

**Supporting Information  
for**

**Insights on Co-Catalyst Promoted Enamine Formation between Dimethylamine and Propanal through  
ab-initio and Density Functional Theory Study**

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Full citation for Ref.23

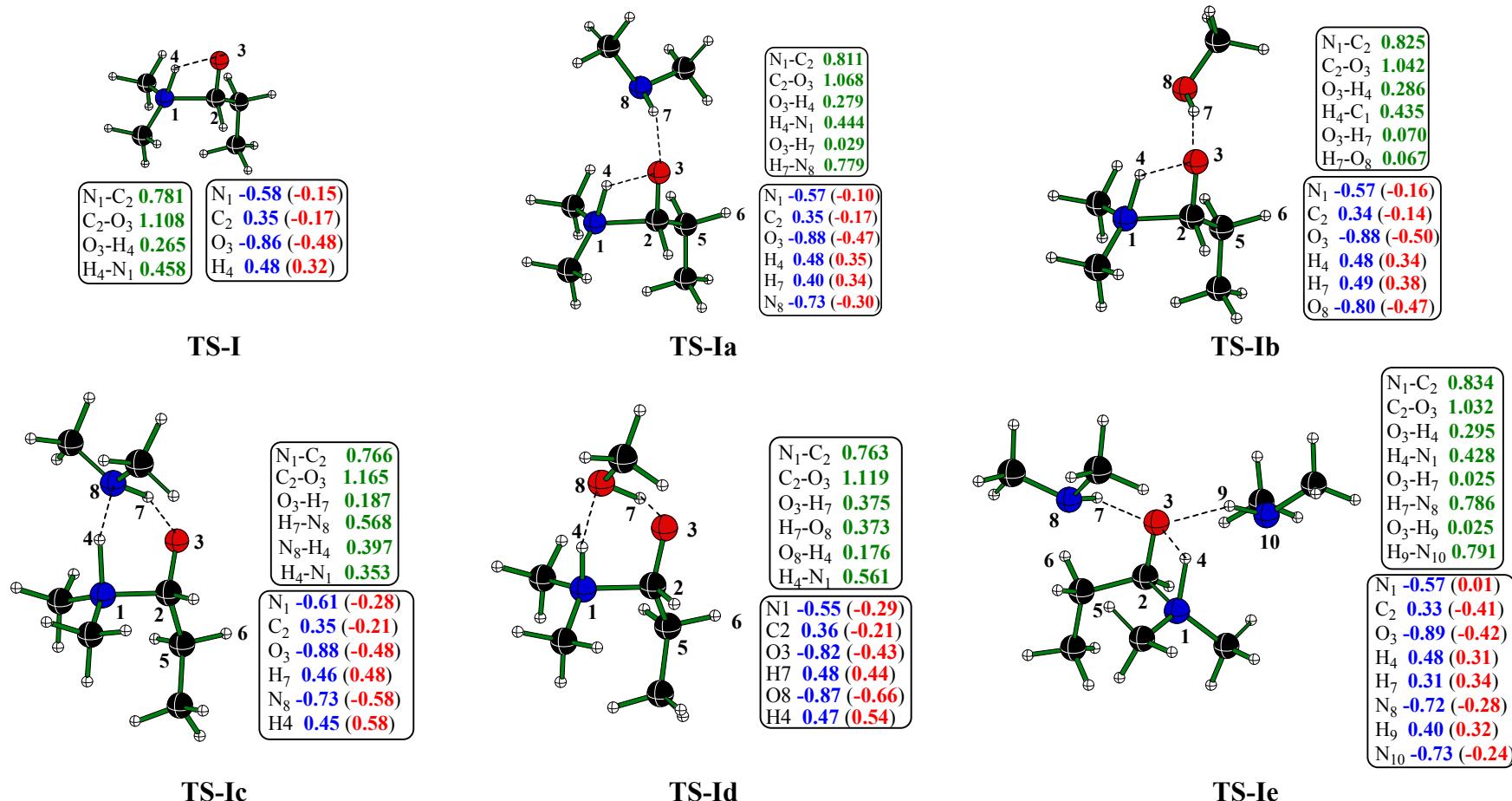
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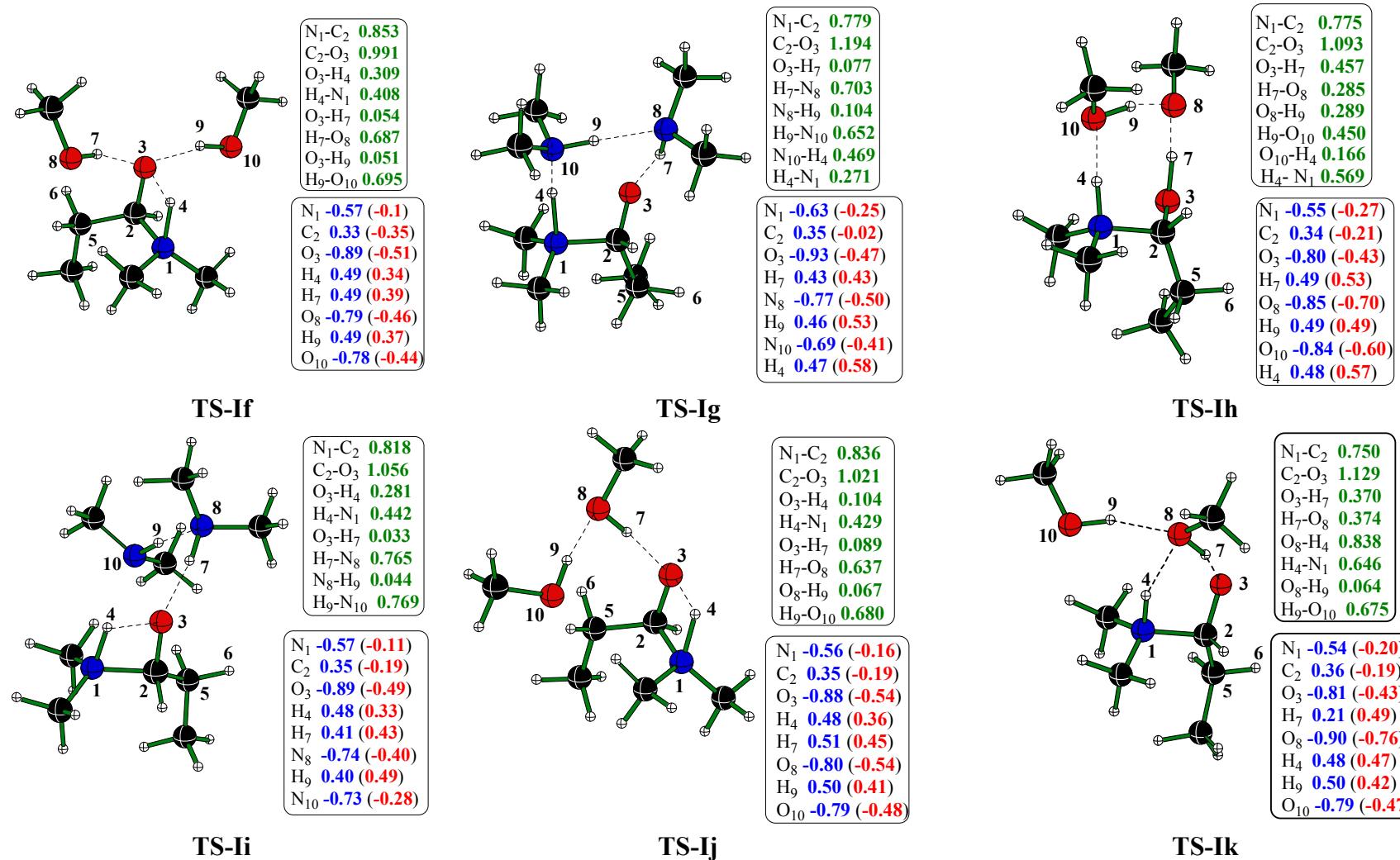
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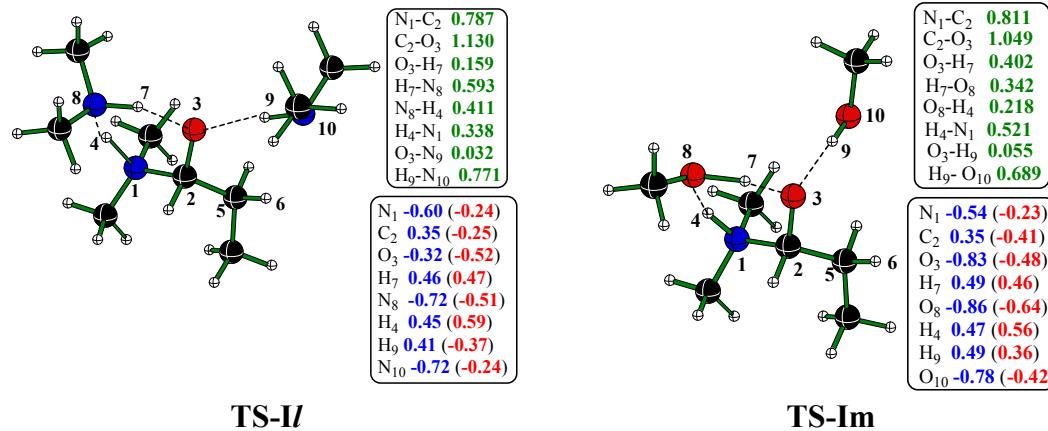
**Figure S1.** Bond Order (in green) for Representative Bonds, Natural (in blue) and Mulliken Charges (in red) for Selected Atoms for the Transition States in Step-I Computed at the mPW1PW91/6-311+G\*\* Level of Theory.



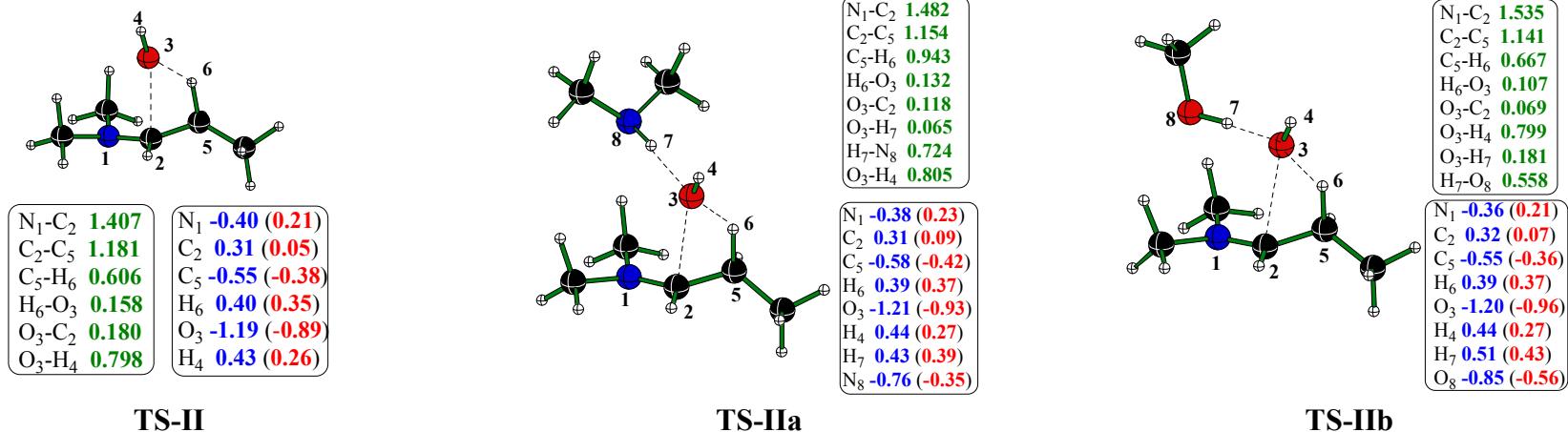
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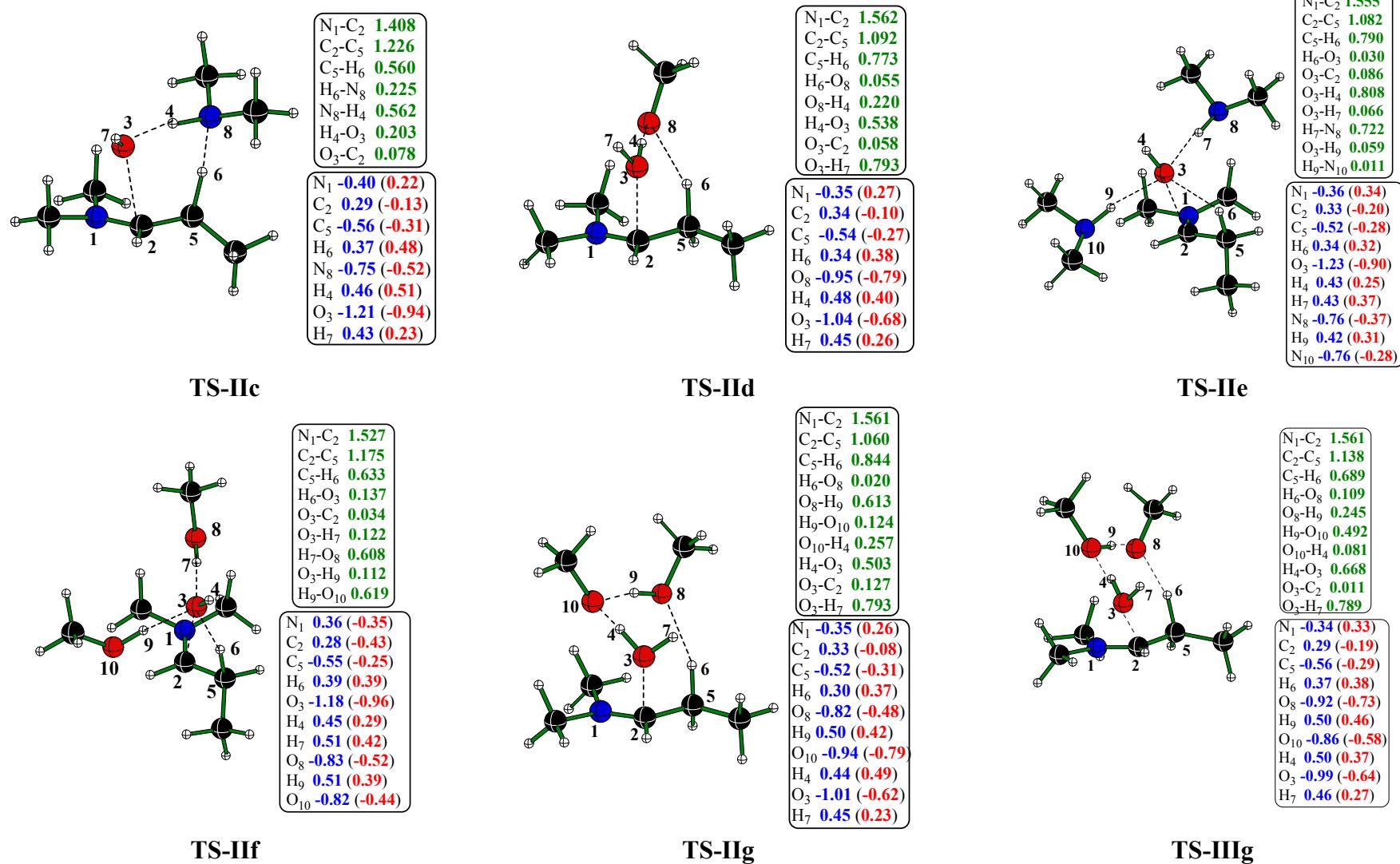
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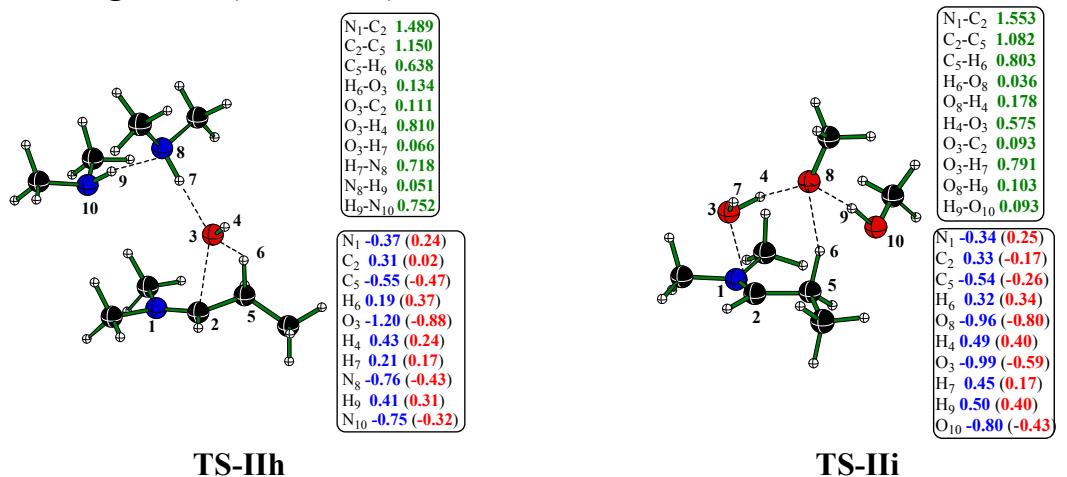
**Figure S2.** Bond Order (in green) for Representative Bonds, Natural (in blue) and Mulliken Charges (in red) for Selected Atoms for the Transition States in step-II Computed at the mPW1PW91/6-311+G\*\* Level of Theory.



