366	1.133868	0.15815		
C	0.106563	-2.40593	0.700217		
C	2.195669	2.024558	-0.111963		
C	-2.425975	1.816422	0.031867		

C	2.541927	-0.732446	0.384093
C	-2.470133	-0.967265	0.45786
C	3.635358	0.039823	0.229273
C	-3.640109	-0.283679	0.363086
C	0.656016	-3.256008	-0.26292
C	-0.374788	-2.934408	1.900677
C	0.713665	-4.624923	-0.027831
C	-0.296908	-4.302108	2.137703
C	0.242455	-5.148256	1.17314
H	2.064163	3.075418	-0.335461
H	-2.396735	2.884603	-0.14496
H	2.653884	-1.78993	0.584631
H	-2.48505	-2.040619	0.596182
H	4.63361	-0.376103	0.295318
H	-4.589322	-0.802365	0.429075
H	-0.796948	-2.271774	2.648616
H	1.12852	-5.282483	-0.782608
H	-0.660144	-4.705654	3.075413
H	0.295109	-6.214957	1.357039
H	5.486714	1.772233	-0.321439
H	4.501356	3.132929	-0.612286
H	-4.85261	2.77812	-0.076039
H	-5.690278	1.284361	0.160114
H	1.023382	-2.84517	-1.197257
O	3.390953	2.200191	1.802713
H	2.84695	1.596571	2.332767

RDA-C4'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.796
O	-0.106144	1.77934	-0.127706	Zero-point Energy Correction	0.295499
N	4.612983	2.161541	-0.295433	Thermal Correction to Energy	0.314301
N	-4.831542	1.82789	0.160852	Thermal Correction to Enthalpy	0.315245
C	0.057877	-0.949227	0.453928	Thermal Correction to Free Energy	0.248265
C	1.204386	-0.207876	0.291283		
C	-1.217214	-0.29117	0.400959		
C	1.089052	1.214298	0.098673		
C	-1.259774	1.084164	0.114323		
C	3.535376	1.467211	-0.090551		
C	-3.652653	1.143132	0.199823		
C	0.122722	-2.414479	0.687236		
C	2.205709	2.019845	-0.155515		
C	-2.433848	1.803025	0.009568		
C	2.552575	-0.73047	0.398881		
C	-2.464073	-0.937829	0.561904		
C	3.63938	0.043751	0.226358		

C	-3.645747	-0.247243	0.473203
C	0.640387	-3.260762	-0.295649
C	-0.327106	-2.952744	1.895583
C	0.70231	-4.632796	-0.073173
C	-0.251249	-4.32329	2.119267
C	0.259876	-5.165321	1.134659
H	2.057984	3.066918	-0.39396
H	-2.398693	2.861417	-0.219515
H	2.67158	-1.781776	0.630974
H	-2.486559	-2.003209	0.754078
H	4.636958	-0.369819	0.31636
H	-4.592079	-0.759793	0.602186
H	-0.725951	-2.295051	2.660347
H	1.099062	-5.284149	-0.842972
H	-0.592738	-4.732754	3.062644
H	0.313232	-6.233604	1.30885
H	4.361071	3.13095	-0.497963
H	-4.833856	2.743174	-0.266542
H	-5.681966	1.293178	0.055306
H	0.988361	-2.841637	-1.233553
O	1.432072	1.864396	2.098077
H	1.131999	2.780447	2.01476

RDA-C4'-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.27
O	-0.10032	1.768515	-0.159539	Zero-point Energy Correction	0.308604
N	4.582659	2.198128	-0.257531	Thermal Correction to Energy	0.327643
N	-4.810382	1.79712	0.069484	Thermal Correction to Enthalpy	0.328587
C	0.045221	-0.953376	0.463707	Thermal Correction to Free Energy	0.26137
C	1.206641	-0.206399	0.303585		
C	-1.210469	-0.297203	0.403329		
C	1.086728	1.216805	0.131473		
C	-1.251811	1.082124	0.090627		
C	3.508285	1.444284	-0.054917		
C	-3.645143	1.134096	0.1636		
C	0.11622	-2.417839	0.693764		
C	2.216447	2.019357	-0.143432		
C	-2.420922	1.795042	-0.03423		
C	2.532329	-0.723561	0.411232		
C	-2.465327	-0.944784	0.566483		
C	3.637342	0.053958	0.247286		
C	-3.640626	-0.260074	0.461064		
C	0.624482	-3.258804	-0.298808		
C	-0.319157	-2.95807	1.906391		
C	0.687423	-4.631409	-0.081555		

C	-0.239283	-4.329251	2.123907
C	0.259335	-5.167484	1.129812
H	2.079737	3.064121	-0.397003
H	-2.387521	2.849732	-0.280083
H	2.659118	-1.776243	0.634593
H	-2.486894	-2.00718	0.77524
H	4.632158	-0.365738	0.336013
H	-4.589381	-0.76753	0.592691
H	-0.707837	-2.30267	2.678598
H	1.073783	-5.280532	-0.858962
H	-0.568896	-4.742207	3.070363
H	0.314333	-6.236765	1.299591
H	5.510438	1.795555	-0.218294
H	4.498108	3.18506	-0.46526
H	-4.832338	2.780923	-0.155229
H	-5.688496	1.318966	0.206572
H	0.959311	-2.837055	-1.240588
O	1.365406	1.843669	1.972796
H	1.092112	2.774572	1.923079

RDA-C4'-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.253
O	-0.102278	1.772367	-0.167315	Zero-point Energy Correction	0.308919
N	4.587335	2.204905	-0.232957	Thermal Correction to Energy	0.328034
N	-4.812335	1.791895	0.055952	Thermal Correction to Enthalpy	0.328978
C	0.043874	-0.951741	0.452172	Thermal Correction to Free Energy	0.261573
C	1.206104	-0.204959	0.287064		
C	-1.209312	-0.293111	0.399643		
C	1.085839	1.222017	0.132148		
C	-1.250154	1.086618	0.084583		
C	3.505048	1.449065	-0.045782		
C	-3.644612	1.132618	0.155511		
C	0.11481	-2.415455	0.686673		
C	2.216434	2.023403	-0.134644		
C	-2.421923	1.79523	-0.043947		
C	2.527056	-0.724583	0.387943		
C	-2.463107	-0.94201	0.568194		
C	3.632964	0.056506	0.233719		
C	-3.638653	-0.259622	0.461656		
C	0.593599	-3.265467	-0.312378		
C	-0.289433	-2.944241	1.914889		
C	0.658817	-4.636188	-0.085337		
C	-0.207056	-4.313485	2.141326		
C	0.262719	-5.160712	1.141405		
H	2.083094	3.071081	-0.378006		

H	-2.39088	2.848705	-0.294411
H	2.651181	-1.779912	0.599367
H	-2.479865	-2.003794	0.780257
H	4.626324	-0.366152	0.321674
H	-4.586143	-0.767983	0.596603
H	-0.653419	-2.280549	2.691925
H	1.021115	-5.293233	-0.867306
H	-0.510897	-4.717892	3.099687
H	0.319796	-6.22834	1.318649
H	5.512732	1.800557	-0.196376
H	4.511566	3.194789	-0.420738
H	-4.840279	2.77192	-0.180602
H	-5.689743	1.313043	0.189365
H	0.902221	-2.852889	-1.266862
O	1.324363	1.787239	1.979099
H	1.12591	2.738209	1.957007

#### RDA-C4-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.799
O	-0.008973	1.777425	-0.030626	Zero-point Energy Correction	0.294802
N	4.693888	2.021834	-0.50939	Thermal Correction to Energy	0.314059
N	-4.708526	1.850655	0.200433	Thermal Correction to Enthalpy	0.315003
C	0.090012	-0.975277	0.420562	Thermal Correction to Free Energy	0.245941
C	1.278086	-0.23968	0.227934		
C	-1.142655	-0.305801	0.373138		
C	1.18546	1.144161	-0.007765		
C	-1.164046	1.101504	0.146766		
C	3.613757	1.354804	-0.228147		
C	-3.552941	1.178252	0.244361		
C	0.143176	-2.435277	0.672532		
C	2.301219	1.953044	-0.174623		
C	-2.324072	1.836986	0.087068		
C	2.605382	-0.812392	0.296869		
C	-2.41221	-0.948024	0.501214		
C	3.706428	-0.065608	0.08119		
C	-3.570368	-0.240914	0.443302		
C	0.683512	-3.293223	-0.289081		
C	-0.346676	-2.957291	1.872342		
C	0.722935	-4.662876	-0.054007		
C	-0.288139	-4.326212	2.109705		
C	0.24182	-5.180144	1.146242		
H	2.17406	3.000798	-0.412294		
H	-2.28005	2.905097	-0.08565		
H	2.69985	-1.864378	0.532125		
H	-2.446856	-2.021239	0.635891		

H	4.696439	-0.503568	0.124111
H	-4.529442	-0.737068	0.535769
H	-0.761184	-2.28865	2.61886
H	1.132684	-5.325054	-0.80737
H	-0.659458	-4.724514	3.046378
H	0.280498	-6.247327	1.330474
H	4.453956	2.999191	-0.690878
H	-4.721448	2.84784	0.04136
H	-5.589145	1.367001	0.300542
H	1.0611	-2.885884	-1.220658
O	2.417302	2.648434	2.216825
H	1.647436	2.103251	2.409494

RDA-C4-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.087984	1.810818	-0.075487	Zero-point Energy Correction	-993.28
N	4.587773	2.217028	-0.353272	Thermal Correction to Energy	0.30787
N	-4.79197	1.814657	0.091744	Thermal Correction to Enthalpy	0.327408
C	0.048548	-0.929706	0.428143	Thermal Correction to Free Energy	0.328352
C	1.224936	-0.176186	0.238314		0.259407
C	-1.19517	-0.282614	0.35743		
C	1.113347	1.208461	-0.016922		
C	-1.235076	1.11599	0.10267		
C	3.508471	1.463931	-0.150807		
C	-3.627258	1.158742	0.166613		
C	0.125003	-2.38448	0.701357		
C	2.216233	2.038309	-0.174412		
C	-2.404719	1.832705	0.011351		
C	2.550067	-0.70795	0.326056		
C	-2.455654	-0.941173	0.483038		
C	3.647523	0.069925	0.135702		
C	-3.625025	-0.254013	0.396696		
C	0.67787	-3.248319	-0.247858		
C	-0.35702	-2.895169	1.909485		
C	0.736834	-4.613775	0.008		
C	-0.277246	-4.259146	2.16748		
C	0.264271	-5.119706	1.216244		
H	2.074854	3.079235	-0.437248		
H	-2.373275	2.897797	-0.184054		
H	2.676693	-1.757435	0.560595		
H	-2.475986	-2.012177	0.640134		
H	4.644855	-0.348828	0.201806		
H	-4.576305	-0.76519	0.489303		
H	-0.78077	-2.221652	2.646787		
H	1.154966	-5.281694	-0.736216		

H	-0.64182	-4.648818	3.110888
H	0.318162	-6.183763	1.416438
H	5.514012	1.815156	-0.305241
H	4.504949	3.207106	-0.540121
H	-4.819604	2.808143	-0.088193
H	-5.668878	1.32387	0.191546
H	1.047125	-2.850359	-1.187084
O	2.412115	2.556868	2.075327
H	1.504723	2.904917	2.099736

RDA-C4-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	-993.262
O	-0.127399	1.803804	-0.075858	Zero-point Energy Correction	0.309103
N	4.539967	2.230426	-0.378707	Thermal Correction to Energy	0.328457
N	-4.835299	1.772515	0.041294	Thermal Correction to Enthalpy	0.329402
C	0.023529	-0.9358	0.429525	Thermal Correction to Free Energy	0.261011
C	1.195845	-0.173764	0.245981		
C	-1.223992	-0.29515	0.349547		
C	1.075638	1.207879	-0.00565		
C	-1.270864	1.102	0.088818		
C	3.473492	1.468479	-0.158635		
C	-3.664275	1.126947	0.128086		
C	0.106106	-2.389447	0.703949		
C	2.178147	2.056901	-0.132308		
C	-2.44565	1.80938	-0.018844		
C	2.523104	-0.704305	0.318552		
C	-2.480157	-0.962735	0.465166		
C	3.616869	0.075252	0.112008		
C	-3.653088	-0.284196	0.364128		
C	0.659385	-3.25283	-0.245374		
C	-0.372771	-2.899921	1.913461		
C	0.721164	-4.617604	0.011636		
C	-0.289061	-4.263025	2.172588		
C	0.252035	-5.122868	1.221036		
H	2.030527	3.063969	-0.49922		
H	-2.4199	2.873718	-0.218436		
H	2.651134	-1.753717	0.551378		
H	-2.491942	-2.033132	0.626415		
H	4.614097	-0.344937	0.161717		
H	-4.600041	-0.804009	0.448607		
H	-0.794624	-2.226122	2.651376		
H	1.137743	-5.286133	-0.732467		
H	-0.649164	-4.652495	3.117416		
H	0.308229	-6.186326	1.421979		
H	5.471719	1.842144	-0.33279		