**Figure S2.** (Continued..)



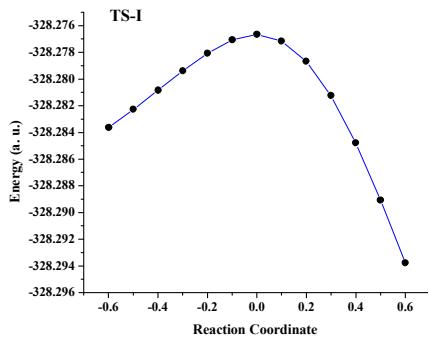
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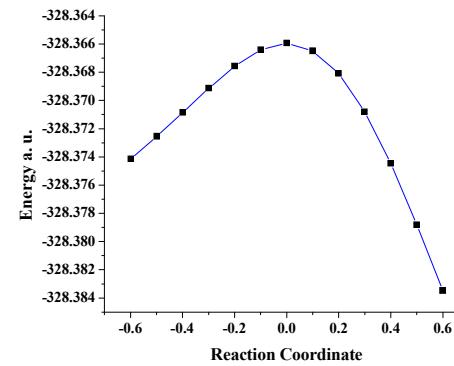
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**TS-I**

mPW1PW91/6-311+G\*\*



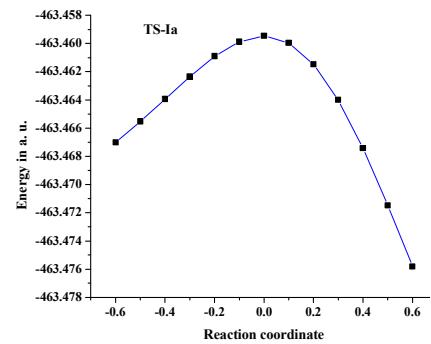
B3LYP/6-311+G\*\*



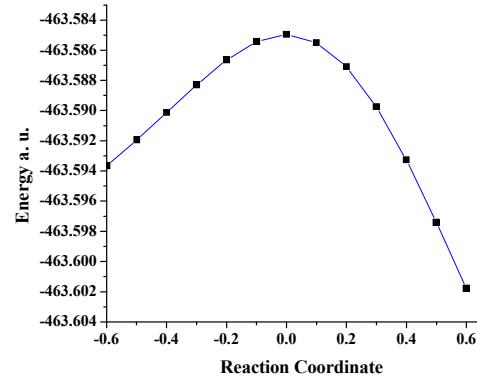
**Figure S3.** (Continued..)

**TS-Ia**

mPW1PW91/6-311+G\*\*

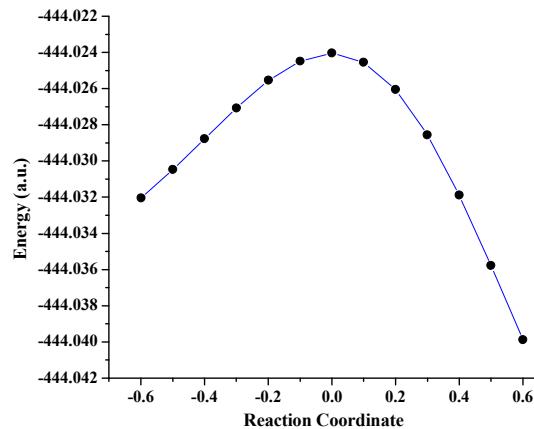


B3LYP/6-311+G\*\*

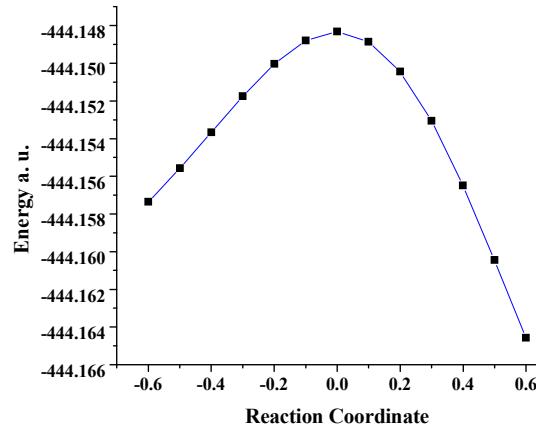


**TS-Ib**

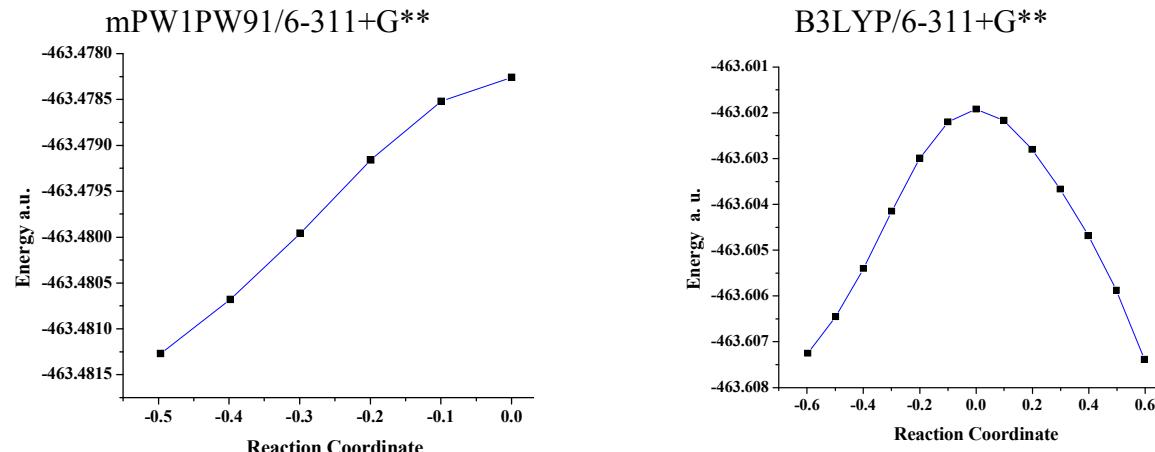
mPW1PW91/6-311+G\*\*



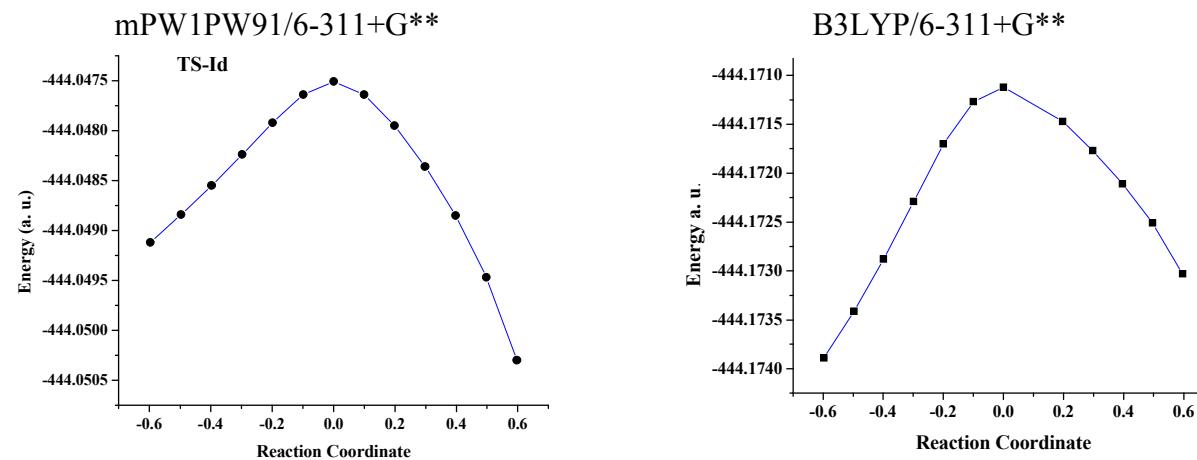
B3LYP/6-311+G\*\*



**Figure S3.** (Continued..)  
**TS-*Ic***



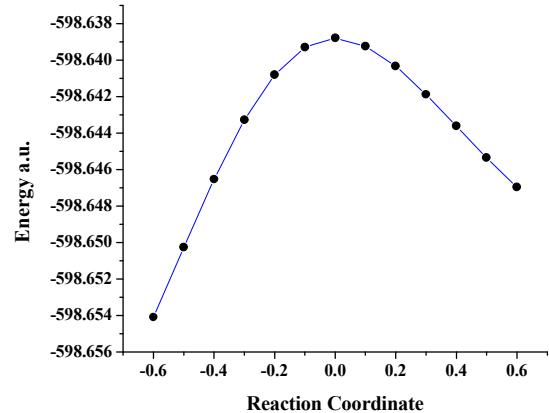
**TS-*Id***



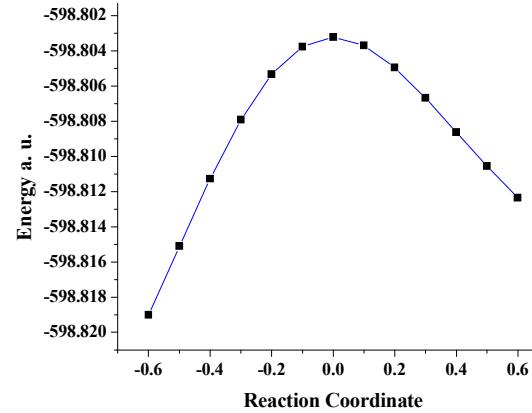
**Figure S3.** (Continued..)

**TS-Ie**

mPW1PW91/6-311+G\*\*

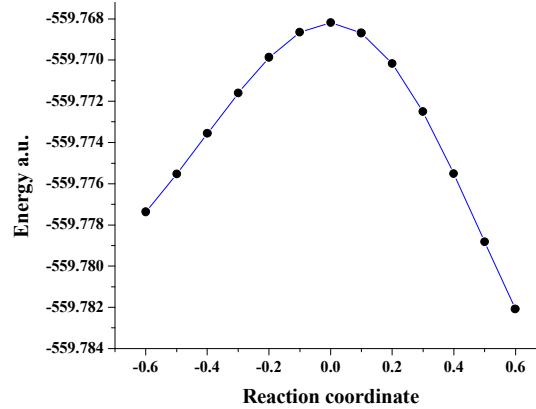


B3LYP/6-311+G\*\*

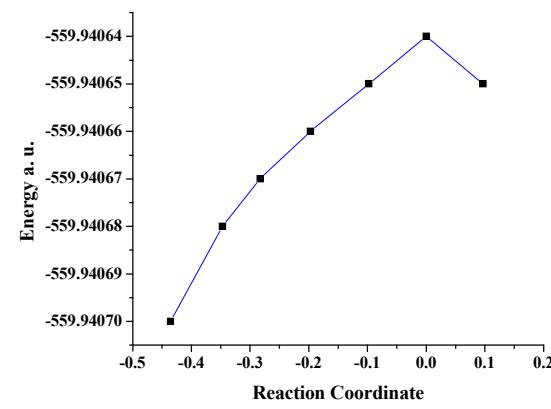


**TS-If**

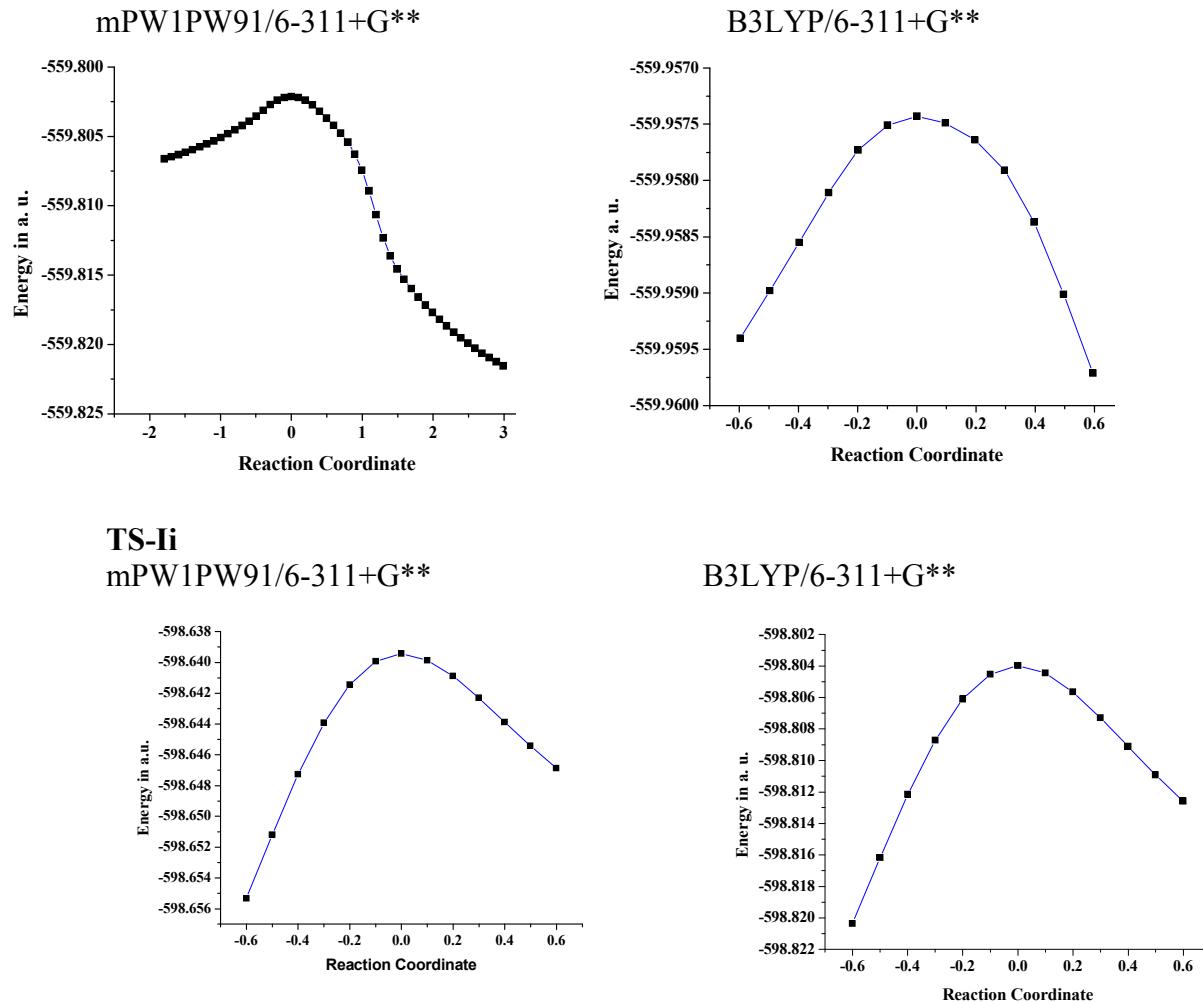
mPW1PW91/6-311+G\*\*



B3LYP/6-311+G\*\*



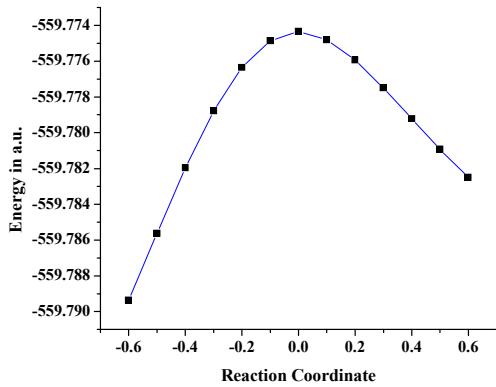
**Figure S3.** (Continued..)  
**TS-Ih**



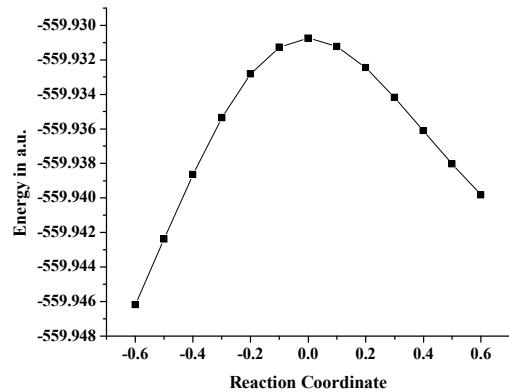
**Figure S3.** (Continued..)

**TS-Ij**

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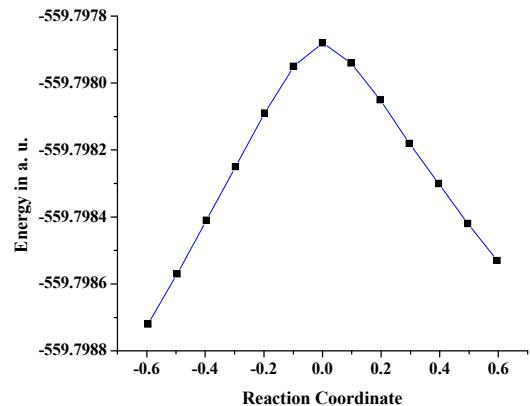


B3LYP/6-311+G\*\*

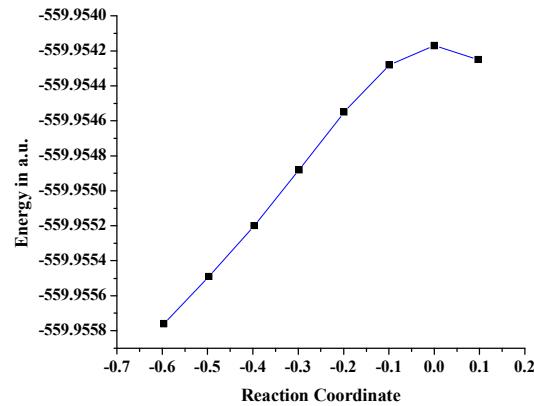


**TS-Ik**

mPW1PW91/6-311+G\*\*



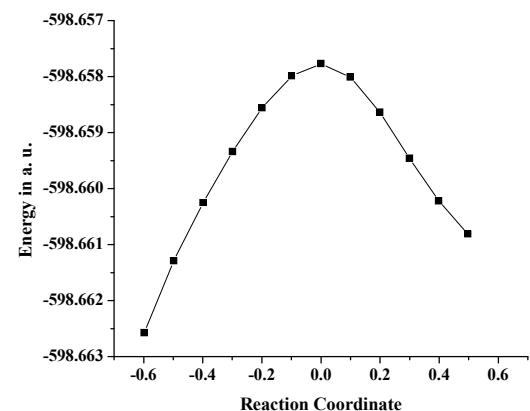
B3LYP/6-311+G\*\*



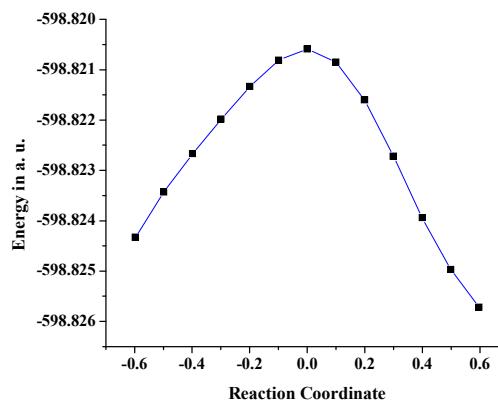
**Figure S3.** (Continued..)

**TS-II**

mPW1PW91/6-311+G\*\*

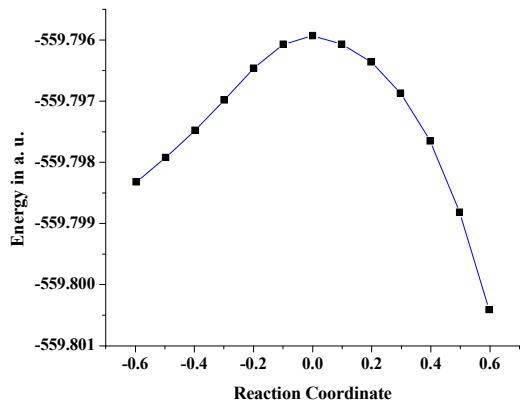


B3LYP/6-311+G\*\*

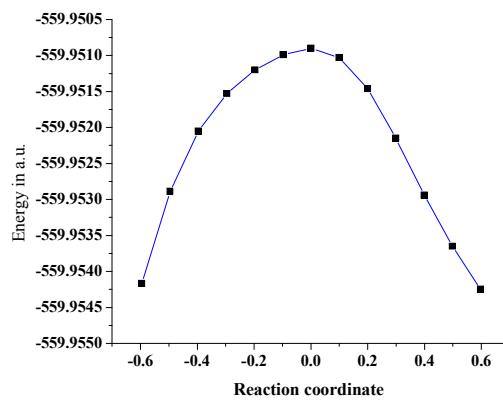


**TS-Im**

mPW1PW91/6-311+G\*\*

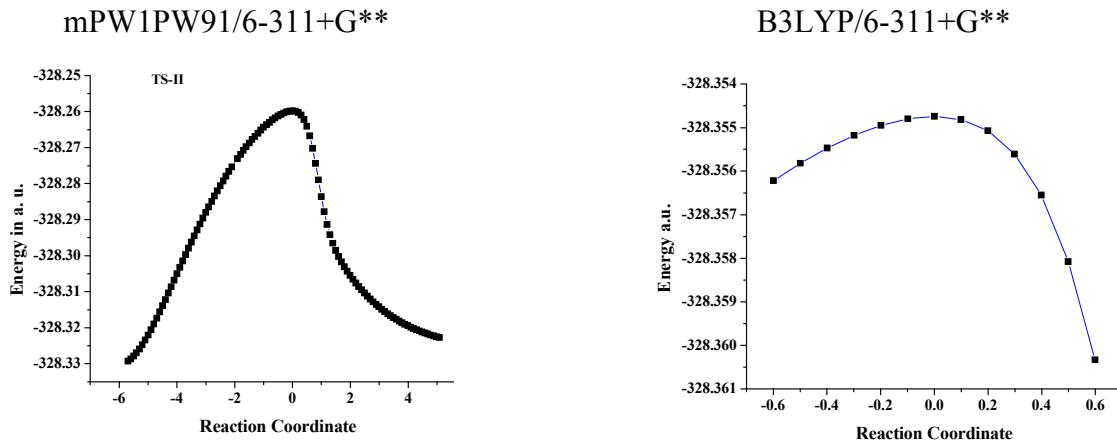


B3LYP/6-311+G\*\*

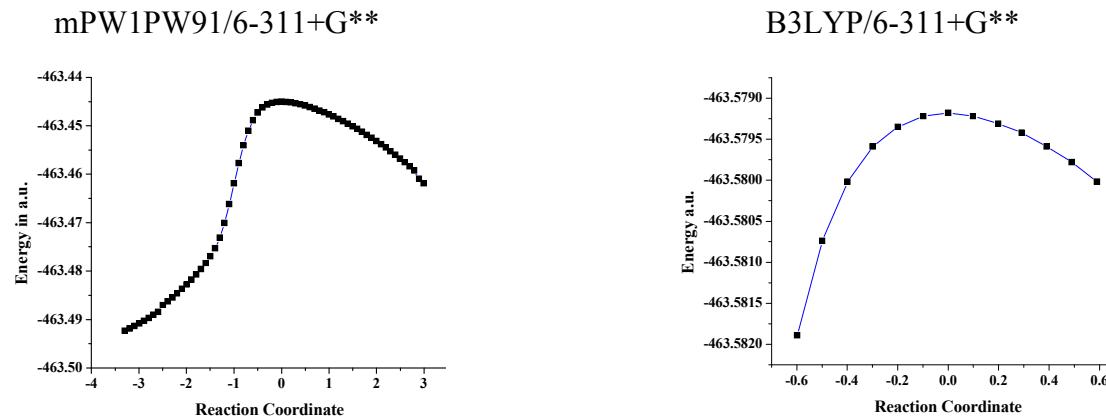


**Figure S4.** The Intrinsic Reaction Coordinate (IRC) Plots of Transition States for Step-II Generated at the mPW1PW91/6-311+G\*\* and B3LYP/6-311+G\*\* Level of Theories. [Extended IRC were performed for all TS in step-II at the mPW1PW91/6-311+G\*\* level. Additional MP2/6-31G\* IRC calculations were also carried out for **TS-IIIf**, **TS-IIg** and **TS-IIIg**]

### TS-II

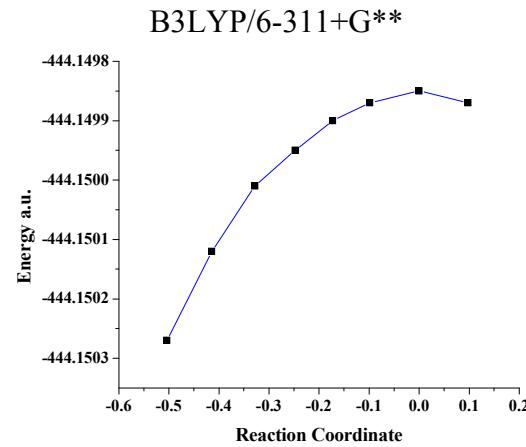
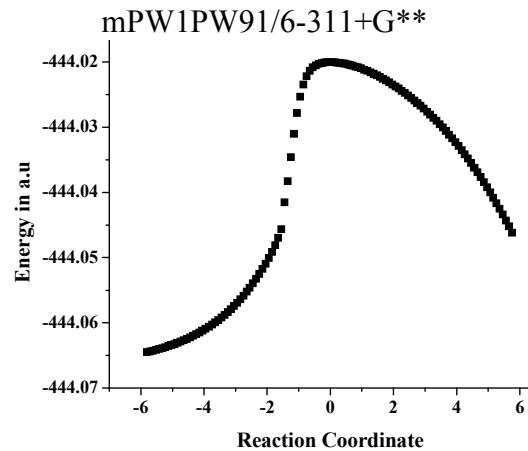


### TS-IIa

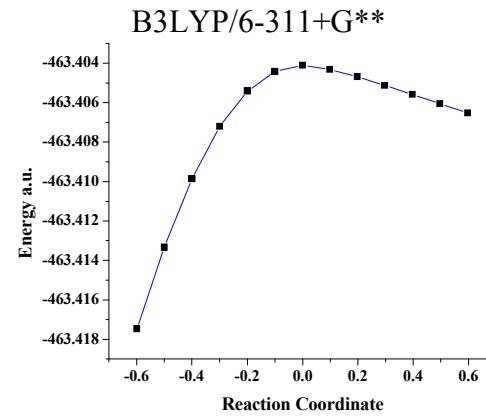
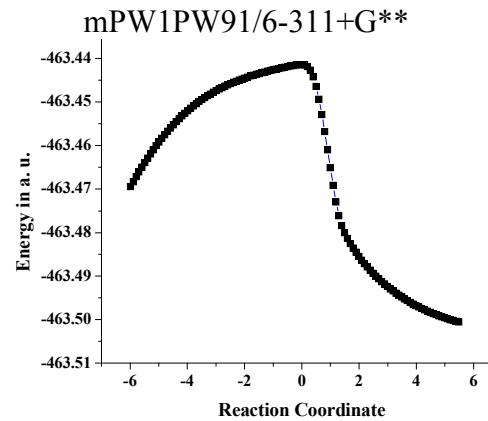


**Figure S4.** (Continued..)

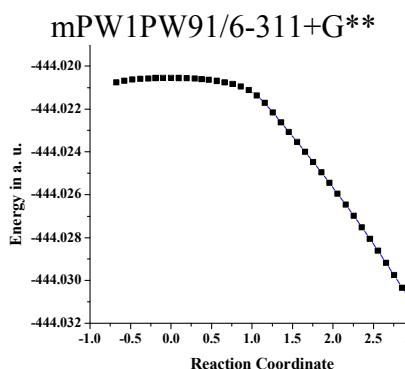
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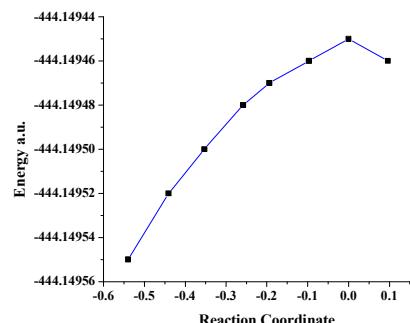
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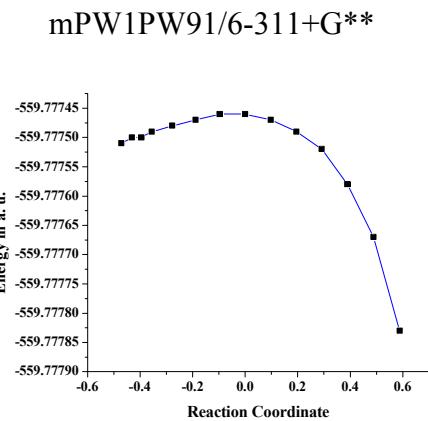
**Figure S4.** (Continued..)  
**TS-IIId**



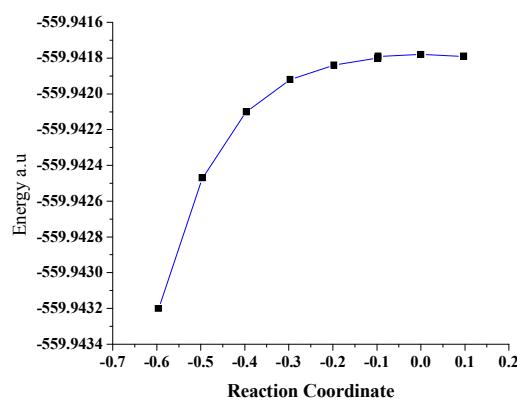
B3LYP/6-311+G\*\*



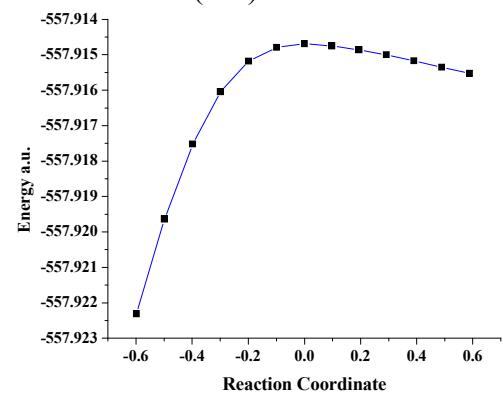
**TS-IIIf**



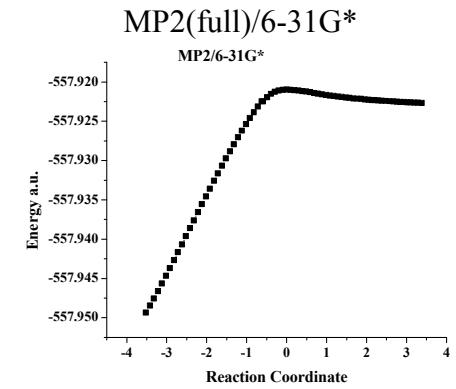
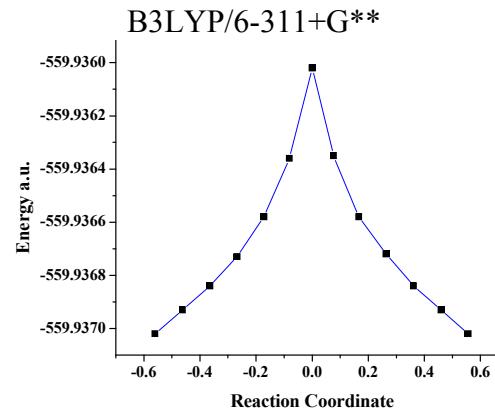
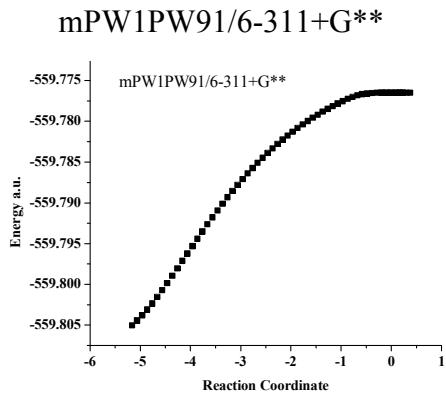
B3LYP/6-311+G\*\*



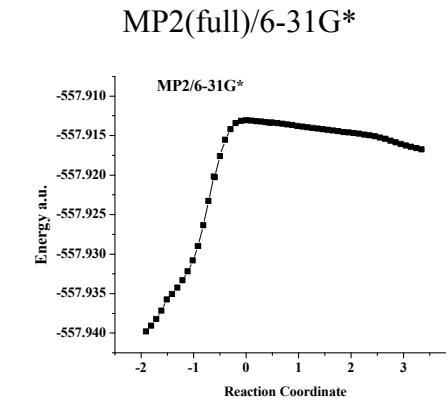
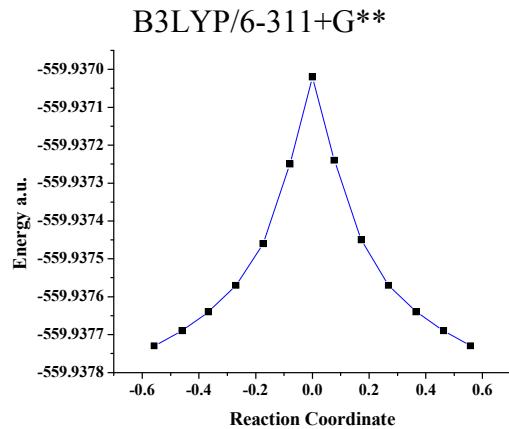
MP2(full)/6-31G\*



**Figure S4.** (Continued..)  
**TS-IIg**



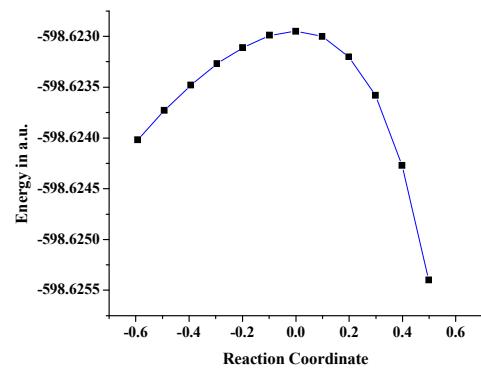
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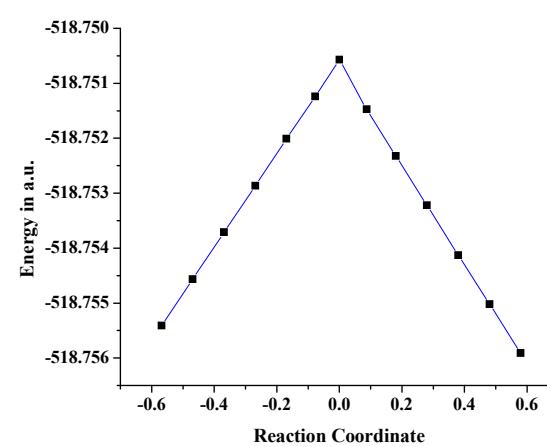
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**Figure S4.** (Continued..)