H	4.450762	3.231694	-0.481497
H	-4.873895	2.763976	-0.143048
H	-5.708806	1.275528	0.132358
H	1.024265	-2.855776	-1.186486
O	2.398397	2.736028	1.817521
H	1.495772	3.070696	1.935197

RDA-C5'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.086507	1.803607	-0.214765	Zero-point Energy Correction	-992.795
N	4.596811	2.169487	-0.351697	Thermal Correction to Energy	0.294612
N	-4.8258	1.763701	0.079039	Thermal Correction to Enthalpy	0.313625
C	0.058008	-0.925826	0.443714	Thermal Correction to Free Energy	0.314569
C	1.208404	-0.173429	0.323238		0.246883
C	-1.203169	-0.265251	0.358509		
C	1.102705	1.263688	0.124081		
C	-1.237329	1.121055	0.050588		
C	3.4795	1.469205	-0.11211		
C	-3.661189	1.156346	0.148061		
C	0.125781	-2.391184	0.683175		
C	2.217288	2.032377	-0.216318		
C	-2.407634	1.821141	-0.056575		
C	2.536678	-0.704842	0.45489		
C	-2.453525	-0.931962	0.529525		
C	3.621826	0.075218	0.261633		
C	-3.63066	-0.258498	0.436715		
C	0.623163	-3.242322	-0.305196		
C	-0.294766	-2.920587	1.905564		
C	0.693904	-4.612775	-0.073879		
C	-0.213151	-4.289565	2.136439		
C	0.27811	-5.137436	1.146579		
H	2.084053	3.073191	-0.483018		
H	-2.388163	2.877911	-0.298524		
H	2.657304	-1.750283	0.70913		
H	-2.453486	-1.994306	0.736363		
H	4.623857	-0.325777	0.364364		
H	-4.577646	-0.766794	0.572334		
H	-0.677237	-2.25728	2.674077		
H	1.076059	-5.268736	-0.847122		
H	-0.533753	-4.693135	3.089623		
H	0.337001	-6.204396	1.326959		
H	5.502608	1.727934	-0.292696		
H	4.550213	3.142549	-0.617351		
H	-4.676085	2.753541	-0.132795		
H	0.949601	-2.828741	-1.253227		

O	0.845762	1.561696	2.237414
H	1.161793	2.471469	2.257255

RDA-C5-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.084983	1.828641	-0.117185	Zero-point Energy Correction	-992.794
N	4.613577	2.220894	-0.390423	Thermal Correction to Energy	0.294422
N	-4.835173	1.772593	0.120302	Thermal Correction to Enthalpy	0.314017
C	0.016073	-0.924163	0.411617	Thermal Correction to Free Energy	0.314962
C	1.225141	-0.164478	0.216474		0.245127
C	-1.197165	-0.286622	0.337491		
C	1.122405	1.206602	-0.049431		
C	-1.250167	1.135424	0.072411		
C	3.5204	1.460155	-0.166312		
C	-3.684437	1.176824	0.16634		
C	0.106434	-2.379456	0.695771		
C	2.231868	2.026283	-0.220879		
C	-2.404989	1.835805	-0.007408		
C	2.533584	-0.696197	0.312325		
C	-2.479315	-0.946612	0.473138		
C	3.648773	0.079351	0.12552		
C	-3.639275	-0.267759	0.395677		
C	0.644722	-3.250298	-0.255503		
C	-0.343208	-2.887167	1.916859		
C	0.719903	-4.613681	0.008772		
C	-0.255105	-4.250011	2.183123		
C	0.27292	-5.115256	1.22896		
H	2.094794	3.072572	-0.466237		
H	-2.377218	2.901215	-0.207356		
H	2.656549	-1.746337	0.547675		
H	-2.489334	-2.017896	0.631997		
H	4.640443	-0.351159	0.199828		
H	-4.588752	-0.781631	0.495003		
H	-0.75688	-2.210672	2.65691		
H	1.129027	-5.283867	-0.738087		
H	-0.601411	-4.634506	3.135262		
H	0.33688	-6.17722	1.435385		
H	5.531193	1.842782	-0.208106		
H	4.522658	3.222972	-0.46827		
H	-4.692577	2.768856	-0.051341		
H	0.99539	-2.857507	-1.20391		
O	2.437251	2.569091	2.159014		
H	1.505558	2.842589	2.104456		

## RDA-C6-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.789
O	-0.092491	1.833504	-0.080799	Zero-point Energy Correction	0.292469
N	4.597906	2.136172	-0.482576	Thermal Correction to Energy	0.312114
N	-4.840503	1.739229	0.122769	Thermal Correction to Enthalpy	0.313058
C	0.018098	-0.932637	0.420612	Thermal Correction to Free Energy	0.243276
C	1.219752	-0.169716	0.246386		
C	-1.199176	-0.292191	0.339478		
C	1.12065	1.21004	-0.013475		
C	-1.254024	1.133941	0.090087		
C	3.522661	1.438506	-0.1123		
C	-3.687121	1.152568	0.16922		
C	0.104186	-2.392397	0.687025		
C	2.223956	2.012544	-0.18584		
C	-2.412651	1.825111	0.010878		
C	2.529569	-0.721951	0.360846		
C	-2.473916	-0.965369	0.461347		
C	3.643033	0.040722	0.193417		
C	-3.638297	-0.293446	0.384273		
C	0.623364	-3.253307	-0.283128		
C	-0.332135	-2.912102	1.907529		
C	0.695392	-4.620297	-0.03684		
C	-0.249101	-4.27883	2.154713		
C	0.261513	-5.134629	1.182612		
H	2.105994	3.067813	-0.400208		
H	-2.393979	2.893203	-0.174746		
H	2.634594	-1.773774	0.593798		
H	-2.474963	-2.037674	0.610597		
H	4.635734	-0.386035	0.274946		
H	-4.585795	-0.812258	0.474012		
H	-0.732628	-2.242802	2.661323		
H	1.090937	-5.283019	-0.797516		
H	-0.585587	-4.67376	3.106065		
H	0.321774	-6.199499	1.374575		
H	5.519987	1.741764	-0.358121		
H	4.525726	3.130722	-0.647733		
H	-4.705733	2.739155	-0.037032		
H	0.963234	-2.849866	-1.231085		
O	3.286446	2.086804	2.172192		
H	2.509552	1.572568	2.429061		

## RDA-C7-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.795
O	-0.10375	1.817466	-0.079613	Zero-point Energy Correction	0.295513
N	4.581044	2.177257	-0.354057	Thermal Correction to Energy	0.313953

N	-4.849602	1.754543	0.111747	Thermal Correction to Enthalpy	0.314897
C	-0.015758	-0.946817	0.429872	Thermal Correction to Free Energy	0.247984
C	1.203997	-0.184237	0.289827		
C	-1.222898	-0.308054	0.334245		
C	1.106217	1.212682	0.009403		
C	-1.270474	1.118905	0.090923		
C	3.486253	1.458981	-0.087873		
C	-3.704578	1.154528	0.158171		
C	0.071676	-2.407581	0.687411		
C	2.201492	2.015892	-0.196819		
C	-2.421671	1.819372	0.009781		
C	2.477922	-0.715793	0.42591		
C	-2.508295	-0.973519	0.437932		
C	3.619249	0.094556	0.348148		
C	-3.666464	-0.294888	0.359613		
C	0.613439	-3.2586	-0.279536		
C	-0.382767	-2.939409	1.895967		
C	0.687974	-4.627005	-0.04283		
C	-0.296273	-4.307696	2.134351		
C	0.235827	-5.153271	1.165013		
H	2.068386	3.060547	-0.45005		
H	-2.394534	2.887936	-0.172499		
H	2.604725	-1.76686	0.650603		
H	-2.516808	-2.047333	0.577612		
H	4.600223	-0.361867	0.309834		
H	-4.618024	-0.808031	0.438175		
H	-0.799478	-2.277966	2.647841		
H	1.100059	-5.281794	-0.801653		
H	-0.646813	-4.711676	3.076804		
H	0.298909	-6.219243	1.349911		
H	5.499028	1.777383	-0.221424		
H	4.51107	3.157656	-0.587215		
H	-4.704099	2.754305	-0.038034		
H	0.968183	-2.846323	-1.218095		
O	3.905597	0.630812	2.355544		
H	4.803715	0.276155	2.390393		

RDA-C8'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.105581	1.846104	-0.077543	Zero-point Energy Correction	-992.795
N	4.625835	2.16278	-0.297412	Thermal Correction to Energy	0.294572
N	-4.794131	1.796741	0.240216	Thermal Correction to Enthalpy	0.313769
C	0.071035	-0.916809	0.435283	Thermal Correction to Free Energy	0.314713
C	1.217943	-0.161117	0.31061		0.246292
C	-1.192648	-0.286659	0.22373		

C	1.121998	1.24333	-0.004762
C	-1.24246	1.138007	0.080362
C	3.540939	1.481545	-0.101849
C	-3.630292	1.148171	0.237465
C	0.131004	-2.376169	0.707406
C	2.203145	2.029395	-0.212785
C	-2.415326	1.84463	0.084312
C	2.555027	-0.690928	0.470768
C	-2.446638	-0.959079	0.387402
C	3.645889	0.073737	0.273742
C	-3.620045	-0.279474	0.386513
C	0.67002	-3.238964	-0.249636
C	-0.356962	-2.89545	1.908745
C	0.720025	-4.607931	-0.005835
C	-0.296873	-4.2636	2.15295
C	0.239327	-5.121403	1.195763
H	2.073893	3.079375	-0.450338
H	-2.404594	2.920444	-0.038985
H	2.661644	-1.730997	0.752407
H	-2.447224	-2.03614	0.49529
H	4.642847	-0.334332	0.392382
H	-4.567127	-0.794534	0.496336
H	-0.777328	-2.224976	2.650786
H	1.135177	-5.272157	-0.754682
H	-0.670084	-4.658877	3.090351
H	0.282055	-6.18744	1.386004
H	4.385235	3.124498	-0.545563
H	-4.829668	2.800669	0.128075
H	-5.664009	1.293607	0.348184
H	1.044046	-2.833623	-1.183761
O	-1.151924	-0.390624	-2.139049
H	-2.078499	-0.129432	-2.203478

RDA-C8-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.789
O	-0.107677	1.852189	0.011872	Zero-point Energy Correction	0.29477
N	4.562325	2.179458	-0.355712	Thermal Correction to Energy	0.313711
N	-4.856683	1.73792	0.076195	Thermal Correction to Enthalpy	0.314655
C	0.044482	-0.922301	0.437759	Thermal Correction to Free Energy	0.247114
C	1.193849	-0.171014	0.326644		
C	-1.224299	-0.271871	0.326697		
C	1.105882	1.246078	0.077667		
C	-1.261731	1.133421	0.131101		
C	3.497218	1.413326	-0.09703		
C	-3.686124	1.139463	0.141681		

C	0.105314	-2.38364	0.697467
C	2.202067	2.023342	-0.109092
C	-2.434689	1.831428	0.045677
C	2.53278	-0.71374	0.521294
C	-2.467935	-0.962102	0.397404
C	3.637909	0.039498	0.165758
C	-3.650247	-0.293278	0.311158
C	0.619404	-3.250508	-0.268316
C	-0.353347	-2.894109	1.914173
C	0.672972	-4.618355	-0.018396
C	-0.287165	-4.260249	2.164351
C	0.222889	-5.124025	1.197894
H	2.098959	3.084443	-0.299727
H	-2.418614	2.905937	-0.098368
H	2.629769	-1.7864	0.58098
H	-2.461311	-2.037621	0.518352
H	4.628421	-0.398058	0.171679
H	-4.595286	-0.819891	0.365205
H	-0.751348	-2.217976	2.663296
H	1.067829	-5.287151	-0.774039
H	-0.635446	-4.649649	3.113651
H	0.26886	-6.189053	1.392858
H	5.491473	1.783511	-0.353119
H	4.455934	3.160815	-0.568522
H	-4.712878	2.743652	-0.04643
H	0.971942	-2.851099	-1.213111
O	2.359024	-0.694241	2.622436
H	3.28241	-0.47405	2.786142