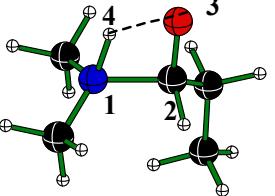
**TS-IIh**  
mPW1PW91/6-311+G\*\*



B3LYP/6-311+G\*\*



**Table S1.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*/mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting complex (PRC) and the Carbinolamine and at the MP2(full)/6-311+G\*\*/MP2(full)/6-31G\* level of theory for **TS-I**

			
	PRC	<b>TS-I</b>	Carbinolamine
	$\rho(r_c)^a$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	-	0.2006	0.2737
C <sub>2</sub> – O <sub>3</sub>	0.4044	0.3151	0.2594
O <sub>3</sub> – H <sub>4</sub>	0.0114	0.1092	0.3631
H <sub>4</sub> – N <sub>1</sub>	0.3381	0.1954	-

<sup>a</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S2.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex (PRC) and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* level of theory for **TS-Ia** and **Ib**

	PRC	<b>TS-Ia</b>	Carbinolamine		PRC	<b>TS-Ib</b>	Carbinolamine
	$\rho(r_c)^b$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0086	0.2119	0.2749	N <sub>1</sub> – C <sub>2</sub>	0.0137	0.2167	0.2780
C <sub>2</sub> – O <sub>3</sub>	0.4008	0.3011	0.2533	C <sub>2</sub> – O <sub>3</sub>	0.3974	0.2941	0.2488
O <sub>3</sub> – H <sub>4</sub>	-	0.1160	0.3616	O <sub>3</sub> – H <sub>4</sub>	-	0.1189	0.3603
H <sub>4</sub> – N <sub>1</sub>	0.3388	0.1877	-	H <sub>4</sub> – N <sub>1</sub>	0.3386	0.1838	-
O <sub>3</sub> –H <sub>7</sub>	0.0151	0.0272	0.0168	O <sub>3</sub> –H <sub>7</sub>	0.0281	0.0419	0.0293
H <sub>7</sub> –N <sub>8</sub>	0.3372	0.3265	0.33733	H <sub>7</sub> –O <sub>8</sub>	0.3530	0.3256	0.2599

<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S3.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*/mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex (PRC) and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* level of theory for **TS-Id** and **Id**

	PRC	TS-Id	Carbinolamine		PRC	TS-Id	Carbinolamine
	$\rho(r_c)$ <sup>b</sup>	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0127	0.2012	0.2635	N <sub>1</sub> – C <sub>2</sub>	0.0142	0.2048	0.2605
C <sub>2</sub> – O <sub>3</sub>	0.4008	0.3203	0.2701	C <sub>2</sub> – O <sub>3</sub>	0.3967	0.3107	0.2689
O <sub>3</sub> – H <sub>7</sub>	0.0162	0.0774	0.3383	O <sub>3</sub> – H <sub>7</sub>	0.0298	0.1677	0.3512
H <sub>7</sub> – N <sub>8</sub>	0.3361	0.2623	0.0355	H <sub>7</sub> – N <sub>8</sub>	0.3506	0.1641	0.0256
N <sub>8</sub> -H <sub>4</sub>	0.0214	0.1681	0.3341	N <sub>8</sub> -H <sub>4</sub>	0.0179	0.0855	0.3371
H <sub>4</sub> -N <sub>1</sub>	0.3307	0.1463	0.0164	H <sub>4</sub> -N <sub>1</sub>	0.3354	0.2586	0.0391

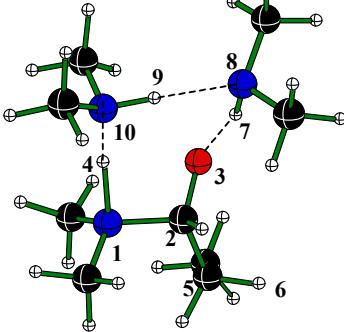
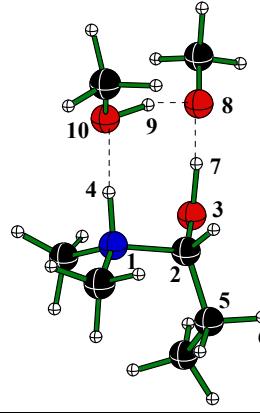
<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S4.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* level of theory for **TS-Ie**<sup>b</sup> and **TS-If**

	PRC	TS-Ie	Carbinolamine		PRC	TS-If	Carbinolamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0159	0.2249	0.2821	N <sub>1</sub> – C <sub>2</sub>	0.1575	0.2289	0.2821
C <sub>2</sub> – O <sub>3</sub>	0.3989	0.2909	0.2498	C <sub>2</sub> – O <sub>3</sub>	0.3379	0.2754	0.2498
O <sub>3</sub> – H <sub>4</sub>	-	0.1200	0.3452	O <sub>3</sub> – H <sub>4</sub>	-	0.1343	0.3452
H <sub>4</sub> –N <sub>1</sub>	0.3217	0.1696	-	H <sub>4</sub> –N <sub>1</sub>	0.3225	0.1688	-
O <sub>3</sub> –H <sub>7</sub>	0.0171	0.0277	0.0175	O <sub>3</sub> –H <sub>7</sub>	0.0464	0.0366	0.0175
H <sub>7</sub> – N <sub>8</sub>	0.3278	0.3188	0.3284	H <sub>7</sub> – O <sub>8</sub>	0.3308	0.3327	0.3284
O <sub>3</sub> –H <sub>9</sub>	0.0169	0.0280	0.01812	O <sub>3</sub> –H <sub>9</sub>	0.0543	0.0365	0.01812
H <sub>9</sub> – N <sub>10</sub>	0.3285	0.3189	0.3287	H <sub>9</sub> – O <sub>10</sub>	0.3184	0.3337	0.3287

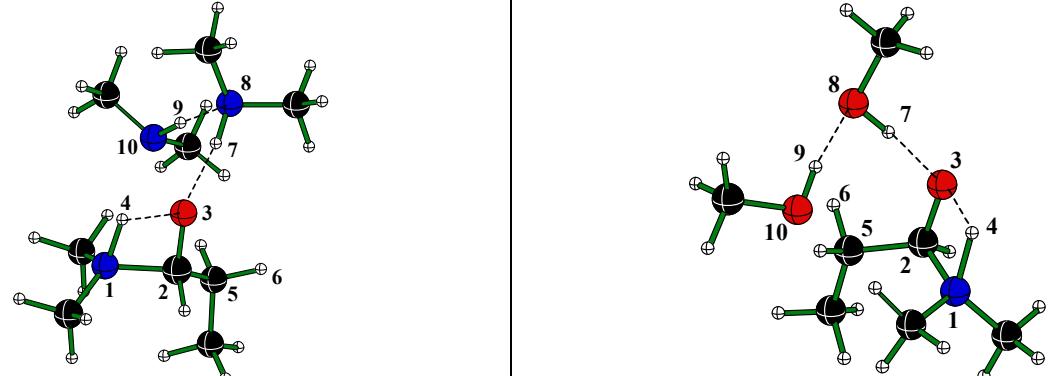
<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup> Analyses performed with the wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and carbinolamine. For **TS-Ie** the MP2(full)/6-31G\* geometry is employed. <sup>c</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S5.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and the carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for **TS-Ig**<sup>b</sup> and **TS-Ih**

							
	PRC	<b>TS-Ig</b>	Carbinolamine		PRC	<b>TS-Ih</b>	Carbinolamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0112	0.2120	0.3274	N <sub>1</sub> – C <sub>2</sub>	0.0138	0.2113	0.1255
C <sub>2</sub> – O <sub>3</sub>	0.402	0.3291	0.2232	C <sub>2</sub> – O <sub>3</sub>	0.3948	0.3038	0.1373
O <sub>3</sub> – H <sub>7</sub>	0.0201	0.0438	0.0519	O <sub>3</sub> – H <sub>7</sub>	0.0359	0.2156	0.1683
H <sub>7</sub> -N <sub>8</sub>	0.3266	0.2997	0.2910	H <sub>7</sub> -O <sub>8</sub>	0.3423	0.1230	0.0181
N <sub>8</sub> -H <sub>9</sub>	0.0255	0.0429	0.0549	O <sub>8</sub> -H <sub>9</sub>	0.0374	0.1328	0.1693
H <sub>9</sub> – N <sub>10</sub>	0.3195	0.2923	0.2767	H <sub>9</sub> – O <sub>10</sub>	0.3422	0.2080	0.0195
N <sub>10</sub> -H <sub>4</sub>	0.0248	0.1879	0.2528	O <sub>10</sub> -H <sub>1</sub>	0.0214	0.08020	0.1605
H <sub>4</sub> – N <sub>1</sub>	0.3199	0.1182	0.0697	H <sub>1</sub> – N <sub>1</sub>	0.3336	0.2685	0.0221

<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup> Analyses performed with wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and carbinolamine. For **TS-Ig** the MP2(full)/6-31G\* geometry is employed. <sup>c</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S6.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* level of theory for the Pre-reacting complex and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* level of theory for **TS-II<sup>b</sup>** and **TS-Ij**



	PRC	<b>TS-II</b>	Carbinolamine		PRC	<b>TS-Ij</b>	Carbinolamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0130	0.2136	0.2818	N <sub>1</sub> – C <sub>2</sub>	0.0169	0.2194	0.2794
C <sub>2</sub> – O <sub>3</sub>	0.4018	0.3033	0.2554	C <sub>2</sub> – O <sub>3</sub>	0.3934	0.2893	0.2445
O <sub>3</sub> – H <sub>4</sub>	–	0.1136	0.3460	O <sub>3</sub> – H <sub>4</sub>	–	0.1235	0.3594
H <sub>4</sub> – N <sub>1</sub>	0.3309	0.1793	–	H <sub>4</sub> – N <sub>1</sub>	0.3343	0.1810	–
O <sub>3</sub> – H <sub>7</sub>	0.0193	0.0327	0.0190	O <sub>3</sub> – H <sub>7</sub>	0.0354	0.0490	0.0334
H <sub>7</sub> – N <sub>8</sub>	0.3270	0.3146	0.3270	H <sub>7</sub> – O <sub>8</sub>	0.3425	0.3151	0.3452
O <sub>3</sub> – H <sub>9</sub>	0.0240	0.0301	0.0232	O <sub>3</sub> – H <sub>9</sub>	0.0371	0.0409	0.0336
H <sub>9</sub> – N <sub>10</sub>	0.3212	0.3143	0.3224	H <sub>9</sub> – O <sub>10</sub>	0.3416	0.3295	0.3480

<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup> Analyses performed with the wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and carbinolamine. For **TS-Ie** the MP2(full)/6-31G\* geometry is employed. <sup>c</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S7.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* level of theory for **TS-Ik** and **TS-II<sup>b</sup>**

	PRC	<b>TS-Ik</b>	Carbinolamine		PRC	<b>TS-II</b>	Carbinolamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.0254	0.1995	0.2607	N <sub>1</sub> – C <sub>2</sub>	0.0102	0.2117	0.2694
C <sub>2</sub> – O <sub>3</sub>	0.3869	0.3142	0.2668	C <sub>2</sub> – O <sub>3</sub>	0.3996	0.3153	0.2687
O <sub>3</sub> – H <sub>7</sub>	0.0403	0.1565	0.3547	O <sub>3</sub> – H <sub>7</sub>	0.0168	0.0680	0.3180
H <sub>7</sub> – O <sub>8</sub>	0.3329	0.1756	0.0212	H <sub>7</sub> – N <sub>8</sub>	0.3281	0.2634	0.0407
O <sub>8</sub> – H <sub>4</sub>	–	0.0463	0.3234	N <sub>8</sub> – H <sub>4</sub>	0.0231	0.1660	0.3662
H <sub>4</sub> – N <sub>1</sub>	0.3293	0.3103	0.0489	H <sub>4</sub> – N <sub>1</sub>	0.3219	0.1366	0.0149
O <sub>8</sub> – H <sub>9</sub>	0.0409	0.0404	0.0307	O <sub>3</sub> – H <sub>9</sub>	0.0166	0.0318	0.0205
H <sub>9</sub> – O <sub>10</sub>	0.3345	0.3289	0.3519	H <sub>9</sub> – O <sub>10</sub>	0.3288	0.4944	0.3273

<sup>a</sup> Refers to cabinolamine-methanol-amine complex. <sup>b</sup> Analyses performed with the wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and carbinolamine. For **TS-II** the MP2(full)/6-31G\* geometry is employed. <sup>c</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S8.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and the Carbinolamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for **TS-Im**

The diagram shows the TS-Im molecule with atom numbering. Atom 1 is the nitrogen of the imine group, bonded to atom 2 (carbon) which is bonded to atom 3 (oxygen) of the methanol molecule. Atom 2 is also bonded to atom 4 (hydrogen) and atom 5 (carbon) of the carbinolamine molecule. Atom 5 is bonded to atom 6 (hydrogen) and atom 7 (hydrogen) of the methanol molecule. Atom 7 is bonded to atom 8 (oxygen) of the carbinolamine molecule, which is also bonded to atom 9 (hydrogen) and atom 10 (oxygen) of the methanol molecule. Partial charges are represented by green lines with '+' signs on the atoms.

	PRC	<b>TS-Im</b>	Carbinolamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.1594	0.2189	0.2639
C <sub>2</sub> – O <sub>3</sub>	0.3378	0.2936	0.2590
O <sub>3</sub> – H <sub>7</sub>	0.0554	0.1848	0.3457
H <sub>7</sub> – O <sub>8</sub>	0.3170	0.1495	0.0300
O <sub>8</sub> – H <sub>4</sub>	0.0343	0.0987	0.3370
H <sub>4</sub> – N <sub>1</sub>	0.3245	0.2478	0.0384
O <sub>3</sub> – H <sub>9</sub>	0.0445	0.0349	0.0294
H <sub>9</sub> – O <sub>10</sub>	0.3328	0.3367	0.3522

<sup>a</sup> Refers to cabinolamine-methanol/amine complex. <sup>b</sup> Analyses performed with the wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and the carbinolamine.

**Table S9.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and the Enamine-water Complex and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for TS-II

	PRC	TS-II	Enamine
	$\rho(r_c)^a$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.2801	0.3396	0.3057
C <sub>2</sub> – C <sub>5</sub>	0.2548	0.2838	0.3288
C <sub>5</sub> – H <sub>6</sub>	0.2739	0.1990	0.0159
H <sub>6</sub> -O <sub>3</sub>	-	0.0845	0.3527
O <sub>3</sub> -C <sub>2</sub>	0.2475	0.0378	-

<sup>a</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S10.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*/mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and Enamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*/MP2(full)/6-31G\* Level of Theory for **TS-IIa** and **IIb**

	PRC	<b>TS-IIa</b>	Enamine		PRC	<b>TS-IIb</b>	Enamine
	$\rho(r_c)^b$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.2824	0.3474	0.3074	N <sub>1</sub> – C <sub>2</sub>	0.2824	0.3460	0.3091
C <sub>2</sub> – C <sub>5</sub>	0.2538	0.2792	0.3275	C <sub>2</sub> – C <sub>5</sub>	0.2538	0.2773	0.3261
C <sub>5</sub> – H <sub>6</sub>	0.2749	0.2139	0.0181	C <sub>5</sub> – H <sub>6</sub>	0.2749	0.2214	0.0200
H <sub>6</sub> –O <sub>3</sub>	-	0.0662	0.3474	H <sub>6</sub> –O <sub>3</sub>	-	0.0669	0.3434
O <sub>3</sub> –C <sub>2</sub>	0.2420	-	-	O <sub>3</sub> –C <sub>2</sub>	0.2420	-	-
O <sub>3</sub> –H <sub>7</sub>	0.0156	0.0408	0.0182	O <sub>3</sub> –H <sub>7</sub>	0.0156	0.0894	0.0301
H <sub>7</sub> –N <sub>8</sub>	0.3374	0.3119	0.33673	H <sub>7</sub> –N <sub>8</sub>	0.3374	0.2550	0.3512

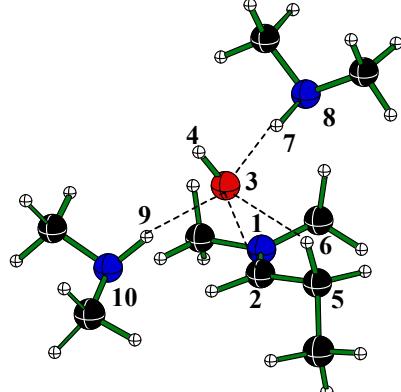
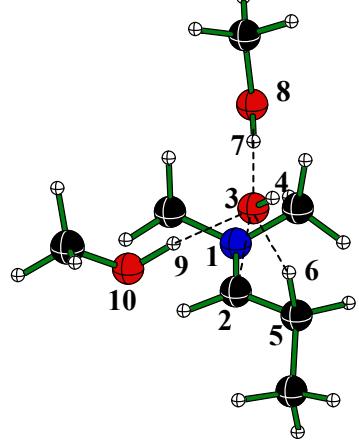
<sup>a</sup> Refers to enamine-methanol/amine complex. <sup>b</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S11.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*/mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and Enamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*/MP2(full)/6-31G\* Level of Theory for **TS-IIc** and **TS-IId**

	PRC	<b>TS-IIc</b>	Enamine		PRC	<b>TS-IId</b>	Enamine
	$\rho(r_c)$ <sup>b</sup>	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.2824	0.3239	0.3069	N <sub>1</sub> – C <sub>2</sub>	0.2854	0.3511	0.3092
C <sub>2</sub> – C <sub>5</sub>	0.2544	0.2923	0.3285	C <sub>2</sub> – C <sub>5</sub>	0.2545	0.2647	0.3262
C <sub>5</sub> – H <sub>6</sub>	0.2750	0.1555	0.0120	C <sub>5</sub> – H <sub>6</sub>	0.2746	0.2690	0.0199
H <sub>6</sub> -N <sub>8</sub>	0.0045	0.1268	0.3335	H <sub>6</sub> -O <sub>8</sub>	-	0.0247	0.3476
N <sub>8</sub> -H <sub>4</sub>	0.3374	0.2326	0.0396	O <sub>8</sub> -H <sub>4</sub>	0.3542	0.0970	0.0329
H <sub>4</sub> -O <sub>3</sub>	0.0155	0.1033	0.3311	H <sub>4</sub> -O <sub>3</sub>	0.0282	0.2457	0.3443
O <sub>3</sub> – C <sub>2</sub>	0.2411	0.0418	-	O <sub>3</sub> – C <sub>2</sub>	0.2356	0.0264	-

<sup>a</sup> Refers to enamine-methanol/amine complex. <sup>b</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S12.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and Enamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for **TS-IIe**<sup>b</sup> and **TS-IIf**

							
	PRC	TS-IIe	Enamine		PRC	TS-IIf	Enamine
	$\rho(r_c)^c$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.2836	0.3494	0.3133	N <sub>1</sub> – C <sub>2</sub>	0.2902	0.3540	0.3101
C <sub>2</sub> – C <sub>5</sub>	0.2570	0.2797	0.3307	C <sub>2</sub> – C <sub>5</sub>	0.2523	0.2660	0.3243
C <sub>5</sub> – H <sub>6</sub>	0.2704	0.2228	0.0219	C <sub>5</sub> – H <sub>6</sub>	0.2705	0.2671	0.0252
H <sub>6</sub> – O <sub>3</sub>	-	0.0599	0.3274	H <sub>6</sub> – O <sub>3</sub>	-	0.0213	0.3326
O <sub>3</sub> - C <sub>2</sub>	0.2555	-	-	O <sub>3</sub> – C <sub>2</sub>	0.2256	0.0139	-
O <sub>3</sub> – H <sub>7</sub>	0.0197	0.0472	0.0188	O <sub>3</sub> – H <sub>7</sub>	0.0264	0.0821	0.0246
H <sub>7</sub> –N <sub>8</sub>	0.3270	0.2967	0.3281	H <sub>7</sub> –O <sub>8</sub>	0.3560	0.2719	0.3565
O <sub>3</sub> – H <sub>9</sub>	-	0.04499	0.0167	O <sub>3</sub> – H <sub>9</sub>	0.0239	0.0775	0.0268
H <sub>9</sub> – N <sub>10</sub>	-	0.2984	0.3283	H <sub>9</sub> – O <sub>10</sub>	0.3575	0.2813	0.3545

<sup>a</sup> Refers to enamine-methanol/amine complex. <sup>b</sup> Analyses performed with the wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and enamine. For **TS-IIe** the MP2(full)/6-31G\* geometry is employed. <sup>c</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S13.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and Iminium ion/Enamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for **TS-IIg** and **IIIg**

	PRC	TS-IIg	Iminium ion		PRC	TS-IIIg	Enamine
	$\rho(r_c)$ <sup>b</sup>	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> -C <sub>2</sub>	0.2936	0.3482	0.3564	N <sub>1</sub> -C <sub>2</sub>	0.3558	0.3417	0.3064
C <sub>2</sub> -C <sub>5</sub>	0.2532	0.2616	0.2649	C <sub>2</sub> -C <sub>5</sub>	0.2673	0.2830	0.3259
C <sub>5</sub> -H <sub>6</sub>	0.2771	0.2764	0.2706	C <sub>5</sub> -H <sub>6</sub>	0.2675	0.1984	0.0211
H <sub>6</sub> -O <sub>8</sub>	0.0087	0.0164	0.0208	H <sub>6</sub> -O <sub>8</sub>	0.0198	0.0853	0.3437
O <sub>8</sub> -H <sub>9</sub>	0.3484	0.3135	0.2935	O <sub>8</sub> -H <sub>9</sub>	0.2731	0.0795	0.0372
H <sub>9</sub> -O <sub>10</sub>	0.0330	0.0051	0.0709	H <sub>9</sub> -O <sub>10</sub>	0.0860	0.2714	0.3410
O <sub>10</sub> -H <sub>4</sub>	0.3442	0.1156	0.0827	O <sub>10</sub> -H <sub>4</sub>	0.0829	0.0380	0.0352
H <sub>4</sub> -O <sub>3</sub>	0.0335	0.2247	0.2729	H <sub>4</sub> -O <sub>3</sub>	0.2723	0.3252	0.3397
O <sub>3</sub> -C <sub>2</sub>	0.2207	0.0411	0.0200	O <sub>3</sub> -C <sub>2</sub>	-	-	-
O <sub>3</sub> -H <sub>7</sub>	0.3624	0.3481	0.3637	O <sub>3</sub> -H <sub>7</sub>	0.3641	0.3535	0.3651

<sup>a</sup> Refers to iminium ion/enamine-methanol complex. <sup>b</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S14.** Summary of Atoms in Molecule (AIM) Analyses Performed Using the Wave Functions Generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-311+G\*\* Level of Theory for the Pre-reacting Complex and Enamine<sup>a</sup> and at the MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* Level of Theory for **TS-IIh**<sup>b</sup> and **TS-IIIi**<sup>c</sup>

	PRC	TS-IIh	Enamine		PRC	TS-IIIi	Enamine
	$\rho(r_c)^d$	$\rho(r_c)$	$\rho(r_c)$		$\rho(r_c)$	$\rho(r_c)$	$\rho(r_c)$
N <sub>1</sub> – C <sub>2</sub>	0.2811	0.3527	0.3127	N <sub>1</sub> – C <sub>2</sub>	0.2936	0.3988	0.3117
C <sub>2</sub> – C <sub>5</sub>	0.2575	0.2782	0.3326	C <sub>2</sub> – C <sub>5</sub>	0.2532	0.2674	0.3242
C <sub>5</sub> – H <sub>6</sub>	0.2705	0.2252	0.0183	C <sub>5</sub> – H <sub>6</sub>	0.2771	0.2623	0.0229
H <sub>6</sub> – O <sub>3</sub>	–	0.0610	0.3331	H <sub>6</sub> – O <sub>8</sub>	–	0.0321	0.3409
O <sub>3</sub> – C <sub>2</sub>	0.2585	–	–	O <sub>8</sub> – H <sub>4</sub>	0.3442	0.0733	0.0180
O <sub>3</sub> – H <sub>7</sub>	0.0176	0.0486	0.0219	H <sub>4</sub> – O <sub>3</sub>	0.0335	0.2822	0.3587
H <sub>7</sub> – N <sub>8</sub>	0.3267	0.2926	0.3267	O <sub>3</sub> – C <sub>2</sub>	0.2270	0.0256	–
N <sub>8</sub> – H <sub>9</sub>	0.0235	0.0213	0.0240	O <sub>8</sub> – H <sub>9</sub>	0.0330	0.0554	0.0288
H <sub>9</sub> – N <sub>10</sub>	0.3197	0.3204	0.3214	H <sub>9</sub> – O <sub>10</sub>	0.3484	0.3116	0.3512

<sup>a</sup> Refers to enamine-methanol/amine complex. <sup>b</sup> Analyses performed with wave functions generated at the MP2(full)/6-31G\*//mPW1PW91/6-311+G\*\* level of theory for the pre-reacting complex and enamine. <sup>c</sup> Analyses performed with the wave functions generated at the MP2(full)/6-311+G\*\*//mPW1PW91/6-31G\* level of theory for **TS-IIIi**. <sup>d</sup>  $\rho(r_c)$  is the electron density at the BCP.

**Table S15.** Computed Activation Energies (in kcal mol<sup>-1</sup>)<sup>a</sup> for Carbinolamine Formation (Step-I) Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-I</b>	<b>TS-Ia</b>	<b>TS-Ib</b>	<b>TS-Ic</b>	<b>TS-ID</b>	<b>TS-Ie</b>	<b>TS-If</b>	<b>TS-Ig</b>	<b>TS-Ih</b>	<b>TS -Ii</b>	<b>TS -Ij</b>	<b>TS -Ik</b>	<b>TS -Il</b>	<b>TS -Im</b>
<i>L1</i>	25.4	13.3	7.9	3.2	-5.5	3.8	-4.9	-11.7	-24.4	4.9	-5.6	-21.8	-7.7	-19.0
<i>L2</i>	25.2	16.3	13.4	4.5	-1.3	9.6	1.3	-4.7	-17.6	9.2	-0.2	-14.9	-2.3	-13.7
<i>L3</i>	24.9	14.9	7.4	0.4	-6.9	0.4	-7.4	-16.5	-24.4	2.2	-6.7	-23.3	-10.1	-22.3
<i>L4</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>L5</i>	31.1	25.8	20.2	14.5	5.9	19.7	3.0	6.3	-7.5	19.3	9.2	-5.5	8.8	-3.4
<i>L6</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>L7</i>	21.6	11.5	7.97	-1.0	-6.1	1.7	-3.9	-15.8	-22.4	1.5	-5.4	-20.3	-9.9	-18.8
<i>L8</i>	22.1	16.4	12.9	-	-	-	-	-	-	-	-	-	-	-

**Table S16.** Computed Activation Energies (in kcal mol<sup>-1</sup>)<sup>a</sup> for Dehydration (step-II) Steps Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-II</b>	<b>TS-IIa</b>	<b>TS-IIb</b>	<b>TS-IIc</b>	<b>TS-IId</b>	<b>TS-IIe</b>	<b>TS-IIf</b>	<b>TS-IIg</b>	<b>TS-IIIg</b>	<b>TS-IIh</b>	<b>TS-IIi</b>
<i>L1</i>	47.0	31.6	22.1	38.0	20.6	18.2	-1.2	0.0	0.1	23.5	1.3
<i>L2</i>	35.7	25.3	16.0	29.7	15.6	15.3	-2.1	-1.5	-0.1	19.5	1.7 <sup>c</sup>
<i>L3</i>	49.9	33.9	19.9	40.5	19.2	15.2	-0.8	-4.8	0.2	21.5	-0.5 <sup>d</sup>
<i>L4</i>	-	-	-	-	-	-	-	-	-	-	-
<i>L5</i>	38.2	28.8	19.2	30.2	18.1	20.0	2.3	3.5	4.8	24.4	5.7
<i>L6</i>	-	-	-	-	-	-	-	-	-	-	-
<i>L7</i>	37.8	24.5	14.6	29.9	13.9	7.6	-4.9	-5.4	-3.3	13.1	-2.4 <sup>e</sup>
<i>L8</i>	36.2	28.5	15.9	-	-	-	-	-	-	-	-

*L1* : mPW1PW91/6-31G\* *L2* : mPW1PW91/6-311+G\*\* *L3* : MP2(full)/6-31G\* *L4* : PCM-mPW1PW91/6-31G\* *L5* : B3LYP/6-311+G\*\* *L6* : PCM-B3LYP/6-31G\* *L7* : MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* *L8* : CBS-QB3

<sup>a</sup> Barriers with respect to separated reactants <sup>b</sup> All energies refer to the optimized geometries at respective levels of theories. <sup>c</sup> Single point energy obtained at the mPW1PW91/6-311+G\*\*//mPW1PW91/6-311G\*\* level of theory. <sup>d</sup> Single point energy obtained at the MP2(full)/6-31G\*\*//mPW1PW91/6-31G\* level of theory. <sup>e</sup> Single point energy obtained at the MP2(full)/6-311+G\*\*//mPW1PW91/6-31G\* level of theory

**Table S17.** Computed Activation Enthalpies (in kcal mol<sup>-1</sup>)<sup>a</sup> for Carbinolamine Formation (Step-I) Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-I</b>	<b>TS-Ia</b>	<b>TS-Ib</b>	<b>TS-Ic</b>	<b>TS-Id</b>	<b>TS-Ie</b>	<b>TS-If</b>	<b>TS-Ig</b>	<b>TS-Ih</b>	<b>TS -Ii</b>	<b>TS -Ij</b>	<b>TS -Ik</b>	<b>TS -Il</b>	<b>TS -Im</b>
<i>L1</i>	24.6	14.2	8.9	2.8	-5.1	6.3	-1.9	-9.5	-23.5	7.2	-2.9	-18.8	-6.3	-17.1
<i>L2</i>	24.6	17.3	14.6	4.1	-0.8	12.0	4.1	-2.9	-16.6	11.5	2.5	-12.1	-0.9	-11.7
<i>L3</i>	24.0	15.6	8.5	0.0	-6.5	2.9	-4.5	-14.5	-23.6	4.3	-4.1	-20.3	-8.6	-20.2
<i>L4</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>L5</i>	30.4	26.6	21.3	14.3	6.4	22.1	5.9	8.5	-21.6	21.5	11.9	-2.6	10.3	-1.3
<i>L6</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>L7</i>	20.8	12.2	9.0	-1.4	-5.7	4.1	-0.9	-13.2	-6.4	3.6	-2.8	-17.3	-8.4	-16.8
<i>L8</i>	21.5	15.2	11.7	-	-	-	-	-	-	-	-	-	-	-

**Table S18.** Computed Activation Enthalpies (in kcal mol<sup>-1</sup>)<sup>a</sup> for Dehydration (step-II) Steps Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-II</b>	<b>TS-IIa</b>	<b>TS-IIb</b>	<b>TS-IIc</b>	<b>TS-IId</b>	<b>TS-IIe</b>	<b>TS-IIf</b>	<b>TS-IIg</b>	<b>TS-IIIg</b>	<b>TS-IIh</b>	<b>TS-IIi</b>
<i>L1</i>	44.8	31.3	21.6	34.9	20.7	20.8	0.6	2.0	0.3	24.5	3.6
<i>L2</i>	34.5	25.6	16.1	27.8	15.3	18.1	-0.4	0.0	0.4	21.1	4.0 <sup>c</sup>
<i>L3</i>	47.7	33.4	20.6	37.5	19.4	16.8	0.2	-2.8	0.4	23.1	-0.4 <sup>d</sup>
<i>L4</i>	-	-	-	-	-	-	-	-	-	-	-
<i>L5</i>	37.0	29.3	19.6	30.4	17.9	23.0	4.1	4.8	5.8	26.1	7.8
<i>L6</i>	-	-	-	-	-	-	-	-	-	-	-
<i>L7</i>	35.6	24.1	15.2	26.9	14.0	9.2	-3.9	-3.5	-3.3	14.7	-2.3 <sup>e</sup>
<i>L8</i>	35.6	27.3	14.7	-	-	-	-	-	-	-	-

*L1* : mPW1PW91/6-31G\* *L2* : mPW1PW91/6-311+G\*\* *L3* : MP2(full)/6-31G\* *L4* : PCM-mPW1PW91/6-31G\* *L5* : B3LYP/6-311+G\*\* *L6* : PCM-B3LYP/6-31G\* *L7* : MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* *L8* : CBS-QB3

<sup>a</sup> Barriers with respect to separated reactants <sup>b</sup> All energies refer to the optimized geometries at respective levels of theories. <sup>c</sup> Single point energy obtained at the mPW1PW91/6-311+G\*\*//mPW1PW91/6-311G\*\* level of theory. Thermal correction to enthalpy is taken from mPW1PW91/6-31G\*\* level of theory. <sup>d</sup> Single point energy obtained at the MP2(full)/6-31G\*\*//mPW1PW91/6-31G\* level of theory. Thermal correction to enthalpy is taken from mPW1PW91/6-31G\* level of theory. <sup>e</sup> Single point energy obtained at the MP2(full)/6-311+G\*\*//mPW1PW91/6-31G\* level of theory. Thermal correction to enthalpy is taken from mPW1PW91/6-31G\* level of theory.