RDA-C9-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.798
O	-0.111503	1.823692	-0.046834	Zero-point Energy Correction	0.294572
N	4.607593	2.143085	-0.456133	Thermal Correction to Energy	0.313475
N	-4.815265	1.727297	-0.085205	Thermal Correction to Enthalpy	0.314419
C	0.045872	-0.889943	0.696304	Thermal Correction to Free Energy	0.247281
C	1.23438	-0.138264	0.3888		
C	-1.197237	-0.274266	0.45835		
C	1.108215	1.219267	0.025018		
C	-1.247678	1.106224	0.122579		
C	3.512036	1.453532	-0.187395		
C	-3.64458	1.09898	0.082235		
C	0.122311	-2.368315	0.853795		
C	2.198447	2.006699	-0.262343		
C	-2.428139	1.78787	-0.057877		
C	2.546854	-0.680262	0.490306		

C	-2.44861	-0.949429	0.568638
C	3.643581	0.074635	0.210316
C	-3.628313	-0.297339	0.390718
C	0.658949	-3.117285	-0.1979
C	-0.393402	-3.024262	1.972538
C	0.683046	-4.506562	-0.126042
C	-0.359717	-4.412357	2.043075
C	0.177923	-5.156494	0.995801
H	2.058815	3.044518	-0.543202
H	-2.411254	2.839843	-0.315
H	2.661859	-1.708021	0.809443
H	-2.454999	-2.007903	0.794636
H	4.642307	-0.337096	0.2895
H	-4.572816	-0.821827	0.473818
H	-0.802253	-2.436764	2.783693
H	1.098866	-5.077941	-0.947427
H	-0.753613	-4.912717	2.91992
H	0.202927	-6.238351	1.05444
H	4.34846	3.098571	-0.716249
H	-4.847441	2.71035	-0.313249
H	-5.685853	1.224816	0.008226
H	1.048715	-2.614267	-1.076417
O	0.346201	-0.386489	2.981471
H	0.567917	0.533469	2.800407

RDA-C9-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.27
O	-0.10653	1.81551	-0.000788	Zero-point Energy Correction	0.309072
N	4.557623	2.164254	-0.451819	Thermal Correction to Energy	0.328008
N	-4.817829	1.739568	-0.092221	Thermal Correction to Enthalpy	0.328952
C	0.048939	-0.90288	0.706266	Thermal Correction to Free Energy	0.262184
C	1.233663	-0.144454	0.451396		
C	-1.208838	-0.281222	0.47426		
C	1.108174	1.22997	0.069875		
C	-1.251759	1.093335	0.150395		
C	3.483049	1.442223	-0.160484		
C	-3.648745	1.098428	0.083316		
C	0.123307	-2.381822	0.856048		
C	2.190908	2.010799	-0.224986		
C	-2.42723	1.7828	-0.039531		
C	2.556331	-0.688115	0.52131		
C	-2.454794	-0.95178	0.571419		
C	3.640667	0.066431	0.227366		
C	-3.636546	-0.293524	0.384089		
C	0.631876	-3.130251	-0.208389		

C	-0.362704	-3.030355	1.991737
C	0.655227	-4.519118	-0.133802
C	-0.328147	-4.418628	2.06432
C	0.178937	-5.164688	1.003333
H	2.055608	3.046104	-0.513903
H	-2.399829	2.836942	-0.288772
H	2.67875	-1.716999	0.835086
H	-2.467188	-2.011868	0.792848
H	4.642591	-0.342499	0.28542
H	-4.580788	-0.820447	0.458358
H	-0.75527	-2.44534	2.814421
H	1.048161	-5.094084	-0.964376
H	-0.698722	-4.917563	2.952422
H	0.2029	-6.246855	1.063259
H	5.482888	1.756304	-0.40621
H	4.477802	3.13679	-0.721179
H	-4.842752	2.722229	-0.321002
H	-5.6939	1.244232	-0.017306
H	1.000251	-2.626087	-1.096111
O	0.634196	-0.328853	2.643726
H	0.244298	0.559655	2.712412

RDA-C9-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.160493	-2.333437	-0.038641	Zero-point Energy Correction	-993.253
N	-4.85224	-2.156321	-0.280056	Thermal Correction to Energy	0.30919
N	4.514898	-2.881972	-0.306867	Thermal Correction to Enthalpy	0.328171
C	0.051181	0.466132	0.156388	Thermal Correction to Free Energy	0.329115
C	-1.225455	-0.168908	0.069196		0.262359
C	1.212505	-0.347533	0.013579		
C	-1.287189	-1.593182	-0.041446		
C	1.070138	-1.750259	-0.056904		
C	-3.680092	-1.536635	-0.160098		
C	3.441751	-2.075078	-0.203906		
C	0.165233	1.943665	0.004279		
C	-2.474357	-2.268774	-0.147041		
C	2.142639	-2.607788	-0.158392		
C	-2.465356	0.54449	0.069266		
C	2.532577	0.164431	-0.048034		
C	-3.647685	-0.105375	-0.043937		
C	3.61393	-0.663028	-0.152899		
C	-0.240635	2.510518	-1.206116		
C	0.722461	2.748389	0.997525		
C	-0.087824	3.8761	-1.420284		
C	0.865786	4.114294	0.779734		

C	0.463693	4.679551	-0.427215
H	-2.479788	-3.348324	-0.233075
H	1.974493	-3.676568	-0.213319
H	-2.441165	1.620877	0.181673
H	2.681003	1.236944	-0.019759
H	-4.586241	0.435828	-0.037037
H	4.616845	-0.25571	-0.204312
H	1.023601	2.302434	1.936865
H	-0.401449	4.309761	-2.362509
H	1.290701	4.738471	1.557092
H	0.578206	5.744491	-0.592731
H	-5.716546	-1.632322	-0.292074
H	-4.909945	-3.162714	-0.355513
H	4.410685	-3.883039	-0.368484
H	5.446254	-2.499412	-0.36193
H	-0.667899	1.88142	-1.980447
O	-0.498121	0.382019	2.15243
H	-0.228259	-0.518805	2.401534

RDA-H2A-C1'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.127739	1.851511	-0.176182	Zero-point Energy Correction	0.323889
N	4.621737	2.277713	-0.314716	Thermal Correction to Energy	0.343042
N	-4.774482	1.8871	0.409618	Thermal Correction to Enthalpy	0.343986
C	-0.013717	-0.909205	0.355425	Thermal Correction to Free Energy	0.27611
C	1.184804	-0.13191	0.233058		
C	-1.245889	-0.276395	0.094067		
C	1.074891	1.232738	-0.079311		
C	-1.273683	1.179687	0.029442		
C	3.424529	1.459695	-0.115571		
C	-3.64424	1.220038	0.317835		
C	0.052588	-2.35418	0.64821		
C	2.189451	2.042857	-0.26987		
C	-2.418435	1.90275	0.114504		
C	2.48134	-0.664717	0.411469		
C	-2.529157	-0.928872	0.320632		
C	3.597022	0.119714	0.23484		
C	-3.666755	-0.222204	0.419223		
C	0.711765	-3.211403	-0.239827		
C	-0.541453	-2.868155	1.804755		
C	0.763432	-4.574282	0.025422		
C	-0.464715	-4.229557	2.074451		
C	0.181809	-5.082928	1.184234		
H	2.068218	3.091007	-0.515586		
H	-2.394184	2.982289	0.035152		

H	2.597765	-1.702409	0.69327
H	-2.549888	-2.009754	0.372948
H	4.593049	-0.284256	0.368407
H	-4.623387	-0.709261	0.566537
H	-1.045129	-2.198767	2.493466
H	1.260432	-5.237992	-0.671807
H	-0.913787	-4.623277	2.978242
H	0.232164	-6.145011	1.393164
H	5.144213	1.966096	-1.143386
H	4.391715	3.269452	-0.442897
H	-4.79262	2.896736	0.330157
H	-5.651488	1.401229	0.553435
H	1.164465	-2.807732	-1.139084
H	5.255482	2.202513	0.490758
O	-1.14635	-0.483367	-1.886398
H	-1.17303	-1.453545	-1.938274

#### RDA-H2A-C1-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.692
O	-0.117232	1.801249	-0.038273	Zero-point Energy Correction	0.323508
N	4.552883	2.192409	-0.274855	Thermal Correction to Energy	0.342884
N	-4.887354	1.839743	0.046684	Thermal Correction to Enthalpy	0.343828
C	0.039331	-0.952117	0.437364	Thermal Correction to Free Energy	0.275052
C	1.181101	-0.203134	0.277323		
C	-1.241667	-0.291201	0.34362		
C	1.087201	1.20789	0.027903		
C	-1.260073	1.089611	0.114039		
C	3.466333	1.455577	-0.092396		
C	-3.619979	1.112884	0.146096		
C	0.099307	-2.405171	0.71221		
C	2.178522	2.018373	-0.152254		
C	-2.445772	1.812702	0.015503		
C	2.519401	-0.737937	0.434939		
C	-2.478628	-0.959343	0.448805		
C	3.619233	0.048153	0.170532		
C	-3.664364	-0.266161	0.35655		
C	0.661795	-3.273971	-0.226217		
C	-0.408791	-2.907383	1.913688		
C	0.710363	-4.638567	0.036078		
C	-0.338463	-4.270143	2.177529		
C	0.215519	-5.136558	1.238226		
H	2.044499	3.076987	-0.335304		
H	-2.420697	2.881202	-0.162315		
H	2.645836	-1.806013	0.537189		
H	-2.496524	-2.030862	0.59714		

H	4.618321	-0.369753	0.207884
H	-4.617101	-0.774846	0.43759
H	-0.84374	-2.229025	2.639605
H	1.137027	-5.311064	-0.698412
H	-0.720443	-4.655086	3.11538
H	0.260474	-6.199673	1.443166
H	5.473327	1.775435	-0.2253
H	4.480442	3.182203	-0.472358
H	-4.736592	2.848865	-0.059474
H	-5.435239	1.515581	-0.760081
H	1.047312	-2.879147	-1.159799
O	2.749927	-0.381762	2.454911
H	3.634377	-0.759154	2.599347
H	-5.461814	1.6917	0.885791

RDA-H2A-C11-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.682
O	-0.163192	1.708127	-0.248466	Zero-point Energy Correction	0.323791
N	4.585219	2.06007	-0.306829	Thermal Correction to Energy	0.342776
N	-4.816298	1.974857	0.226326	Thermal Correction to Enthalpy	0.34372
C	-0.149428	-1.028992	0.337433	Thermal Correction to Free Energy	0.276711
C	1.090182	-0.291781	0.208006		
C	-1.338394	-0.323882	0.337003		
C	1.01942	1.071437	-0.114358		
C	-1.322511	1.08654	0.040446		
C	3.373237	1.258857	-0.127274		
C	-3.696621	1.264908	0.259762		
C	-0.089492	-2.514075	0.513052		
C	2.153007	1.857231	-0.313019		
C	-2.449748	1.85887	-0.013264		
C	2.375941	-0.833966	0.433796		
C	-2.638709	-0.891151	0.605626		
C	3.509201	-0.072141	0.268289		
C	-3.757587	-0.136453	0.583664		
C	0.87767	-3.277098	-0.225394		
C	-0.536698	-3.04368	1.765272		
C	1.216716	-4.553152	0.174106		
C	-0.171964	-4.312758	2.152413		
C	0.690337	-5.079378	1.355506		
H	2.050267	2.899744	-0.589329		
H	-2.375803	2.909622	-0.263555		
H	2.483139	-1.856716	0.767127		
H	-2.712924	-1.941002	0.839513		
H	4.492786	-0.49116	0.442716		
H	-4.725739	-0.570998	0.803174		

H	-1.157016	-2.43217	2.408858
H	1.901055	-5.138938	-0.426474
H	-0.536555	-4.712269	3.090774
H	0.967655	-6.077716	1.671774
H	5.330598	1.509274	-0.749344
H	4.408718	2.884632	-0.892067
H	-4.80057	2.958995	-0.006715
H	-5.708365	1.538476	0.416811
H	1.280071	-2.855916	-1.138693
O	-1.465646	-2.988884	-0.784998
H	-1.370608	-3.954572	-0.784796
H	4.945548	2.392088	0.597565