**Table S19.** Computed Gibbs Free Energies of Activation (in kcal mol<sup>-1</sup>)<sup>a</sup> for Carbinolamine Formation (Step-I) Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-I</b>	<b>TS-Ia</b>	<b>TS-Ib</b>	<b>TS-Ic</b>	<b>TS-Id</b>	<b>TS-Ie</b>	<b>TS-If</b>	<b>TS-Ig</b>	<b>TS-Ih</b>	<b>TS -Ii</b>	<b>TS -Ij</b>	<b>TS -Ik</b>	<b>TS -Il</b>	<b>TS -Im</b>
<i>L1</i>	38.4	38.2	32.8	28.5	20.1	39.7	30.9	27.8	10.9	40.2	30.6	15.2	27.8	17.4
<i>L2</i>	38.4	40.7	37.6	29.8	24.3	44.6	35.3	33.9	18.9	44.2	35.3	21.7	33.2	22.9
<i>L3</i>	38.2	38.1	32.3	26.0	18.7	36.5	29.4	22.7	11.0	37.1	28.9	14.0	25.3	15.8
<i>L4<sup>c</sup></i>	24.4	19.0	13.3	4.1	-4.2	11.5	2.7	-5.6	-17.9	11.8	1.51	-15.0	-1.3 <sup>d</sup>	-14.5
<i>L5</i>	44.0	48.1	43.9	39.8	31.3	54.3	37.7	44.9	29.1	53.9	44.3	31.2	43.3	33.4
<i>L6<sup>c</sup></i>	30.3	25.7	19.0	12.1	2.0	18.9	7.8	3.2	-11.9	19.4	6.7	-9.6	8.2 <sup>e</sup>	-8.7
<i>L7</i>	34.9	34.8	32.9	24.6	19.5	37.7	32.9	23.4	13.0	36.4	30.3	17.0	25.4	19.2
<i>L8</i>	35.1	37.3	34.3	-	-	-	-	-	-	-	-	-	-	-

**Table S20.** Computed Gibbs Free Energies of Activation (in kcal mol<sup>-1</sup>)<sup>a</sup> for Dehydration (step-II) Steps Obtained at Different Levels of Theories<sup>b</sup>

	<b>TS-II</b>	<b>TS-IIa</b>	<b>TS-IIb</b>	<b>TS-IIc</b>	<b>TS-IId</b>	<b>TS-IIe</b>	<b>TS-IIf</b>	<b>TS-IIg</b>	<b>TS-IIIg</b>	<b>TS-IIh</b>	<b>TS-IIi</b>
<i>L1</i>	57.5	54.0	44.2	58.1	43.9	53.0	32.7	34.9	32.8	56.0	36.5
<i>L2</i>	46.7	47.8	38.6	51.0	37.4	49.8	31.1	32.9	33.0	51.5	36.5 <sup>f</sup>
<i>L3</i>	60.3	56.0	43.5	60.6	42.1	50.1	33.5	32.1	32.2	57.2	32.4 <sup>g</sup>
<i>L4<sup>c</sup></i>	47.3	36.3	26.8	39.4	24.2	24.7	5.7	6.0	7.5	30.8	6.4
<i>L5</i>	49.1	51.3	42.1	53.5	40.6	54.3	35.7	36.7	38.2	56.2	39.6
<i>L6<sup>c</sup></i>	49.0	38.8	28.3	43.3	22.8	27.8	6.6	3.9	9.2 <sup>e</sup>	35.3 <sup>e</sup>	9.0 <sup>e</sup>
<i>L7</i>	48.2	46.7	38.2	50.0	36.7	42.6	29.4	31.5	28.5	48.8	30.5 <sup>h</sup>
<i>L8</i>	48.1	50.5	37.5	-	-	-	-	-	-	-	-

*L1* : mPW1PW91/6-31G\* *L2* : mPW1PW91/6-311+G\*\* *L3* : MP2(full)/6-31G\* *L4* : PCM-mPW1PW91/6-31G\* *L5* : B3LYP/6-311+G\*\* *L6* : PCM-B3LYP/6-31G\* *L7* : MP2(full)/6-311+G\*\*//MP2(full)/6-31G\* *L8* : CBS-QB3 <sup>a</sup>Barriers with respect to separated reactants <sup>b</sup>All energies refer to the optimized geometries at respective levels of theories <sup>c</sup>Activation energies in THF obtained using the PCM (Polarized Continuum Model) solvation model and UAKS radii. <sup>d</sup>Single point energy obtained at the PCM-mPW1PW91/6-31G\*/mPW1PW91/6-31G\* level of theory. <sup>e</sup>Single point energy obtained at the PCM-B3LYP/6-

<sup>f</sup>PCM-B3LYP/6-31G\*//B3LYP/6-31G\* <sup>g</sup>PCM-B3LYP/6-31G\*//B3LYP/6-31G\* <sup>h</sup>PCM-B3LYP/6-31G\*//B3LYP/6-31G\*

$31G^*/mPW1PW91/6-31G^*$  level of theory.<sup>f</sup> Single point energy obtained at the  $mPW1PW91/6-311+G^{**}/mPW1PW91/6-311G^{**}$  level of theory. Thermal correction to free energy is taken from  $mPW1PW91/6-311G^{**}$  level of theory. <sup>g</sup> Single point energy obtained at the  $MP2(full)/6-31G^*/mPW1PW91/6-31G^*$  level of theory. Thermal correction to free energy is taken from  $mPW1PW91/6-31G^*$  level of theory. <sup>h</sup> Single point energy obtained at the  $MP2(full)/6-311+G^{**}/mPW1PW91/6-31G^*$  level of theory. Thermal correction to enthalpy is taken from  $mPW1PW91/6-31G^*$  level of theory.

**Table S21.** Selected Bond Distances and Angles (in Å and °) of Transition State **TS-I** Computed at the Various Levels of Theories

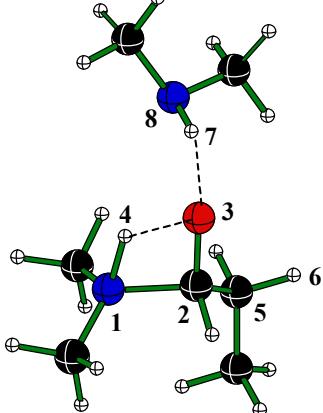
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Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>
mPW1PW91/6-31G*	1.594	1.338	1.384	1.202	114.8
mPW1PW91/6-311+G**	1.586	1.344	1.375	1.950	115.8
MP2/6-31G*	1.583	1.351	1.405	1.209	113.3
PCM-mPW1PW91/6-31G*	1.570	1.353	1.367	1.213	114.9
B3LYP/6-311+G**	1.607	1.353	1.363	1.214	116.4
PCM-B3LYP/6-31G*	1.592	1.359	1.364	1.227	115.3

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**Table S22.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ia** Computed at the Various Levels of Theories

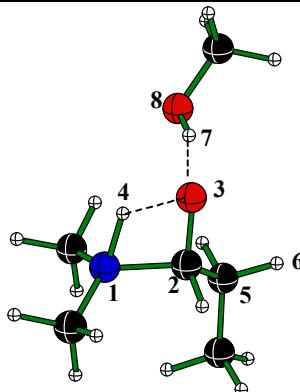
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Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>
mPW1PW91/6-31G*	1.567	1.358	1.361	1.217	1.950	1.026	115.1	162.3
mPW1PW91/6-311+G**	1.563	1.360	1.356	1.209	2.016	1.022	115.6	160.8
MP2/6-31G*	1.562	1.372	1.378	1.225	1.958	1.028	114.1	163.3
PCM-mPW1PW91/6-31G*	1.554	1.369	1.345	1.229	1.957	1.028	115.1	165.6
B3LYP/6-311+G**	1.682	1.369	1.350	1.226	2.060	1.022	115.9	161.0
PCM-B3LYP/6-31G*	1.577	1.372	1.346	1.236	1.965	1.026	115.0	173.2

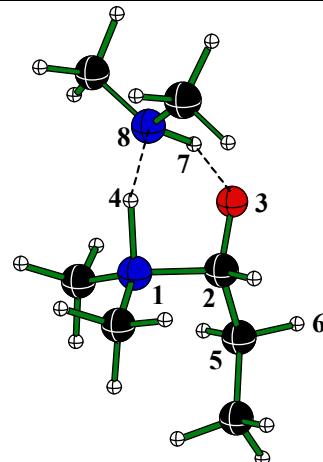
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**Table S23.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ib** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>
mPW1PW91/6-31G*	1.557	1.369	1.350	1.226	1.719	0.992	114.8	165.1
mPW1PW91/6-311+G**	1.554	1.370	1.344	1.219	1.727	0.983	115.3	165.4
MP2/6-31G*	1.554	1.377	1.370	1.225	1.776	0.988	113.0	162.7
PCM-mPW1PW91/6-31G*	1.544	1.380	1.331	1.241	1.708	0.993	114.9	169.3
B3LYP/6-311+G**	1.572	1.379	1.340	1.235	1.763	0.984	115.6	165.0
PCM-B3LYP/6-31G*	1.562	1.387	1.334	1.252	1.733	0.995	115.1	168.9

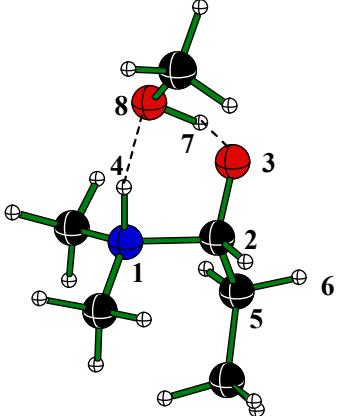
**Table S24.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-1c** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	N <sub>1</sub> -H <sub>4</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>
mPW1PW91/6-31G*	1.594	1.322	1.486	1.113	1.279	1.324	157.9	149.6
mPW1PW91/6-311+G**	1.587	1.326	1.479	1.109	1.288	1.307	159.1	150.9
MP2/6-31G*	1.585	1.334	1.530	1.101	1.272	1.336	157.8	147.4
PCM-mPW1PW91/6-31G*	1.580	1.327	1.576	1.086	1.257	1.346	158.6	146.8
B3LYP/6-311+G**	1.621	1.328	1.528	1.098	1.263	1.354	159.1	149.1
PCM-B3LYP/6-31G*	1.611	1.328	1.615	1.081	1.248	1.376	158.6	145.7

**Table S25.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-1d** Computed at the Various Levels of Theories

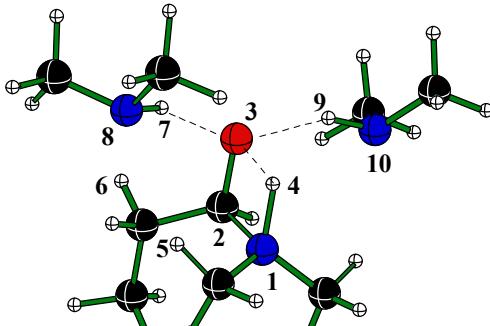
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Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>
mPW1PW91/6-31G*	1.591	1.335	1.205	1.218	1.479	1.112	158.5	154.8
mPW1PW91/6-311+G**	1.587	1.335	1.206	1.203	1.490	1.098	159.1	154.5
MP2/6-31G*	1.577	1.349	1.218	1.227	1.487	1.113	158.3	154.8
PCM-mPW1PW91/6-31G*	1.579	1.344	1.185	1.237	1.531	1.097	160.1	154.6
B3LYP/6-311+G**	1.610	1.344	1.177	1.249	1.507	1.098	158.5	154.2
PCM-B3LYP/6-31G*	1.601	1.351	1.167	1.275	1.545	1.098	159.8	154.7

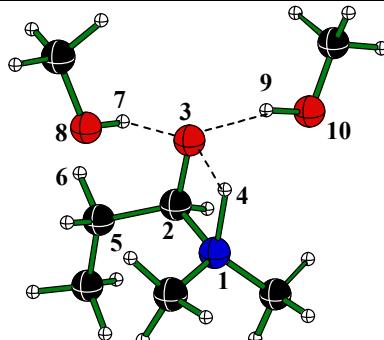
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**Table S26.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ie** Computed at the Various Levels of Theories



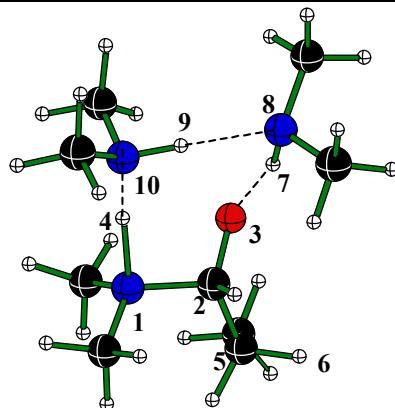
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>9</sub> -N <sub>10</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub> -N <sub>10</sub>
mPW1PW91/6-31G*	1.548	1.378	1.331	1.235	1.994	1.024	1.993	1.024	115.8	157.4	161.3
mPW1PW91/6-311+G**	1.549	1.376	1.330	1.224	2.043	1.020	2.046	1.020	116.3	156.4	160.6
MP2/6-31G*	1.544	1.394	1.345	1.246	1.991	1.026	1.993	1.026	114.8	157.3	161.9
PCM-mPW1PW91/6-31G*	1.542	1.384	1.322	1.243	1.998	1.024	1.997	1.023	115.8	159.8	164.6
B3LYP/6-311+G**	1.567	1.385	1.330	1.238	2.080	1.021	2.080	1.022	116.4	157.4	160.9
PCM-B3LYP/6-31G*	1.560	1.392	1.325	1.254	2.037	1.025	2.029	1.251	115.9	164.4	160.3

**Table S27.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-If** Computed at the Various Levels of Theories



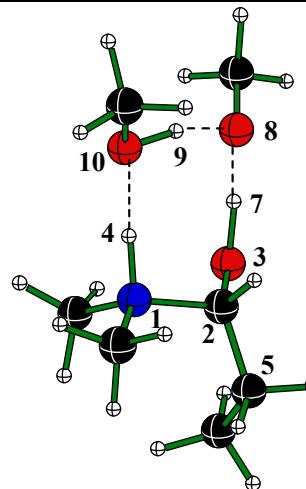
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub> -O <sub>10</sub>
mPW1PW91/6-31G*	1.536	1.397	1.306	1.254	1.777	0.984	1.785	0.983	115.9	161.6	157.1
mPW1PW91/6-311+G**	1.535	1.395	1.305	1.245	1.776	0.978	1.781	0.977	116.1	162.6	158.5
MP2/6-31G*	1.532	1.410	1.318	1.268	1.801	0.988	1.807	0.988	114.8	163.9	157.8
PCM-mPW1PW91/6-31G*	1.528	1.399	1.301	1.264	1.760	0.986	1.744	0.985	114.9	166.4	166.5
B3LYP/6-311+G**	1.552	1.403	1.306	1.258	1.809	0.980	1.808	0.980	116.7	162.0	158.5
PCM-B3LYP/6-31G*	1.545	1.411	1.298	1.275	1.799	0.987	1.790	0.987	115.9	164.7	160.7

**Table S28.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ig** Computed at the Various Levels of Theories



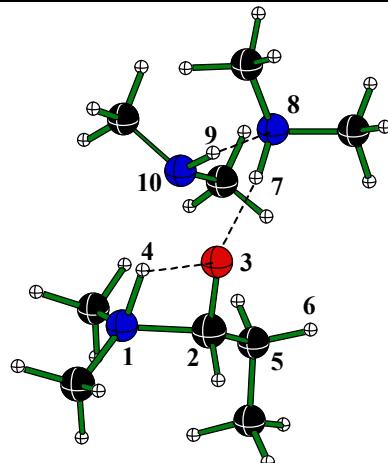
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -N <sub>10</sub>	N <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub> -N <sub>10</sub>	N <sub>10</sub> -H <sub>4</sub> -N <sub>1</sub>
mPW1PW91/6-31G*	1.570	1.315	1.731	1.048	1.793	1.060	1.200	1.426	159.2	164.9	173.3
mPW1PW91/6-311+G**	1.565	1.317	1.731	1.045	1.805	1.056	1.200	1.422	160.6	166.4	174.2
MP2/6-31G*	1.564	1.327	1.770	1.045	1.835	1.054	1.214	1.403	158.6	164.1	172.5
PCM-mPW1PW91/6-31G*	1.565	1.317	1.761	1.045	1.815	1.055	1.216	1.400	161.0	164.3	174.0
B3LYP/6-311+G**	1.596	1.319	1.780	1.043	1.854	1.053	1.196	1.450	160.3	166.8	174.6
PCM-B3LYP/6-31G*	1.594	1.319	1.801	1.044	1.861	1.054	1.216	1.422	161.2	163.8	174.1

**Table S29.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ih** Computed at the Various Levels of Theories



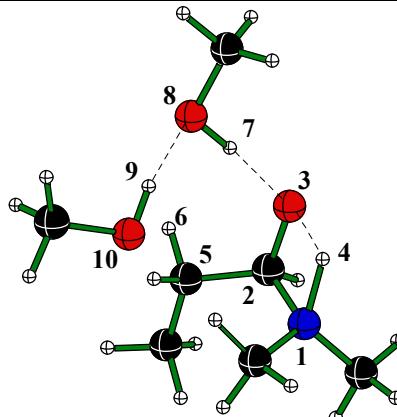
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub> -N <sub>1</sub>
mPW1PW91/6-31G*	1.578	1.339	1.123	1.308	1.283	1.136	1.497	1.100	171.7	168.5	173.7
mPW1PW91/6-311+G**	1.575	1.339	1.118	1.299	1.291	1.119	1.508	1.100	171.6	167.1	174.7
MP2/6-31G*	1.568	1.354	1.123	1.329	1.301	1.138	1.506	1.100	170.8	169.1	175.5
PCM-mPW1PW91/6-31G*	1.532	1.349	1.087	1.374	1.303	1.123	1.532	1.100	172.8	169.9	174.9
B3LYP/6-311+G**	1.596	1.347	1.096	1.354	1.283	1.137	1.533	1.088	170.9	166.9	174.9
PCM-B3LYP/6-31G*	1.584	1.357	1.074	1.423	1.285	1.147	1.543	1.093	172.7	170.0	174.8

**Table S30.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-II** Computed at the Various Levels of Theories



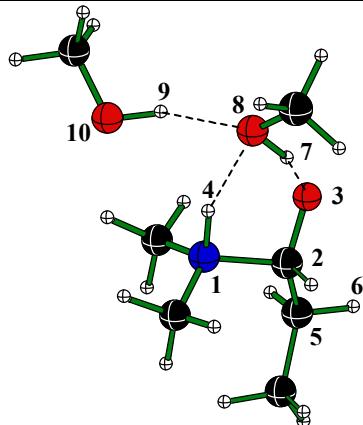
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -N <sub>10</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub> -N <sub>10</sub>
mPW1PW91/6-31G*	1.567	1.361	1.351	1.218	1.889	1.028	2.033	1.029	115.6	174.5	171.3
mPW1PW91/6-311+G**	1.561	1.364	1.346	1.212	1.929	1.024	2.094	1.025	116.1	173.4	172.5
MP2/6-31G*	1.564	1.376	1.364	1.224	1.894	1.030	2.025	1.030	114.9	175.3	171.7
PCM-mPW1PW91/6-31G*	1.556	1.370	1.337	1.229	1.900	1.028	2.041	1.028	115.7	175.1	171.0
B3LYP/6-311+G**	1.579	1.373	1.341	1.229	1.964	1.025	2.148	1.025	116.2	173.6	172.9
PCM-B3LYP/6-31G*	1.574	1.377	1.338	1.241	1.928	1.030	2.089	1.030	115.9	176.3	171.1

**Table S31.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ij** Computed at the Various Levels of Theories



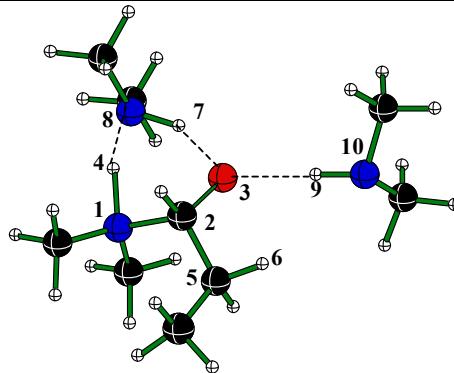
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>	N <sub>1</sub> -H <sub>4</sub> -O <sub>3</sub>
mPW1PW91/6-31G*	1.559	1.375	1.332	1.232	1.635	1.001	1.711	0.988	176.7	169.6	115.4
mPW1PW91/6-311+G**	1.549	1.378	1.326	1.226	1.638	0.994	1.741	0.980	173.7	168.7	115.4
MP2/6-31G*	1.549	1.388	1.349	1.239	1.665	1.002	1.742	0.990	176.9	170.3	114.1
PCM-mPW1PW91/6-31G*	1.542	1.384	1.316	1.246	1.626	1.003	1.720	0.987	177.4	172.0	115.4
B3LYP/6-311+G**	1.566	1.387	1.324	1.241	1.672	0.994	1.774	0.981	173.2	168.3	116.1
PCM-B3LYP/6-31G*	1.559	1.392	1.319	1.257	1.649	1.004	1.742	0.990	177.9	172.0	115.5

**Table S32.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Ik** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub> -N <sub>1</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>
mPW1PW91/6-31G*	1.606	1.328	1.235	1.184	1.727	1.050	1.737	0.986	162.6	150.6	157.6
mPW1PW91/6-311+G**	1.598	1.331	1.211	1.194	1.736	1.047	1.715	0.983	163.4	151.1	161.4
MP2/6-31G*	1.587	1.343	1.242	1.197	1.740	1.051	1.752	0.991	162.2	151.1	157.6
PCM-mPW1PW91/6-31G*	1.608	1.331	1.251	1.167	1.740	1.049	1.721	0.986	162.6	149.9	166.8
B3LYP/6-311+G**	1.621	1.340	1.180	1.243	1.738	1.050	1.732	0.987	162.7	151.3	161.6
PCM-B3LYP/6-31G*	1.632	1.339	1.215	1.213	1.745	1.052	1.727	0.991	162.4	149.9	166.9

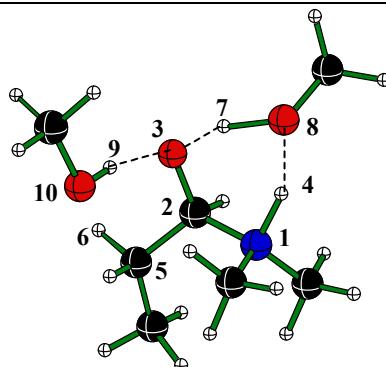
**Table S33.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-II** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>9</sub>	H <sub>9</sub> -N <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>4</sub> -N <sub>1</sub>	O <sub>3</sub> -H <sub>9</sub> -N <sub>10</sub>
mPW1PW91/6-31G*	1.575	1.335	1.538	1.094	1.263	1.343	1.908	1.026	147.2	158.3	174.2
mPW1PW91/6-311+G**	1.571	1.336	1.527	1.092	1.271	1.326	1.935	1.023	148.7	159.4	177.2
MP2/6-31G*	1.565	1.348	1.578	1.086	1.262	1.348	1.916	1.027	144.9	158.4	174.4
PCM-mPW1PW91/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—
B3LYP/6-311+G**	1.599	1.339	1.574	1.084	1.256	1.363	1.963	1.024	147.1	159.4	178.0
PCM-B3LYP/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—

<sup>a</sup> The transition state could not be located at this level of theory.

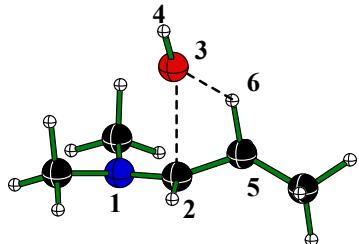
**Table S34.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-Im** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -N <sub>1</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub> -N <sub>1</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>
mPW1PW91/6-31G*	1.555	1.360	1.193	1.230	1.400	1.148	1.790	0.981	157.4	155.7	166.8
mPW1PW91/6-311+G**	1.555	1.360	1.172	1.237	1.419	1.128	1.777	0.977	158.4	156.5	165.7
MP2/6-31G*	1.550	1.372	1.182	1.261	1.430	1.137	1.817	0.985	157.9	156.6	160.2
PCM-mPW1PW91/6-31G*	1.549	1.369	1.148	1.281	1.427	1.135	1.773	0.983	158.3	156.8	165.4
B3LYP/6-311+G**	1.568	1.376	1.133	1.321	1.453	1.131	1.812	0.984	157.8	156.7	164.6
PCM-B3LYP/6-31G*	1.576	1.369	1.152	1.279	1.447	1.122	1.817	0.978	157.7	156.1	164.6

**Table S35.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-II** Computed at the Various Levels of Theories

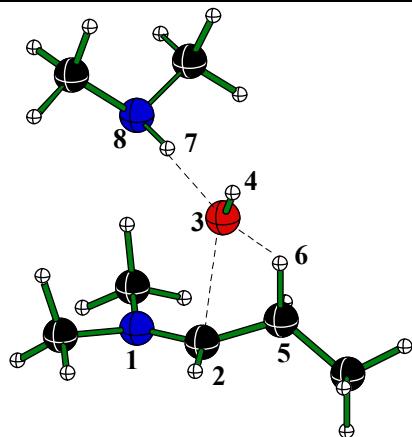
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Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	C <sub>5</sub> -H <sub>6</sub> -O <sub>3</sub>
mPW1PW91/6-31G*	1.330	1.438	1.251	1.444	2.215	137.0
mPW1PW91/6-311+G**	1.313	1.437	1.194	1.535	2.332	136.3
MP2/6-31G*	1.324	1.435	1.222	1.477	2.241	134.1
PCM-mPW1PW91/6-31G*	1.323	1.440	1.238	1.481	2.288	139.7
B3LYP/6-311+G**	1.316	1.443	1.189	1.563	2.410	137.4
PCM-B3LYP/6-31G*	1.325	1.446	1.228	1.520	2.368	140.6

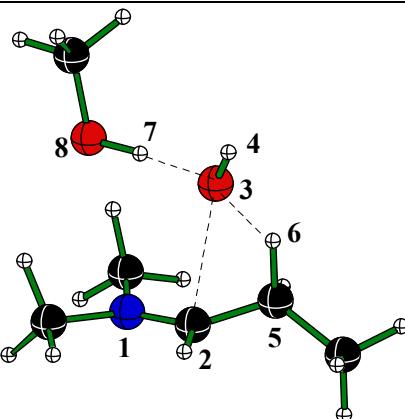
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**Table S36.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIa** Computed at the Various Levels of Theories



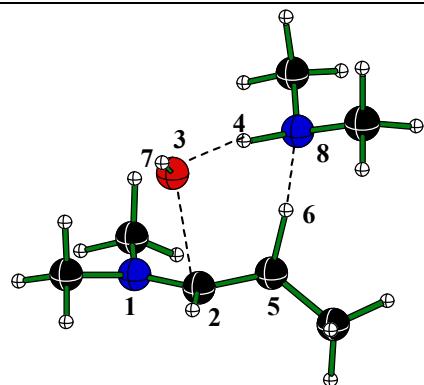
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>4</sub>	C <sub>5</sub> -H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>
mPW1PW91/6-31G*	1.310	1.443	1.200	1.564	2.381	1.767	1.042	0.966	139.1	171.3
mPW1PW91/6-311+G**	1.302	1.443	1.175	1.600	2.487	1.815	1.038	0.959	140.7	172.8
MP2/6-31G*	1.305	1.441	1.196	1.589	2.423	1.714	1.044	0.972	140.8	172.9
PCM-mPW1PW91/6-31G*	1.306	1.448	1.189	1.585	2.439	1.741	1.047	0.967	140.2	174.1
B3LYP/6-311+G**	1.306	1.449	1.171	1.622	2.564	1.849	1.038	0.963	141.8	172.9
PCM-B3LYP/6-31G*	1.311	1.450	1.186	1.600	2.495	1.765	1.047	0.972	140.7	174.7

**Table S37.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIb** Computed at the Various Levels of Theories



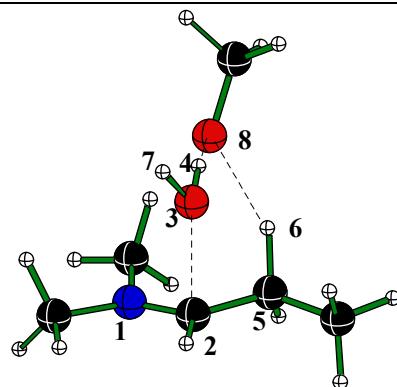
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>4</sub>	C <sub>5</sub> -H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>
mPW1PW91/6-31G*	1.302	1.449	1.176	1.592	2.518	1.445	1.058	0.965	140.9	173.4
mPW1PW91/6-311+G**	1.295	1.448	1.161	1.649	2.629	1.477	1.042	0.978	143.7	173.0
MP2/6-31G*	1.301	1.451	1.182	1.573	2.603	1.441	1.070	0.970	145.1	175.1
PCM-mPW1PW91/6-31G*	1.298	1.451	1.162	1.679	2.573	1.436	1.062	0.966	141.5	174.8
B3LYP/6-311+G**	1.300	1.453	1.160	1.667	2.694	1.516	1.035	0.962	144.8	172.9
PCM-B3LYP/6-31G*	1.303	1.456	1.165	1.679	2.612	1.475	1.056	0.971	142.1	174.4

**Table S38.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIc** Computed at the Various Levels of Theories



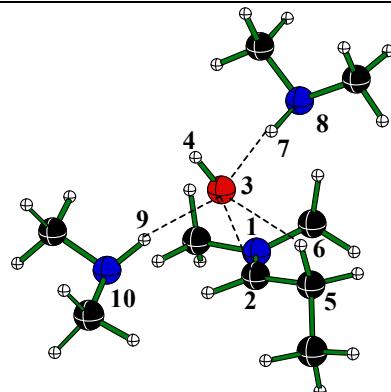
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	C <sub>5</sub> -H <sub>6</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>4</sub> -N <sub>8</sub>
mPW1PW91/6-31G*	1.338	1.426	1.292	1.437	1.186	1.316	2.305	0.967	169.8	162.9
mPW1PW91/6-311+G**	1.314	1.425	1.249	1.523	1.111	1.448	2.576	0.958	174.7	163.7
MP2/6-31G*	1.343	1.419	1.318	1.394	1.142	1.402	2.244	0.974	169.3	159.0
PCM-mPW1PW91/6-31G*	1.315	1.425	1.264	1.526	1.141	1.422	2.695	0.967	169.2	169.1
B3LYP/6-311+G**	1.318	1.426	1.264	1.518	1.110	1.469	2.721	0.962	175.5	164.7
PCM-B3LYP/6-31G*	1.322	1.427	1.282	1.508	1.156	1.408	2.736	0.972	169.9	168.8