RDA-H2A-C12-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.692
O	-0.108499	1.80876	-0.078273	Zero-point Energy Correction	0.323027
N	4.637966	2.259968	-0.275738	Thermal Correction to Energy	0.34262
N	-4.800522	1.771671	0.077783	Thermal Correction to Enthalpy	0.343564
C	0.009651	-0.939723	0.426015	Thermal Correction to Free Energy	0.274303
C	1.216396	-0.172484	0.249293		
C	-1.20871	-0.298533	0.346905		
C	1.096761	1.200556	-0.006313		
C	-1.252283	1.116238	0.091968		
C	3.444344	1.43276	-0.090508		
C	-3.641577	1.131907	0.152097		
C	0.095443	-2.389481	0.702058		
C	2.208428	2.021783	-0.186898		
C	-2.420943	1.820269	0.001046		
C	2.514169	-0.717189	0.355644		
C	-2.476469	-0.970646	0.464455		
C	3.624793	0.075167	0.185017		
C	-3.639482	-0.291475	0.376867		
C	0.657353	-3.25746	-0.216825		
C	-0.351319	-2.878746	1.960805		
C	0.715483	-4.627226	0.062102		
C	-0.331893	-4.271893	2.198897		
C	0.21783	-5.131429	1.264073		
H	2.081749	3.079012	-0.386757		
H	-2.40381	2.885739	-0.190739		
H	2.636038	-1.767285	0.584817		
H	-2.488507	-2.04293	0.613681		
H	4.623746	-0.334969	0.267963		
H	-4.592995	-0.799157	0.460669		
H	-0.94212	-2.234023	2.599411		
H	1.142651	-5.300211	-0.671473		

H	-0.72919	-4.649108	3.133571
H	0.253112	-6.196102	1.459389
H	5.17395	1.952262	-1.096905
H	4.402143	3.249908	-0.406584
H	-4.834276	2.768198	-0.092324
H	-5.673627	1.271686	0.179831
H	1.031097	-2.878174	-1.161221
O	1.3349	-2.368432	3.004645
H	1.068912	-2.799398	3.832934
H	5.261668	2.190166	0.538191

RDA-H2A-C13-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.114269	1.816689	-0.118075	Zero-point Energy Correction	0.323154
N	4.634242	2.257295	-0.316051	Thermal Correction to Energy	0.342611
N	-4.805211	1.792528	0.043977	Thermal Correction to Enthalpy	0.343555
C	0.000841	-0.920115	0.450471	Thermal Correction to Free Energy	0.274586
C	1.207818	-0.155584	0.263421		
C	-1.217066	-0.281954	0.349379		
C	1.090466	1.210159	-0.027958		
C	-1.258549	1.128497	0.067541		
C	3.438702	1.437839	-0.110113		
C	-3.648007	1.150771	0.128861		
C	0.092644	-2.367387	0.75172		
C	2.203615	2.025366	-0.226143		
C	-2.425625	1.833221	-0.035167		
C	2.504517	-0.697708	0.391627		
C	-2.487051	-0.94862	0.477061		
C	3.616868	0.088433	0.203786		
C	-3.64856	-0.268333	0.377262		
C	0.660541	-3.242528	-0.19347		
C	-0.381126	-2.858741	1.953334		
C	0.71551	-4.610638	0.057702		
C	-0.234171	-4.234628	2.259891		
C	0.250007	-5.113243	1.261202		
H	2.078677	3.077206	-0.453524		
H	-2.405931	2.895054	-0.246019		
H	2.626293	-1.740816	0.652727		
H	-2.500571	-2.017352	0.646305		
H	4.615105	-0.319829	0.303336		
H	-4.603027	-0.772821	0.469019		
H	-0.820396	-2.190047	2.684819		
H	1.115762	-5.277981	-0.695291		
H	-0.75891	-4.638436	3.115321		
H	0.283642	-6.177113	1.464171		

H	5.160114	1.937698	-1.139287
H	4.401826	3.246857	-0.455528
H	-4.836057	2.786026	-0.143388
H	-5.679649	1.297007	0.155471
H	1.029424	-2.845332	-1.132756
O	1.482781	-4.079246	3.342716
H	1.660076	-5.03231	3.388025
H	5.265744	2.193102	0.492207

RDA-H2A-C14-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.10789	1.792889	-0.101865	Zero-point Energy Correction	0.323094
N	4.642373	2.211916	-0.284003	Thermal Correction to Energy	0.342626
N	-4.799597	1.792818	0.032857	Thermal Correction to Enthalpy	0.34357
C	-0.009395	-0.94457	0.465263	Thermal Correction to Free Energy	0.274337
C	1.203186	-0.186867	0.281966		
C	-1.223966	-0.29955	0.360098		
C	1.093273	1.179962	-0.007877		
C	-1.256649	1.110772	0.077252		
C	3.442808	1.397397	-0.081932		
C	-3.646319	1.145092	0.123749		
C	0.071135	-2.390426	0.766988		
C	2.210741	1.990278	-0.201582		
C	-2.419501	1.821353	-0.032228		
C	2.497228	-0.734521	0.414876		
C	-2.497962	-0.960335	0.478111		
C	3.6136	0.046995	0.231739		
C	-3.655428	-0.27446	0.370648		
C	0.648772	-3.263699	-0.163885		
C	-0.444363	-2.880133	1.980226		
C	0.719823	-4.614908	0.115255		
C	-0.35402	-4.222561	2.273018		
C	0.288498	-5.107312	1.371052		
H	2.090583	3.042694	-0.428764		
H	-2.392901	2.883094	-0.24274		
H	2.613764	-1.778472	0.674509		
H	-2.519245	-2.02941	0.645003		
H	4.609582	-0.365926	0.334651		
H	-4.612884	-0.774537	0.455209		
H	-0.906545	-2.192876	2.679628		
H	1.140164	-5.301097	-0.610231		
H	-0.742933	-4.605646	3.208316		
H	0.190217	-6.174793	1.51658		
H	5.16714	1.893071	-1.108254		
H	4.414454	3.203029	-0.419856		

H	-4.82411	2.78682	-0.15295
H	-5.677372	1.301624	0.137408
H	1.014647	-2.877027	-1.108239
O	2.123739	-5.126923	2.274599
H	2.594019	-5.548997	1.537927
H	5.27322	2.141761	0.524268

RDA-H2A-C2-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.695
O	-0.092202	1.80695	-0.072277	Zero-point Energy Correction	0.323343
N	4.568096	2.199191	-0.406874	Thermal Correction to Energy	0.342833
N	-4.855929	1.834102	0.107205	Thermal Correction to Enthalpy	0.343777
C	0.079522	-0.94184	0.447249	Thermal Correction to Free Energy	0.274536
C	1.227019	-0.188222	0.258433		
C	-1.19931	-0.283108	0.377194		
C	1.117968	1.221669	-0.022585		
C	-1.22629	1.094994	0.120928		
C	3.488464	1.477866	-0.171329		
C	-3.585458	1.112823	0.198054		
C	0.148215	-2.395001	0.708644		
C	2.198022	2.030902	-0.247367		
C	-2.416264	1.812584	0.03164		
C	2.548783	-0.720254	0.353845		
C	-2.435517	-0.951939	0.513933		
C	3.651549	0.087898	0.22025		
C	-3.623153	-0.263199	0.432999		
C	0.730681	-3.247893	-0.233428		
C	-0.370548	-2.917628	1.897346		
C	0.786142	-4.615088	0.011673		
C	-0.29096	-4.28248	2.145103		
C	0.281207	-5.132282	1.201413		
H	2.056083	3.078863	-0.479058		
H	-2.398283	2.877479	-0.167382		
H	2.686799	-1.767442	0.587709		
H	-2.450254	-2.021187	0.676305		
H	4.645887	-0.338179	0.183181		
H	-4.573077	-0.772395	0.539204		
H	-0.818319	-2.252702	2.627678		
H	1.226599	-5.274661	-0.726308		
H	-0.679791	-4.68219	3.073868		
H	0.332614	-6.197484	1.393531		
H	5.489648	1.78725	-0.33287		
H	4.495312	3.178255	-0.653517		
H	-4.709723	2.843516	-0.003385		
H	-5.408597	1.505167	-0.6946		

H	1.123269	-2.83888	-1.15781
O	3.835148	0.58812	2.264503
H	3.937126	-0.32193	2.589744
H	-5.4234	1.685821	0.951087

RDA-H2A-C3-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.686
O	-0.095309	1.802448	0.013649	Zero-point Energy Correction	0.324195
N	4.553554	2.100166	-0.5636	Thermal Correction to Energy	0.343181
N	-4.863323	1.825334	0.064822	Thermal Correction to Enthalpy	0.344126
C	0.071309	-0.95355	0.471831	Thermal Correction to Free Energy	0.276532
C	1.219111	-0.197712	0.311719		
C	-1.207123	-0.293445	0.389371		
C	1.10095	1.20339	0.077188		
C	-1.234556	1.089628	0.158011		
C	3.524608	1.468663	-0.006454		
C	-3.592646	1.107637	0.175298		
C	0.132706	-2.411874	0.714814		
C	2.200672	2.034329	-0.076062		
C	-2.422165	1.810739	0.049917		
C	2.56837	-0.736887	0.408832		
C	-2.446089	-0.963771	0.489364		
C	3.653377	0.035482	0.260103		
C	-3.630789	-0.273329	0.389783		
C	0.714084	-3.255697	-0.235262		
C	-0.39296	-2.946934	1.894399		
C	0.761885	-4.6263	-0.00744		
C	-0.323744	-4.315787	2.124649		
C	0.24831	-5.156454	1.17306		
H	2.066658	3.077932	-0.330276		
H	-2.397067	2.878705	-0.131147		
H	2.683794	-1.79268	0.614023		
H	-2.464154	-2.035141	0.636532		
H	4.655722	-0.370085	0.328621		
H	-4.582435	-0.785091	0.465329		
H	-0.8413	-2.289082	2.630941		
H	1.202865	-5.278626	-0.751566		
H	-0.720241	-4.725254	3.045938		
H	0.292994	-6.224335	1.351537		
H	5.481033	1.7083	-0.466566		
H	4.478785	3.084632	-0.784872		
H	-4.718726	2.833705	-0.056797		
H	-5.408856	1.485242	-0.737197		
H	1.114801	-2.836985	-1.151906		
O	3.273431	2.235415	1.736157		

H	2.814929	1.575428	2.280849
H	-5.437438	1.686532	0.905981

RDA-H2A-C4'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.099322	1.765388	-0.16157	Zero-point Energy Correction	-993.692
N	4.572813	2.168264	-0.311893	Thermal Correction to Energy	0.324164
N	-4.868394	1.829422	0.077483	Thermal Correction to Enthalpy	0.343138
C	0.067543	-0.959884	0.473856	Thermal Correction to Free Energy	0.344082
C	1.205743	-0.211357	0.316795		0.276718
C	-1.216451	-0.292978	0.403187		
C	1.08852	1.21531	0.104252		
C	-1.243109	1.070434	0.089458		
C	3.500941	1.433587	-0.08885		
C	-3.600406	1.104241	0.183403		
C	0.131454	-2.421895	0.703613		
C	2.21056	2.012789	-0.175123		
C	-2.427663	1.788422	-0.029751		
C	2.546175	-0.731584	0.436706		
C	-2.451309	-0.947786	0.581022		
C	3.637467	0.040142	0.248134		
C	-3.639115	-0.256667	0.482961		
C	0.68055	-3.257766	-0.271505		
C	-0.348443	-2.965392	1.898476		
C	0.740942	-4.630175	-0.054362		
C	-0.268948	-4.335799	2.116354		
C	0.270243	-5.169442	1.139361		
H	2.076787	3.053095	-0.445994		
H	-2.406248	2.843342	-0.276013		
H	2.669537	-1.77648	0.691801		
H	-2.470171	-2.008239	0.793298		
H	4.636974	-0.366049	0.345231		
H	-4.589022	-0.756479	0.628237		
H	-0.768641	-2.31341	2.656489		
H	1.158858	-5.275999	-0.817312		
H	-0.630315	-4.752089	3.049033		
H	0.323494	-6.238332	1.309292		
H	5.497688	1.756977	-0.263391		
H	4.4931	3.151659	-0.543273		
H	-4.717429	2.836462	-0.047246		
H	-5.419774	1.491957	-0.721418		
H	1.04861	-2.831177	-1.19812		
O	1.450223	1.885935	1.969289		
H	1.135336	2.802561	1.899		
H	-5.43918	1.696609	0.92139		

## RDA-H2A-C4-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.080703	1.807793	-0.044331	Zero-point Energy Correction	-993.698 0.323627
N	4.57374	2.184347	-0.416244	Thermal Correction to Energy	0.343046
N	-4.846631	1.848579	0.081688	Thermal Correction to Enthalpy	0.343991
C	0.08149	-0.938441	0.460177	Thermal Correction to Free Energy	0.275196
C	1.229229	-0.1865	0.271741		
C	-1.195641	-0.276971	0.387735		
C	1.114606	1.212989	0.013565		
C	-1.21996	1.10162	0.134756		
C	3.509366	1.450181	-0.16295		
C	-3.577579	1.126868	0.185768		
C	0.14569	-2.391917	0.720453		
C	2.216277	2.042304	-0.135927		
C	-2.40662	1.824351	0.033066		
C	2.568223	-0.719511	0.354871		
C	-2.435351	-0.943211	0.51134		
C	3.655014	0.052217	0.14146		
C	-3.619019	-0.250765	0.418655		
C	0.735197	-3.244992	-0.216971		
C	-0.38485	-2.914056	1.90413		
C	0.78515	-4.61244	0.027463		
C	-0.310376	-4.279235	2.151587		
C	0.268416	-5.129364	1.212325		
H	2.077896	3.074199	-0.432033		
H	-2.382289	2.889341	-0.16475		
H	2.694144	-1.764891	0.603879		
H	-2.454789	-2.012804	0.670559		
H	4.655591	-0.359293	0.196845		
H	-4.571347	-0.757929	0.512996		
H	-0.837618	-2.248661	2.630952		
H	1.230895	-5.272478	-0.706889		
H	-0.708401	-4.67886	3.076466		
H	0.315855	-6.194815	1.404068		
H	5.498514	1.771829	-0.404713		
H	4.48845	3.173152	-0.617867		
H	-4.699441	2.857444	-0.032906		
H	-5.393388	1.515498	-0.722553		
H	1.137208	-2.836215	-1.137394		
O	2.376407	2.530542	1.999776		
H	1.585245	3.092379	1.966539		
H	-5.420559	1.704711	0.92207		

RDA-H2A-C5'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.688
O	-0.108273	1.792373	-0.171462	Zero-point Energy Correction	0.323156
N	4.643153	2.245985	-0.313557	Thermal Correction to Energy	0.342454
N	-4.793357	1.771989	0.059175	Thermal Correction to Enthalpy	0.343398
C	0.006831	-0.950774	0.450662	Thermal Correction to Free Energy	0.275134
C	1.209232	-0.184149	0.289125		
C	-1.208213	-0.297426	0.37344		
C	1.083092	1.227334	0.117547		
C	-1.252229	1.1104	0.066214		
C	3.445435	1.438751	-0.081548		
C	-3.641962	1.128766	0.143645		
C	0.093923	-2.406907	0.708776		
C	2.217504	2.032538	-0.155945		
C	-2.416479	1.808853	-0.048176		
C	2.501092	-0.718586	0.387384		
C	-2.478676	-0.961096	0.523423		
C	3.613534	0.078541	0.205116		
C	-3.641892	-0.285185	0.422357		
C	0.64882	-3.254083	-0.254264		
C	-0.373375	-2.93331	1.915414		
C	0.720509	-4.621333	-0.014153		
C	-0.282465	-4.299834	2.156018		
C	0.259226	-5.144633	1.191228		
H	2.084036	3.083689	-0.385269		
H	-2.401325	2.865484	-0.284293		
H	2.631931	-1.77093	0.60091		
H	-2.489695	-2.025925	0.71465		
H	4.610901	-0.339051	0.273598		
H	-4.595553	-0.786711	0.535388		
H	-0.795963	-2.270584	2.662597		
H	1.139029	-5.276947	-0.76835		
H	-0.638018	-4.703139	3.096583		
H	0.32261	-6.210074	1.378441		
H	5.188859	1.875476	-1.101793		
H	4.410694	3.223665	-0.522627		
H	-4.822247	2.762585	-0.147584		
H	-5.669476	1.283725	0.19467		
H	1.009232	-2.841939	-1.190425		
O	1.081775	1.603752	2.120513		
H	1.309486	2.548923	2.103089		
H	5.254944	2.239139	0.512802		

RDA-H2A-C5-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.699
------	---	---	---	------------------------	----------

O	-0.147563	1.809068	-0.156986	Zero-point Energy Correction	0.322415
N	4.587636	2.302827	-0.347642	Thermal Correction to Energy	0.342259
N	-4.835689	1.762426	0.061359	Thermal Correction to Enthalpy	0.343204
C	-0.01104	-0.933823	0.400805	Thermal Correction to Free Energy	0.273014
C	1.1896	-0.160224	0.195384		
C	-1.232962	-0.296669	0.319999		
C	1.060739	1.207513	-0.08657		
C	-1.285605	1.113593	0.042313		
C	3.408954	1.44936	-0.194645		
C	-3.674334	1.125724	0.131989		
C	0.085996	-2.379627	0.699444		
C	2.165551	2.030382	-0.295522		
C	-2.457012	1.813817	-0.04383		
C	2.490792	-0.694622	0.296681		
C	-2.498783	-0.968606	0.459593		
C	3.597657	0.099264	0.099935		
C	-3.665019	-0.293591	0.375662		
C	0.670683	-3.248298	-0.22717		
C	-0.41043	-2.878659	1.906624		
C	0.742527	-4.608228	0.049457		
C	-0.31563	-4.237369	2.185813		
C	0.254858	-5.102949	1.256761		
H	2.031742	3.08295	-0.515269		
H	-2.444326	2.876121	-0.252893		
H	2.621935	-1.739366	0.54444		
H	-2.506117	-2.038139	0.623181		
H	4.598978	-0.305045	0.183339		
H	-4.615717	-0.803632	0.475479		
H	-0.856709	-2.199902	2.624982		
H	1.182265	-5.280844	-0.677131		
H	-0.691493	-4.618645	3.127634		
H	0.320207	-6.162732	1.473193		
H	5.411447	1.756882	-0.624466		
H	4.436099	3.03266	-1.054161		
H	-4.873392	2.756111	-0.123388		
H	-5.706313	1.26218	0.180833		
H	1.051905	-2.85828	-1.164554		
O	3.092727	2.611669	2.299359		
H	2.140122	2.578434	2.507758		
H	4.8075	2.77341	0.540814		

RDA-H2A-C6-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.139049	1.80327	-0.059822	Zero-point Energy Correction	0.323126
N	4.596458	2.206838	-0.474994	Thermal Correction to Energy	0.342419

N	-4.828017	1.749226	0.081946	Thermal Correction to Enthalpy	0.343363
C	-0.012459	-0.954921	0.437383	Thermal Correction to Free Energy	0.275057
C	1.189684	-0.181451	0.264944		
C	-1.232127	-0.312374	0.354346		
C	1.069253	1.196294	0.0131		
C	-1.279962	1.105602	0.104034		
C	3.435921	1.440608	-0.022833		
C	-3.669348	1.1132	0.157423		
C	0.075797	-2.409161	0.701472		
C	2.171114	2.012252	-0.178591		
C	-2.449057	1.805891	0.012614		
C	2.492606	-0.732892	0.35604		
C	-2.49951	-0.987831	0.463764		
C	3.600705	0.048922	0.185454		
C	-3.664047	-0.311921	0.375248		
C	0.651315	-3.258297	-0.248147		
C	-0.421688	-2.934269	1.896659		
C	0.714781	-4.6252	-0.005508		
C	-0.337162	-4.300466	2.141206		
C	0.225599	-5.146584	1.189866		
H	2.04922	3.066228	-0.398597		
H	-2.434834	2.872139	-0.175037		
H	2.611274	-1.787251	0.564907		
H	-2.507869	-2.060086	0.607699		
H	4.600808	-0.361983	0.250739		
H	-4.616548	-0.822724	0.451419		
H	-0.862713	-2.270615	2.632233		
H	1.148406	-5.282376	-0.749704		
H	-0.715255	-4.702609	3.073394		
H	0.283386	-6.21193	1.379393		
H	5.442211	1.899166	0.01951		
H	4.469577	3.208352	-0.286536		
H	-4.864224	2.746614	-0.084857		
H	-5.700521	1.246625	0.180139		
H	1.03302	-2.847926	-1.176663		
O	3.800053	2.097782	1.869088		
H	3.140127	1.593772	2.375812		
H	4.746439	2.08235	-1.483957		

RDA-H2A-C7-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.117001	1.799161	-0.108319	Zero-point Energy Correction	-993.691
N	4.618703	2.286596	-0.287435	Thermal Correction to Energy	0.323412
N	-4.806038	1.779629	0.097286	Thermal Correction to Enthalpy	0.342755
C	-0.001286	-0.947816	0.426632	Thermal Correction to Free Energy	0.343699
					0.275226

C	1.203455	-0.173943	0.237191
C	-1.219277	-0.305192	0.346335
C	1.079276	1.196771	-0.040206
C	-1.264726	1.107351	0.082218
C	3.422973	1.46535	-0.152347
C	-3.651639	1.13343	0.164552
C	0.092654	-2.39599	0.711602
C	2.191842	2.031712	-0.248692
C	-2.427505	1.816802	-0.002146
C	2.497338	-0.709215	0.337349
C	-2.489424	-0.970954	0.474876
C	3.624805	0.106895	0.204428
C	-3.651379	-0.287913	0.393908
C	0.686391	-3.255147	-0.218302
C	-0.414669	-2.90673	1.90934
C	0.756822	-4.617524	0.045995
C	-0.321357	-4.267966	2.176075
C	0.258463	-5.124038	1.243996
H	2.046975	3.083512	-0.464628
H	-2.407263	2.880773	-0.201847
H	2.636634	-1.758862	0.558601
H	-2.503498	-2.042009	0.627754
H	4.605793	-0.335221	0.084764
H	-4.605559	-0.792991	0.485341
H	-0.86741	-2.235065	2.630264
H	1.203435	-5.282878	-0.683055
H	-0.705491	-4.658589	3.110669
H	0.322822	-6.185774	1.450894
H	5.262572	1.895378	-0.986824
H	4.398101	3.251249	-0.560467
H	-4.835103	2.775548	-0.078124
H	-5.681506	1.285589	0.209277
H	1.075161	-2.856101	-1.148814
O	4.007118	0.51601	2.158825
H	4.270334	-0.384414	2.410556
H	5.1218	2.31449	0.611412

RDA-H2A-C8'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.684
O	-0.093716	1.858879	0.033192	Zero-point Energy Correction	0.323505
N	4.625663	2.212248	-0.531887	Thermal Correction to Energy	0.342745
N	-4.778476	1.787755	0.094876	Thermal Correction to Enthalpy	0.343689
C	0.008468	-0.913508	0.527896	Thermal Correction to Free Energy	0.275592
C	1.225257	-0.088479	0.562426		
C	-1.193313	-0.282215	0.357298		

C	1.106795	1.261237	0.102237
C	-1.238526	1.148826	0.171982
C	3.44267	1.430469	-0.180455
C	-3.628885	1.143825	0.160856
C	0.111832	-2.369222	0.761021
C	2.210494	2.036459	-0.22536
C	-2.401832	1.849285	0.089554
C	2.540418	-0.67189	0.503542
C	-2.465635	-0.968835	0.361051
C	3.628649	0.082485	0.172614
C	-3.628627	-0.293348	0.277981
C	0.769899	-3.185223	-0.163947
C	-0.455935	-2.930064	1.908192
C	0.845757	-4.555432	0.054469
C	-0.35904	-4.299523	2.12923
C	0.286598	-5.11265	1.202172
H	2.083057	3.071777	-0.51797
H	-2.389016	2.923119	-0.048965
H	2.661753	-1.70896	0.784995
H	-2.471015	-2.048331	0.437036
H	4.624585	-0.343284	0.170382
H	-4.582502	-0.807116	0.288215
H	-0.95949	-2.290217	2.624429
H	1.343219	-5.187241	-0.671536
H	-0.791705	-4.729938	3.024339
H	0.354536	-6.180498	1.373383
H	5.118482	1.791665	-1.330798
H	4.385331	3.178486	-0.781714
H	-4.807408	2.795166	-0.00134
H	-5.656133	1.284281	0.132173
H	1.204702	-2.747307	-1.05583
H	5.289543	2.244923	0.252852
O	1.065644	0.28982	2.419834
H	1.979743	0.545025	2.627858

RDA-H2A-C8-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.126429	1.800858	-0.077202	Zero-point Energy Correction	0.323016
N	4.617567	2.269483	-0.247582	Thermal Correction to Energy	0.342518
N	-4.819952	1.791273	0.072445	Thermal Correction to Enthalpy	0.343462
C	-0.019607	-0.949765	0.420084	Thermal Correction to Free Energy	0.274327
C	1.17929	-0.181049	0.251376		
C	-1.238846	-0.302977	0.330731		
C	1.070235	1.186192	0.009211		
C	-1.275985	1.112375	0.08368		

C	3.432071	1.429742	-0.071478
C	-3.664051	1.143567	0.140936
C	0.067166	-2.399235	0.705607
C	2.190195	2.01229	-0.157272
C	-2.439698	1.825018	-0.006014
C	2.491185	-0.723791	0.428535
C	-2.508939	-0.967742	0.441731
C	3.614616	0.076822	0.191633
C	-3.668749	-0.280545	0.355256
C	0.643871	-3.263757	-0.229237
C	-0.427881	-2.902611	1.911327
C	0.710419	-4.625886	0.038355
C	-0.339204	-4.263762	2.180695
C	0.224094	-5.125899	1.243987
H	2.059765	3.070627	-0.350913
H	-2.41462	2.891757	-0.18958
H	2.618094	-1.795052	0.487302
H	-2.525721	-2.040105	0.585545
H	4.610586	-0.345881	0.246901
H	-4.624958	-0.784196	0.433605
H	-0.867861	-2.225714	2.635366
H	1.144167	-5.295934	-0.694195
H	-0.714181	-4.649739	3.12094
H	0.284672	-6.187431	1.453097
H	5.311626	1.808409	-0.848649
H	4.382185	3.172694	-0.674554
H	-4.847699	2.788977	-0.090926
H	-5.695794	1.296131	0.173403
H	1.023691	-2.868781	-1.165278
O	2.567032	-0.557504	2.471236
H	3.477507	-0.868967	2.610179
H	5.070886	2.458027	0.655646

RDA-H2A-C9-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.69
O	-0.08675	1.78336	-0.127366	Zero-point Energy Correction	0.324338
N	4.656312	2.171408	-0.508894	Thermal Correction to Energy	0.343296
N	-4.777745	1.736558	-0.042326	Thermal Correction to Enthalpy	0.34424
C	0.039998	-0.905512	0.716202	Thermal Correction to Free Energy	0.276803
C	1.245657	-0.154684	0.405997		
C	-1.198442	-0.272379	0.512476		
C	1.12185	1.1743	-0.009316		
C	-1.233343	1.108547	0.103218		
C	3.468945	1.382215	-0.177303		
C	-3.625309	1.111372	0.116896		

C	0.128345	-2.383443	0.8725
C	2.229502	1.960023	-0.315158
C	-2.399802	1.789134	-0.084306
C	2.53961	-0.685935	0.554272
C	-2.461011	-0.940925	0.665678
C	3.652289	0.072745	0.26303
C	-3.625394	-0.284128	0.483094
C	0.69302	-3.103435	-0.187051
C	-0.377165	-3.067966	1.979251
C	0.747256	-4.491098	-0.13751
C	-0.305256	-4.456191	2.027981
C	0.253725	-5.170151	0.972675
H	2.100069	2.984738	-0.642161
H	-2.386148	2.826411	-0.394658
H	2.662301	-1.699871	0.911621
H	-2.466468	-1.989039	0.933651
H	4.651161	-0.33041	0.376095
H	-4.578559	-0.785887	0.599452
H	-0.816109	-2.518904	2.800928
H	1.179172	-5.038848	-0.96642
H	-0.690079	-4.978664	2.895632
H	0.304326	-6.251768	1.014619
H	5.100336	1.819386	-1.366725
H	4.429186	3.161225	-0.655601
H	-4.807605	2.713986	-0.306452
H	-5.654424	1.248152	0.093081
H	1.076357	-2.578867	-1.055207
O	-0.273245	-0.300867	2.755563
H	-0.150339	0.663616	2.701327
H	5.355727	2.115146	0.241172

RDA-HA-C1-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.264
O	-0.123713	1.803698	-0.036676	Zero-point Energy Correction	0.307901
N	4.560639	2.224219	-0.226145	Thermal Correction to Energy	0.3274
N	-4.835095	1.805565	0.048331	Thermal Correction to Enthalpy	0.328345
C	0.005473	-0.943448	0.429096	Thermal Correction to Free Energy	0.259752
C	1.1746	-0.192018	0.269948		
C	-1.243441	-0.297183	0.337776		
C	1.080729	1.201621	0.037577		
C	-1.277689	1.101628	0.107008		
C	3.463893	1.474433	-0.060856		
C	-3.670545	1.144561	0.131403		
C	0.077956	-2.39829	0.705408		
C	2.1798	2.025826	-0.123286		

C	-2.446194	1.820423	0.008153
C	2.50186	-0.725912	0.428182
C	-2.501507	-0.957521	0.434709
C	3.610894	0.071068	0.181154
C	-3.672008	-0.268867	0.339193
C	0.630117	-3.266816	-0.239277
C	-0.407773	-2.90212	1.914685
C	0.687691	-4.63118	0.023188
C	-0.330526	-4.265119	2.178904
C	0.212158	-5.130762	1.23285
H	2.036295	3.085222	-0.295723
H	-2.412637	2.888645	-0.167117
H	2.632566	-1.796633	0.491416
H	-2.522175	-2.030347	0.578462
H	4.607271	-0.353647	0.218798
H	-4.624358	-0.780922	0.411017
H	-0.833783	-2.224146	2.646155
H	1.10612	-5.302804	-0.716952
H	-0.698345	-4.650224	3.12246
H	0.26409	-6.193579	1.437895
H	5.47943	1.808341	-0.176421
H	4.485733	3.212699	-0.419275
H	-4.854416	2.800984	-0.117449
H	-5.712149	1.312154	0.124599
H	1.001711	-2.872376	-1.178769
O	2.747784	-0.474909	2.445069
H	3.654325	-0.806009	2.556637

RDA-HA-C11-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.255
O	-0.157534	1.71836	-0.2165	Zero-point Energy Correction	0.308489
N	4.532557	2.024524	-0.316614	Thermal Correction to Energy	0.32754
N	-4.826905	1.991423	0.249335	Thermal Correction to Enthalpy	0.328484
C	-0.11419	-1.021495	0.328182	Thermal Correction to Free Energy	0.261966
C	1.091962	-0.299787	0.20214		
C	-1.335078	-0.31629	0.326616		
C	1.033269	1.090282	-0.095741		
C	-1.319787	1.079435	0.05288		
C	3.419282	1.30097	-0.135829		
C	-3.697371	1.26938	0.271774		
C	-0.064714	-2.508515	0.508562		
C	2.148345	1.873396	-0.287892		
C	-2.453164	1.859311	0.009431		
C	2.403519	-0.833033	0.404377		
C	-2.622268	-0.882123	0.587958		

C	3.519231	-0.072549	0.246689
C	-3.752263	-0.126217	0.574057
C	0.905317	-3.283504	-0.212337
C	-0.538731	-3.034174	1.752655
C	1.229998	-4.561036	0.196615
C	-0.189679	-4.30434	2.149925
C	0.680819	-5.080095	1.37015
H	2.033431	2.921617	-0.534794
H	-2.371537	2.914131	-0.221968
H	2.519097	-1.858274	0.728547
H	-2.70055	-1.935695	0.804904
H	4.503028	-0.492469	0.420886
H	-4.716562	-0.572889	0.786496
H	-1.166542	-2.417446	2.383759
H	1.919311	-5.153531	-0.391695
H	-0.572866	-4.69856	3.083169
H	0.944908	-6.079717	1.693718
H	5.442281	1.605812	-0.190637
H	4.479964	2.998975	-0.575046
H	-4.80806	2.974118	0.019175
H	-5.719092	1.552601	0.422519
H	1.32284	-2.869604	-1.121979
O	-1.422381	-2.981075	-0.817432
H	-1.319218	-3.945787	-0.822547

RDA-HA-C12-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.265
O	-0.102626	1.817225	-0.05459	Zero-point Energy Correction	0.307468
N	4.583232	2.228228	-0.263469	Thermal Correction to Energy	0.327219
N	-4.810953	1.790622	0.078819	Thermal Correction to Enthalpy	0.328163
C	0.042845	-0.927204	0.428362	Thermal Correction to Free Energy	0.258782
C	1.217408	-0.177825	0.25349		
C	-1.205436	-0.285433	0.35587		
C	1.111128	1.218465	0.006355		
C	-1.24814	1.112665	0.110131		
C	3.490012	1.471995	-0.095941		
C	-3.642116	1.139377	0.158288		
C	0.11574	-2.38078	0.698595		
C	2.204768	2.032801	-0.171741		
C	-2.423308	1.821564	0.01606		
C	2.537478	-0.712678	0.344968		
C	-2.46042	-0.95308	0.471		
C	3.632596	0.074627	0.174654		
C	-3.634644	-0.273202	0.381461		
C	0.655518	-3.253938	-0.228137		

C	-0.326897	-2.870424	1.958991
C	0.701397	-4.625382	0.046064
C	-0.324491	-4.264913	2.191748
C	0.207667	-5.128209	1.250269
H	2.068803	3.090892	-0.358677
H	-2.399436	2.887862	-0.172031
H	2.663409	-1.765188	0.563902
H	-2.475406	-2.025392	0.623128
H	4.631629	-0.338502	0.248894
H	-4.58356	-0.789236	0.467618
H	-0.903927	-2.220884	2.605056
H	1.115114	-5.300916	-0.692978
H	-0.719777	-4.640636	3.128008
H	0.23117	-6.193952	1.441656
H	5.503953	1.819046	-0.201596
H	4.504493	3.217338	-0.449799
H	-4.839049	2.784332	-0.096753
H	-5.683885	1.291875	0.168373
H	1.02352	-2.875864	-1.175178
O	1.377902	-2.390216	2.992333
H	1.159446	-2.89782	3.79042

RDA-HA-C13-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.264
O	-0.107286	1.823153	-0.097119	Zero-point Energy Correction	0.307587
N	4.581193	2.220753	-0.299562	Thermal Correction to Energy	0.327176
N	-4.813978	1.813505	0.043541	Thermal Correction to Enthalpy	0.32812
C	0.031941	-0.909467	0.453309	Thermal Correction to Free Energy	0.259169
C	1.207896	-0.163597	0.26868		
C	-1.214541	-0.269341	0.359498		
C	1.105496	1.224697	-0.016095		
C	-1.253774	1.124617	0.084572		
C	3.485274	1.471456	-0.115303		
C	-3.647716	1.159848	0.135064		
C	0.11021	-2.361977	0.745748		
C	2.201663	2.032225	-0.211749		
C	-2.426624	1.834883	-0.022556		
C	2.525919	-0.69746	0.383539		
C	-2.472471	-0.929885	0.489148		
C	3.623966	0.082477	0.196477		
C	-3.644306	-0.248005	0.386458		
C	0.650568	-3.240546	-0.210825		
C	-0.34901	-2.854545	1.952623		
C	0.698566	-4.610984	0.035233		
C	-0.211483	-4.232717	2.252702		

C	0.248904	-5.113452	1.243997
H	2.068344	3.08526	-0.42699
H	-2.399472	2.897109	-0.232065
H	2.650313	-1.743245	0.635847
H	-2.489623	-1.997871	0.665449
H	4.621738	-0.329961	0.28945
H	-4.594809	-0.759052	0.48407
H	-0.770352	-2.184735	2.693708
H	1.081076	-5.279097	-0.726361
H	-0.726372	-4.634358	3.115141
H	0.276131	-6.178187	1.443541
H	5.500677	1.811802	-0.221021
H	4.505565	3.204766	-0.511862
H	-4.838494	2.803937	-0.150298
H	-5.68866	1.320376	0.146164
H	1.007161	-2.843638	-1.154906
O	1.523941	-4.098186	3.313777
H	1.698472	-5.052311	3.340836

RDA-HA-C14-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.264
O	-0.100522	1.799308	-0.07744	Zero-point Energy Correction	0.307618
N	4.58905	2.17694	-0.267609	Thermal Correction to Energy	0.327222
N	-4.807925	1.811726	0.037605	Thermal Correction to Enthalpy	0.328166
C	0.023682	-0.935317	0.46417	Thermal Correction to Free Energy	0.259227
C	1.204576	-0.195806	0.283263		
C	-1.220044	-0.288556	0.368048		
C	1.108959	1.194649	0.004106		
C	-1.251258	1.105792	0.096259		
C	3.490009	1.431616	-0.08843		
C	-3.645262	1.152167	0.132921		
C	0.09122	-2.385666	0.75898		
C	2.208887	1.997998	-0.185945		
C	-2.420199	1.821904	-0.015141		
C	2.520504	-0.735217	0.400551		
C	-2.48154	-0.944204	0.486314		
C	3.622002	0.040892	0.219093		
C	-3.649684	-0.256759	0.378515		
C	0.644049	-3.264314	-0.180783		
C	-0.412114	-2.873499	1.978365		
C	0.708447	-4.61689	0.096208		
C	-0.330523	-4.216793	2.268858		
C	0.290923	-5.107067	1.357188		
H	2.08029	3.052244	-0.398081		
H	-2.386632	2.884599	-0.221275		

H	2.640407	-1.78234	0.648855
H	-2.505918	-2.013106	0.656778
H	4.617794	-0.376094	0.313101
H	-4.60298	-0.764149	0.467571
H	-0.859008	-2.183238	2.684803
H	1.113337	-5.305832	-0.63555
H	-0.709451	-4.597292	3.209398
H	0.185031	-6.173749	1.503128
H	5.50682	1.764018	-0.189185
H	4.517714	3.161678	-0.478262
H	-4.826566	2.803114	-0.151967
H	-5.685579	1.32227	0.132233
H	0.999594	-2.879516	-1.129745
O	2.139992	-5.146332	2.239639
H	2.600983	-5.554011	1.48935

RDA-HA-C2-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.27
O	-0.092227	1.811705	-0.078014	Zero-point Energy Correction	0.30786
N	4.583609	2.218572	-0.369329	Thermal Correction to Energy	0.327394
N	-4.7906	1.795551	0.131518	Thermal Correction to Enthalpy	0.328338
C	0.047204	-0.937838	0.427001	Thermal Correction to Free Energy	0.259453
C	1.228916	-0.180683	0.242985		
C	-1.192415	-0.293457	0.359438		
C	1.121577	1.216111	-0.024857		
C	-1.23581	1.108652	0.109209		
C	3.495483	1.479844	-0.156682		
C	-3.627971	1.140552	0.193728		
C	0.128587	-2.393363	0.691818		
C	2.207494	2.031201	-0.233947		
C	-2.406666	1.819653	0.031188		
C	2.532441	-0.712174	0.334672		
C	-2.452569	-0.956698	0.489396		
C	3.64713	0.092396	0.199443		
C	-3.623633	-0.273864	0.415932		
C	0.692819	-3.248054	-0.259181		
C	-0.360816	-2.914944	1.892217		
C	0.755696	-4.614897	-0.012823		
C	-0.276987	-4.280302	2.141059		
C	0.275832	-5.13158	1.18797		
H	2.063919	3.081945	-0.4529		
H	-2.383524	2.885331	-0.160166		
H	2.668686	-1.763086	0.555429		
H	-2.467486	-2.028238	0.641145		
H	4.637703	-0.342317	0.171103		

H	-4.573973	-0.785262	0.512682
H	-0.794054	-2.248402	2.629821
H	1.182168	-5.275265	-0.758435
H	-0.647451	-4.678291	3.078184
H	0.332729	-6.196427	1.380752
H	5.50431	1.809062	-0.295903
H	4.507391	3.202489	-0.586236
H	-4.816486	2.790508	-0.040612
H	-5.665227	1.30225	0.239061
H	1.067708	-2.841147	-1.191875
O	3.905028	0.613724	2.313558
H	3.678935	-0.269994	2.646044

RDA-HA-C3-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.106819	1.807843	-0.022018	Zero-point Energy Correction	-993.262
N	4.567709	2.1267	-0.526391	Thermal Correction to Energy	0.308309
N	-4.809239	1.779204	0.085691	Thermal Correction to Enthalpy	0.327473
C	0.033603	-0.94279	0.450567	Thermal Correction to Free Energy	0.328418
C	1.213587	-0.182675	0.286649		0.260824
C	-1.207203	-0.298389	0.369349		
C	1.09968	1.199731	0.045169		
C	-1.25181	1.108204	0.129496		
C	3.514486	1.467931	-0.018497		
C	-3.643011	1.133578	0.165965		
C	0.109307	-2.401947	0.701781		
C	2.198973	2.023379	-0.13001		
C	-2.423638	1.817639	0.03229		
C	2.545567	-0.729208	0.38533		
C	-2.467133	-0.966321	0.472574		
C	3.640356	0.042062	0.232078		
C	-3.636707	-0.284486	0.38021		
C	0.674016	-3.247914	-0.256275		
C	-0.388266	-2.934629	1.893507		
C	0.72933	-4.617798	-0.025635		
C	-0.313529	-4.303531	2.126409		
C	0.24	-5.146232	1.166323		
H	2.067864	3.073043	-0.360854		
H	-2.398734	2.884833	-0.149572		
H	2.658034	-1.785697	0.590004		
H	-2.482427	-2.038636	0.617343		
H	4.639401	-0.371624	0.301029		
H	-4.587593	-0.798743	0.455339		
H	-0.822764	-2.274696	2.636377		
H	1.156767	-5.271447	-0.776593		

H	-0.691872	-4.71076	3.056383
H	0.290144	-6.213596	1.346607
H	5.491347	1.757347	-0.343785
H	4.497337	3.128565	-0.647192
H	-4.840083	2.775193	-0.080244
H	-5.681804	1.278417	0.17485
H	1.056579	-2.831827	-1.181935
O	3.371714	2.173118	1.849167
H	2.770989	1.583383	2.329729

RDA-HA-C4'-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.262
O	-0.100433	1.770445	-0.160152	Zero-point Energy Correction	0.308597
N	4.582986	2.194152	-0.265016	Thermal Correction to Energy	0.327655
N	-4.81126	1.797978	0.079895	Thermal Correction to Enthalpy	0.328599
C	0.04493	-0.953029	0.466214	Thermal Correction to Free Energy	0.261413
C	1.206384	-0.206115	0.305972		
C	-1.21107	-0.29676	0.40673		
C	1.087646	1.216981	0.132822		
C	-1.253498	1.082315	0.093935		
C	3.508872	1.441213	-0.059191		
C	-3.645982	1.134171	0.170798		
C	0.116109	-2.417232	0.694718		
C	2.217726	2.017601	-0.146043		
C	-2.422508	1.795233	-0.028686		
C	2.532126	-0.724322	0.411947		
C	-2.465813	-0.944502	0.569976		
C	3.637544	0.051706	0.244931		
C	-3.641299	-0.25975	0.466336		
C	0.646868	-3.25434	-0.289385		
C	-0.341228	-2.961903	1.897281		
C	0.709951	-4.627114	-0.074208		
C	-0.260898	-4.333144	2.113402		
C	0.259838	-5.167362	1.127292		
H	2.083012	3.062343	-0.399612		
H	-2.390804	2.849643	-0.274449		
H	2.658174	-1.776569	0.636104		
H	-2.487345	-2.006805	0.777271		
H	4.632311	-0.367791	0.331491		
H	-4.590045	-0.766607	0.597824		
H	-0.747761	-2.309441	2.662257		
H	1.113574	-5.272915	-0.844978		
H	-0.607539	-4.749246	3.051867		
H	0.314951	-6.236456	1.29557		
H	5.509054	1.788172	-0.227701		

H	4.495023	3.179848	-0.47583
H	-4.829985	2.781147	-0.146244
H	-5.687514	1.316863	0.215853
H	0.999294	-2.828651	-1.222535
O	1.366369	1.854279	1.97266
H	1.095054	2.783815	1.900733

RDA-HA-C4-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.086223	1.814787	-0.070222	Zero-point Energy Correction	-993.273
N	4.590299	2.211952	-0.367453	Thermal Correction to Energy	0.307811
N	-4.790932	1.814979	0.097545	Thermal Correction to Enthalpy	0.327364
C	0.049497	-0.928292	0.432427	Thermal Correction to Free Energy	0.328308
C	1.226378	-0.175049	0.242308		0.259387
C	-1.19397	-0.28107	0.36263		
C	1.115999	1.209319	-0.013009		
C	-1.234786	1.117641	0.108834		
C	3.510557	1.462055	-0.153205		
C	-3.626242	1.158942	0.172482		
C	0.125645	-2.383009	0.703296		
C	2.219458	2.03768	-0.173474		
C	-2.404389	1.833693	0.018061		
C	2.551306	-0.707368	0.330289		
C	-2.45439	-0.940228	0.487124		
C	3.649217	0.069361	0.137535		
C	-3.623956	-0.253526	0.401189		
C	0.695123	-3.242918	-0.239722		
C	-0.373792	-2.898381	1.902293		
C	0.753289	-4.608846	0.01295		
C	-0.294628	-4.262765	2.157728		
C	0.26347	-5.119274	1.212407		
H	2.079624	3.078473	-0.436656		
H	-2.374841	2.898596	-0.176708		
H	2.677261	-1.756365	0.565877		
H	-2.474123	-2.011101	0.642894		
H	4.646427	-0.349261	0.201738		
H	-4.575417	-0.763969	0.492899		
H	-0.81098	-2.2278	2.633887		
H	1.184175	-5.273362	-0.726401		
H	-0.672708	-4.655943	3.09384		
H	0.316768	-6.183374	1.410284		
H	5.514279	1.805306	-0.323647		
H	4.50505	3.19992	-0.5622		
H	-4.815205	2.8081	-0.082878		
H	-5.665983	1.321349	0.196109		

H	1.078083	-2.840727	-1.171221
O	2.393407	2.55634	2.087138
H	1.486824	2.905639	2.069002

RDA-HA-C9-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-993.262
O	-0.106624	1.819876	0.000997	Zero-point Energy Correction	0.308948
N	4.558271	2.162486	-0.455491	Thermal Correction to Energy	0.327951
N	-4.819444	1.737603	-0.082509	Thermal Correction to Enthalpy	0.328895
C	0.050195	-0.901676	0.707971	Thermal Correction to Free Energy	0.261974
C	1.234796	-0.143916	0.449441		
C	-1.208096	-0.280121	0.477687		
C	1.109893	1.23095	0.068775		
C	-1.253327	1.094283	0.153784		
C	3.4841	1.440538	-0.164725		
C	-3.649616	1.096738	0.089734		
C	0.124052	-2.380335	0.856669		
C	2.192347	2.010524	-0.227185		
C	-2.429315	1.782425	-0.034642		
C	2.557126	-0.689172	0.515358		
C	-2.453449	-0.9519	0.575297		
C	3.641625	0.064445	0.220434		
C	-3.636053	-0.294816	0.389412		
C	0.649924	-3.128102	-0.199705		
C	-0.380971	-3.030063	1.983441		
C	0.67204	-4.516979	-0.125655		
C	-0.347359	-4.418164	2.056079		
C	0.177418	-5.163385	1.003088		
H	2.05944	3.046079	-0.515134		
H	-2.404783	2.836304	-0.283766		
H	2.678962	-1.718609	0.826341		
H	-2.464657	-2.011836	0.795783		
H	4.643426	-0.344496	0.274932		
H	-4.57986	-0.821837	0.463779		
H	-0.788971	-2.445901	2.798825		
H	1.078283	-5.091037	-0.94987		
H	-0.732921	-4.917418	2.937066		
H	0.200449	-6.24518	1.062595		
H	5.48197	1.751448	-0.410554		
H	4.475247	3.135053	-0.722872		
H	-4.841789	2.718662	-0.316855		
H	-5.692896	1.23761	-0.012707		
H	1.032372	-2.62354	-1.080756		
O	0.634683	-0.324424	2.647892		
H	0.248086	0.566025	2.699247		

## RDA-HA-N17-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.119767	1.833037	-0.07543	Zero-point Energy Correction	-993.268
N	4.558098	2.21373	-0.319536	Thermal Correction to Energy	0.305377
N	-4.81099	1.768354	0.129849	Thermal Correction to Enthalpy	0.324559
C	0.037022	-0.923611	0.431379	Thermal Correction to Free Energy	0.325503
C	1.209094	-0.161421	0.246172		0.256557
C	-1.206331	-0.281107	0.360606		
C	1.097077	1.236892	-0.018302		
C	-1.258396	1.126865	0.10883		
C	3.47859	1.476252	-0.134807		
C	-3.649074	1.129928	0.19274		
C	0.120851	-2.380337	0.696203		
C	2.182336	2.043495	-0.213683		
C	-2.431447	1.824904	0.030314		
C	2.529605	-0.701934	0.344719		
C	-2.460594	-0.959659	0.491059		
C	3.624908	0.075663	0.160225		
C	-3.635515	-0.289315	0.416612		
C	0.676589	-3.233792	-0.260271		
C	-0.358654	-2.902101	1.900084		
C	0.74184	-4.600835	-0.015439		
C	-0.274501	-4.26797	2.14654		
C	0.270686	-5.118409	1.188394		
H	2.052543	3.100002	-0.414032		
H	-2.422032	2.890827	-0.160697		
H	2.64978	-1.750941	0.580821		
H	-2.463078	-2.030825	0.643778		
H	4.625361	-0.33282	0.238085		
H	-4.582898	-0.806175	0.512617		
H	-0.785997	-2.236131	2.641787		
H	1.162876	-5.260468	-0.764746		
H	-0.638342	-4.666804	3.085875		
H	0.328429	-6.183481	1.379601		
H	5.558322	1.771287	-0.257706		
H	4.478986	3.203937	-0.516365		
H	-4.848339	2.764483	-0.044334		
H	-5.682528	1.265537	0.235818		
H	1.044357	-2.825939	-1.195516		
O	6.772458	1.169805	-0.851825		
H	7.287559	1.704	-1.472607		

## RDA-N17-TS-H

Atom	X	Y	Z	Electronic Energy (EE)	-992.796
O	-0.086245	1.741384	-0.053291	Zero-point Energy Correction	0.294996
N	4.656126	2.029853	-0.236701	Thermal Correction to Energy	0.314112
N	-4.787069	1.812433	0.132614	Thermal Correction to Enthalpy	0.315056
C	0.006504	-1.014733	0.415446	Thermal Correction to Free Energy	0.246522
C	1.1999	-0.279155	0.257022		
C	-1.225032	-0.346178	0.343393		
C	1.119485	1.117423	0.010892		
C	-1.241103	1.059763	0.115223		
C	3.521982	1.333012	-0.076639		
C	-3.633785	1.135281	0.186502		
C	0.055998	-2.476595	0.657815		
C	2.231044	1.909248	-0.154885		
C	-2.401696	1.79302	0.041874		
C	2.508326	-0.840067	0.370396		
C	-2.496328	-0.988268	0.453033		
C	3.619215	-0.070766	0.210108		
C	-3.655281	-0.282628	0.382912		
C	0.611102	-3.326131	-0.302928		
C	-0.452023	-3.009622	1.845182		
C	0.646825	-4.697986	-0.079858		
C	-0.396381	-4.380589	2.071263		
C	0.147833	-5.226079	1.108162		
H	2.112665	2.971708	-0.334465		
H	-2.356974	2.861207	-0.130832		
H	2.607775	-1.893835	0.59637		
H	-2.531985	-2.061638	0.587121		
H	4.609256	-0.501859	0.300201		
H	-4.615102	-0.77902	0.464866		
H	-0.87812	-2.347877	2.591305		
H	1.067664	-5.353293	-0.833154		
H	-0.781528	-4.787366	2.998674		
H	0.18353	-6.294903	1.283256		
H	4.424895	3.002896	-0.434132		
H	-4.794809	2.810025	-0.023477		
H	-5.670231	1.331995	0.224671		
H	1.002534	-2.910262	-1.224859		
O	4.706396	2.967891	1.914698		
H	4.682611	2.042806	2.181177		

RDA-N17-TS-M

Atom	X	Y	Z	Electronic Energy (EE)	-993.274
O	-0.119767	1.833037	-0.07543	Zero-point Energy Correction	0.305385
N	4.558098	2.21373	-0.319536	Thermal Correction to Energy	0.324601
N	-4.81099	1.768354	0.129849	Thermal Correction to Enthalpy	0.325545

C	0.037022	-0.923611	0.431379	Thermal Correction to Free Energy	0.25652
C	1.209094	-0.161421	0.246172		
C	-1.206331	-0.281107	0.360606		
C	1.097077	1.236892	-0.018302		
C	-1.258396	1.126865	0.10883		
C	3.47859	1.476252	-0.134807		
C	-3.649074	1.129928	0.19274		
C	0.120851	-2.380337	0.696203		
C	2.182336	2.043495	-0.213683		
C	-2.431447	1.824904	0.030314		
C	2.529605	-0.701934	0.344719		
C	-2.460594	-0.959659	0.491059		
C	3.624908	0.075663	0.160225		
C	-3.635515	-0.289315	0.416612		
C	0.676589	-3.233792	-0.260271		
C	-0.358654	-2.902101	1.900084		
C	0.74184	-4.600835	-0.015439		
C	-0.274501	-4.26797	2.14654		
C	0.270686	-5.118409	1.188394		
H	2.052543	3.100002	-0.414032		
H	-2.422032	2.890827	-0.160697		
H	2.64978	-1.750941	0.580821		
H	-2.463078	-2.030825	0.643778		
H	4.625361	-0.33282	0.238085		
H	-4.582898	-0.806175	0.512617		
H	-0.785997	-2.236131	2.641787		
H	1.162876	-5.260468	-0.764746		
H	-0.638342	-4.666804	3.085875		
H	0.328429	-6.183481	1.379601		
H	5.558322	1.771287	-0.257706		
H	4.478986	3.203937	-0.516365		
H	-4.848339	2.764483	-0.044334		
H	-5.682528	1.265537	0.235818		
H	1.044357	-2.825939	-1.195516		
O	6.772458	1.169805	-0.851825		
H	7.287559	1.704	-1.472607		

RDA-N17-TS-P

Atom	X	Y	Z	Electronic Energy (EE)	
O	-0.050818	1.822742	0.013024	Zero-point Energy Correction	-993.251
N	4.653058	2.242476	-0.002521	Thermal Correction to Energy	0.304408
N	-4.752731	1.800848	0.012623	Thermal Correction to Enthalpy	0.323897
C	0.067934	-0.931515	0.474203	Thermal Correction to Free Energy	0.324841
C	1.260632	-0.168092	0.34147		0.255476
C	-1.1629	-0.284529	0.362768		

C	1.15506	1.21982	0.101779
C	-1.195454	1.125895	0.133391
C	3.535784	1.469983	0.062587
C	-3.589624	1.152994	0.111407
C	0.139892	-2.38964	0.725673
C	2.261576	2.034552	-0.055795
C	-2.365019	1.836813	0.016522
C	2.569846	-0.709449	0.466629
C	-2.4285	-0.953241	0.418373
C	3.674438	0.078832	0.333841
C	-3.592378	-0.26941	0.302248
C	0.722016	-3.23452	-0.223352
C	-0.375733	-2.923043	1.90992
C	0.775098	-4.603866	0.008044
C	-0.299605	-4.291135	2.144473
C	0.269886	-5.132248	1.192894
H	2.130225	3.091417	-0.254505
H	-2.333882	2.905792	-0.154576
H	2.684603	-1.763338	0.683458
H	-2.446566	-2.028145	0.541969
H	4.670148	-0.336441	0.429912
H	-4.54462	-0.785454	0.337004
H	-0.820816	-2.263963	2.647437
H	1.214376	-5.257422	-0.736214
H	-0.688038	-4.699237	3.069972
H	0.320689	-6.199361	1.374854
H	5.584646	1.76674	-0.331013
H	4.516863	3.185277	-0.358958
H	-4.785521	2.799762	-0.132324
H	-5.630619	1.305158	0.071679
H	1.117372	-2.818886	-1.143944
O	6.278082	1.151258	-1.33834
H	6.31948	1.7375	-2.1098

## References

- (1) Evans, M. G.; Polanyi, M. Some Applications of the Transition State Method to the Calculation of Reaction Velocities, Especially in Solution. *Trans. Faraday Soc.* **1935**, *31*, 875-894.
- (2) Eyring, H. The Activated Complex in Chemical Reactions. *J. Chem. Phys.* **1935**, *3*, 107-115.
- (3) Truhlar, D. G.; Hase, W. L.; Hynes, J. T. Current Status of Transition-State Theory. *J. Phys. Chem.* **1983**, *87*, 2664-2682.
- (4) Furuncuoglu, T.; Ugur, I.; Degirmenci, I.; Aviyente, V. Role of Chain Transfer Agents in Free Radical Polymerization Kinetics. *Macromolecules* **2010**, *43*, 1823-1835.
- (5) Vélez, E.; Quijano, J.; Notario, R.; Pabón, E.; Murillo, J.; Leal, J.; Zapata, E.; Alarcón, G. A Computational Study of Stereospecificity in the Thermal Elimination Reaction of Menthyl Benzoate in the Gas Phase. *J. Phys. Org. Chem.* **2009**, *22*, 971-977.
- (6) Pollak, E.; Pechukas, P. Symmetry Numbers, Not Statistical Factors, Should Be Used in Absolute Rate Theory and in Broensted Relations. *J. Am. Chem. Soc.* **1978**, *100*, 2984-2991.
- (7) Fernández-Ramos, A.; Ellingson, B. A.; Meana-Pañeda, R.; Marques, J. M.; Truhlar, D. G. Symmetry Numbers and Chemical Reaction Rates. *Theor. Chem. Acc.* **2007**, *118*, 813-826.
- (8) Eckart, C. The Penetration of a Potential Barrier by Electrons. *Phy. Rev.* **1930**, *35*, 1303.
- (9) Marcus, R. A. Chemical and Electrochemical Electron-Transfer Theory. *Annu. Rev. Phys. Chem.* **1964**, *15*, 155-196.
- (10) Marcus, R. A. Electron Transfer Reactions in Chemistry. Theory and Experiment. *Rev. Mod. Phys.* **1993**, *65*, 599.
- (11) Lu, Y.; Wang, A.; Shi, P.; Zhang, H. A Theoretical Study on the Antioxidant Activity of Piceatannol and Isorhapontigenin Scavenging Nitric Oxide and Nitrogen Dioxide Radicals. *PloS one* **2017**, *12*, e0169773.
- (12) Lu, Y.; Wang, A.; Shi, P.; Zhang, H.; Li, Z. Quantum Chemical Study on the Antioxidation Mechanism of Piceatannol and Isorhapontigenin toward Hydroxyl and Hydroperoxyl Radicals. *PloS one* **2015**, *10*, e0133259.
- (13) Nelsen, S. F.; Blackstock, S. C.; Kim, Y. Estimation of Inner Shell Marcus Terms for Amino Nitrogen Compounds by Molecular Orbital Calculations. *J. Am. Chem. Soc.* **1987**, *109*, 677-682.
- (14) Nelsen, S. F.; Weaver, M. N.; Luo, Y.; Pladziewicz, J. R.; Ausman, L. K.; Jentzsch, T. L.; O'Konek, J. J. Estimation of Electronic Coupling for Intermolecular Electron Transfer from Cross-Reaction Data. *J. Phys. Chem. A* **2006**, *110*, 11665-11676.
- (15) Galano, A.; Alvarez-Idaboy, J. R. A Computational Methodology for Accurate Predictions of Rate Constants in Solution: Application to the Assessment of Primary Antioxidant Activity. *J. Comput. Chem.* **2013**, *34*, 2430-2445.
- (16) Collins, F. C.; Kimball, G. E. Diffusion-Controlled Reaction Rates. *J. Colloid Sci.* **1949**, *4*, 425-437.
- (17) Von Smoluchowski, M. Mathematical Theory of the Kinetics of the Coagulation of Colloidal Solutions. *Z. Phys. Chem* **1917**, *92*, 129-68.
- (18) Truhlar, D. G. Nearly Encounter-Controlled Reactions: The Equivalence of the Steady-State and Diffusional Viewpoints. *J. Chem. Educ.* **1985**, *62*, 104.
- (19) Einstein, A. On the Motion of Small Particles Suspended in Liquids at Rest Required by the Molecular-Kinetic Theory of Heat. *Ann. Phys.* **1905**, *17*, 549-560.

(20) Stokes, G. G., *Mathematical and Physical Papers*. University Press: Cambridge, 1905.