**Table S39.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIId** Computed at the Various Levels of Theories



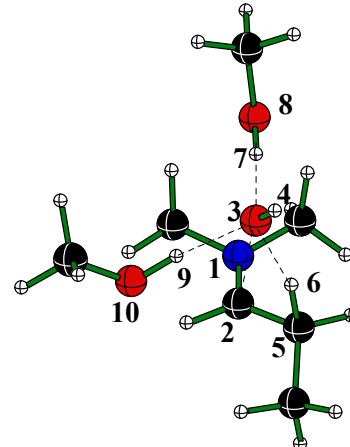
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	C <sub>5</sub> -H <sub>6</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>4</sub> -O <sub>8</sub>
mPW1PW91/6-31G*	1.302	1.458	1.152	1.690	1.502	1.038	2.510	0.964	154.3	166.6
mPW1PW91/6-311+G**	1.291	1.467	1.120	1.896	1.397	1.073	2.516	0.956	149.0	167.7
MP2/6-31G*	1.295	1.479	1.107	2.048	1.418	1.077	2.421	0.970	142.5	169.5
PCM-mPW1PW91/6-31G*	1.305	1.449	1.175	1.602	1.566	1.020	2.700	0.965	161.1	168.1
B3LYP/6-311+G**	1.296	1.478	1.116	1.928	1.363	1.099	2.521	0.961	147.9	168.8
PCM-B3LYP/6-31G*	1.305	1.455	1.171	1.638	1.602	1.019	2.799	0.970	158.6	168.3

**Table S40.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIe** Computed at the Various Levels of Theories



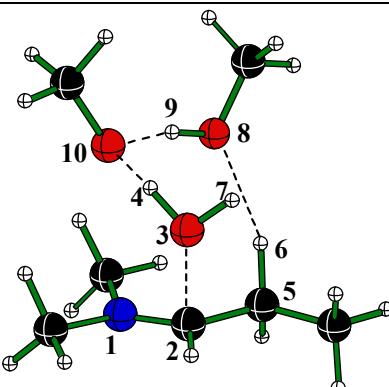
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>4</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub>	H <sub>9</sub> -N <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub> -N <sub>10</sub>
mPW1PW91/6-31G*	1.300	1.469	1.119	1.833	2.450	0.968	1.778	1.046	1.801	1.042	178.9	168.6
mPW1PW91/6-311+G**	1.292	1.468	1.111	1.962	2.488	0.960	1.829	1.039	1.868	1.036	177.4	168.5
MP2/6-31G*	1.299	1.449	1.168	1.631	2.709	0.972	1.754	1.049	1.775	1.047	173.3	170.0
PCM-mPW1PW91/6-31G*	1.295	1.471	1.113	1.885	2.518	0.969	1.781	1.046	1.771	1.045	176.8	171.5
B3LYP/6-311+G**	1.297	1.474	1.110	1.984	2.526	0.964	1.870	1.039	1.929	1.034	177.1	168.6
PCM-B3LYP/6-31G*	1.300	1.477	1.114	1.895	2.554	0.973	1.811	1.046	1.808	1.044	176.9	171.0

**Table S41.** Selected Bond Distances and Angles (in Å and °) of Transition State TS-IIIf Computed at the Various Levels of Theories



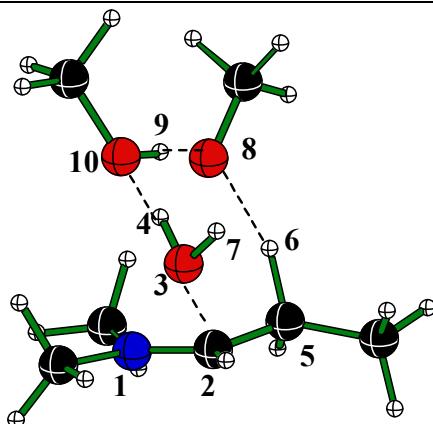
Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>4</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub> -O <sub>8</sub>	O <sub>3</sub> -H <sub>9</sub> -O <sub>10</sub>
mPW1PW91/6-31G*	1.294	1.455	1.153	1.730	2.870	0.964	1.508	1.034	1.544	1.026	174.0	168.9
mPW1PW91/6-311+G**	1.297	1.439	1.184	1.607	2.983	0.958	1.578	1.010	1.605	1.005	172.5	167.4
MP2/6-31G*	1.307	1.431	1.233	1.471	2.895	0.971	1.598	1.017	1.650	1.007	174.2	165.9
PCM-mPW1PW91/6-31G*	1.288	1.476	1.107	2.130	2.705	0.965	1.475	1.047	1.500	1.038	175.2	172.2
B3LYP/6-311+G**	1.306	1.437	1.205	1.552	3.031	0.962	1.631	1.000	1.661	1.000	171.8	166.2
PCM-B3LYP/6-31G*	1.290	1.485	1.105	2.184	2.720	0.970	1.495	1.049	1.527	1.037	174.6	171.8

**Table S42.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIg** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub> -O <sub>3</sub>
mPW1PW91/6-31G*	1.289	1.480	1.106	2.125	1.035	1.514	1.513	1.034	2.561	0.964	170.1	170.6
mPW1PW91/6-311+G**	1.291	1.484	1.099	2.175	1.009	1.579	1.339	1.097	2.362	0.957	169.8	171.8
MP2/6-31G*	1.300	1.489	1.095	2.241	1.006	1.671	1.352	1.107	2.228	0.973	171.1	173.3
PCM-mPW1PW91/6-31G*	1.287	1.480	1.105	2.165	1.039	1.497	1.552	1.024	2.744	0.966	172.4	172.8
B3LYP/6-311+G**	1.296	1.492	1.100	2.219	1.000	1.619	1.311	1.125	2.375	0.962	169.1	172.1
PCM-B3LYP/6-31G*	1.307	1.503	1.096	2.410	1.023	1.601	1.510	1.051	2.213	0.979	163.8	161.6

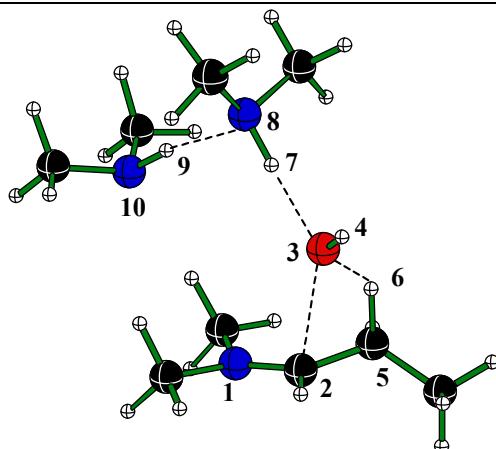
**Table S43.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIIg** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub> -O <sub>3</sub>
mPW1PW91/6-31G*	1.293	1.464	1.136	1.796	1.291	1.137	1.654	1.001	2.921	0.963	171.9	170.2
mPW1PW91/6-311+G**	1.294	1.450	1.159	1.674	1.361	1.085	1.657	0.994	3.021	0.956	172.8	169.0
MP2/6-31G*	1.306	1.436	1.221	1.491	1.491	1.047	1.766	0.991	3.059	0.969	173.6	169.6
PCM-mPW1PW91/6-31G*	1.302	1.440	1.202	1.542	1.464	1.048	1.719	0.991	3.057	0.965	173.2	172.2
B3LYP/6-311+G**	1.300	1.453	1.168	1.656	1.438	1.059	1.700	0.993	3.068	0.960	168.6	172.6
PCM-B3LYP/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—	—

<sup>a</sup> The transition state could not be located at this level of theory.

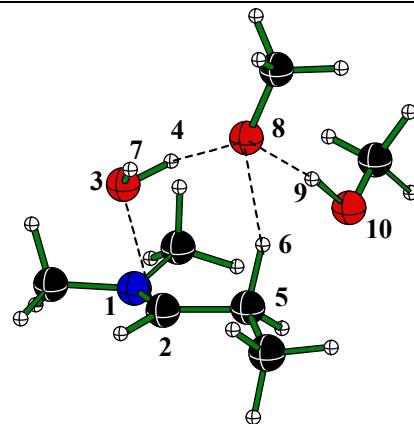
**Table S44.** Selected Bond Distances and Angles (in Å and °) for Transition State **TS-IIh** Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>	H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -N <sub>10</sub>	O <sub>3</sub> -H <sub>4</sub>	O <sub>3</sub> -H <sub>7</sub> -N <sub>8</sub>	N <sub>8</sub> -H <sub>9</sub> -N <sub>10</sub>
mPW1PW91/6-31G*	1.309	1.442	1.208	1.552	2.403	1.742	1.045	1.998	1.032	0.967	177.5	175.9
mPW1PW91/6-311+G**	1.301	1.445	1.176	1.600	2.524	1.803	1.040	2.023	1.030	0.960	177.5	176.9
MP2/6-31G*	1.298	1.454	1.163	1.628	2.557	1.739	1.053	2.164	1.025	0.973	173.2	160.0
PCM-mPW1PW91/6-31G*	1.305	1.445	1.197	1.575	2.458	1.715	1.050	2.003	1.032	0.968	177.1	177.2
B3LYP/6-311+G**	1.305	1.450	1.172	1.618	2.602	1.842	1.039	2.065	1.030	0.964	177.3	177.3
PCM-B3LYP/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—	—

<sup>a</sup> The transition state could not be located at this level of theory.

**Table S45.** Selected Bond Distances and Angles (in Å and °) for Transition State TS-IIIi Computed at the Various Levels of Theories



Level of theory	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>3</sub> -H <sub>7</sub>	O <sub>8</sub> -H <sub>4</sub> -O <sub>3</sub>	O <sub>8</sub> -H <sub>9</sub> -O <sub>10</sub>
mPW1PW91/6-31G*	1.297	1.471	1.116	1.911	1.525	1.033	2.443	1.632	1.005	0.964	170.8	173.2
mPW1PW91/6-311G**	1.292	1.472	1.106	2.009	1.459	1.043	2.414	1.625	1.005	0.957	173.3	172.8
mPW1PW91/6-311+G** <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—	—
MP2/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—	—
PCM-mPW1PW91/6-31G*	1.296	1.485	1.101	2.099	1.492	1.042	2.345	1.611	1.008	0.966	173.4	175.7
B3LYP/6-311+G**	1.292	1.482	1.101	2.246	1.463	1.053	2.554	1.631	1.006	0.961	173.6	172.8
PCM-B3LYP/6-31G* <sup>a</sup>	—	—	—	—	—	—	—	—	—	—	—	—

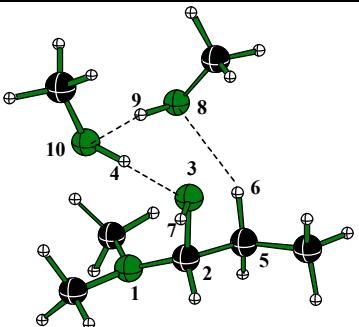
<sup>a</sup> The transition state could not be located at this level of theory.

**Table S46.** The Second-Order Perturbation Energy of Delocalization and C<sub>2</sub>-O<sub>3</sub> Bond Distances (in Å) for the Pre-reacting Complexes Computed at the NBO//mPW1PW91/6-311+G\*\* level of theory.<sup>a</sup>

PRC of	n <sub>N</sub> →σ*(C <sub>2</sub> -O <sub>3</sub> )	C <sub>2</sub> - O <sub>3</sub>
<b>TS-II</b>	16.96	1.433
<b>TS-IIa</b>	17.46	1.441
<b>TS-IIb</b>	18.67	1.448
<b>TS-IIc</b>	17.83	1.441
<b>TS-IId</b>	19.06	1.450
<b>TS-IIe</b>	15.75	1.426
<b>TS-IIf</b>	21.12	1.468
<b>TS-IIg</b>	19.86	1.467
<b>TS-IIh</b>	15.39	1.420
<b>TS-IIi</b>	19.86	1.467

<sup>a</sup> The second order perturbation energies and bond distance are reported respectively in kcal mol<sup>-1</sup> and Å.

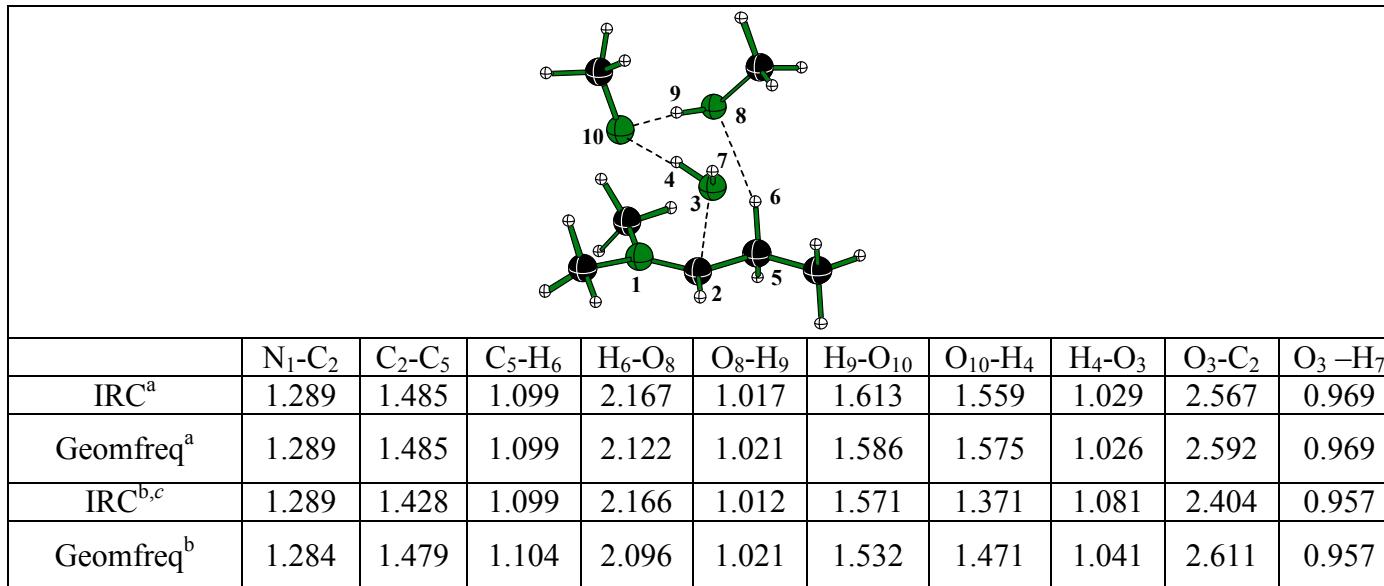
**Table S47.** Selected Bond Distances (in Å) for Pre-Reacting Complex Obtained through Intrinsic Reaction Coordinate (IRC) and *geomfreq* Calculations on **TS-IIg** Performed at the MP2(full)/6-31G\* and mPW1PW91/6-311+G\*\* Levels of Theories



	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>
IRC <sup>a</sup>	1.388	1.511	1.092	2.299	0.984	1.771	0.999	1.562	1.653	0.976
Geomfreq <sup>a</sup>	1.435	1.516	1.092	2.436	0.983	1.834	0.984	1.809	1.462	0.974
IRC <sup>b</sup>	1.407	1.520	1.093	2.262	0.975	1.737	0.979	1.661	1.488	0.960
Geomfreq <sup>b</sup>	1.419	1.522	1.093	2.487	0.972	1.816	0.975	1.809	1.466	0.959

<sup>a</sup>MP2(full)/6-31G\* <sup>b</sup>mPW1PW91/6-311+G\*\* (See computational section for further details)

**Table S48.** Selected Bond Distances (in Å) of Iminium Ion Intermediate Obtained through Intrinsic Reaction Coordinate (IRC) and *geomfreq* Calculation on TS-IIg Performed at the MP2(full)/6-31G\* and mPW1PW91/6-311+G\*\* Levels of Theories



<sup>a</sup> MP2(full)/6-31G\*<sup>b</sup> mPW1PW91/6-311+G\*\*<sup>c</sup> The IRC runs were normally terminated within eleven optimization steps in this case. (See computational section for further details)

**Table S49.** Selected Bond Distances (in Å) of Iminium Ion Intermediate Obtained through Intrinsic Reaction Coordinate (IRC) and *geomfreq* Calculation on **TS-IIIg** Performed at the MP2(full)/6-31G\* and mPW1PW91/6-311+G\*\* Levels of Theories

	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>
IRC <sup>a</sup>	1.292	1.478	1.107	1.906	1.089	1.380	1.648	1.014	2.958	0.967
<i>geomfreq</i> <sup>a</sup>	1.289	1.485	1.099	2.122	1.021	1.586	1.574	1.026	2.592	0.969
IRC <sup>b,c</sup>	1.293	1.453	1.152	1.705	1.340	1.096	1.650	0.995	3.013	0.956
<i>geomfreq</i> <sup>b</sup>	1.284	1.475	1.106	2.138	1.043	1.453	1.466	1.042	2.903	0.956

<sup>a</sup> MP2(full)/6-31G\* <sup>b</sup> mPW1PW91/6-311+G\*\* (See computational section for further details) <sup>c</sup> The IRC runs were normally terminated within five optimization steps in this case.

**Table S50.** Selected Bond Distances (in Å) of Enamine obtained by Intrinsic Reaction Coordinate (IRC) and *geomfreq* Calculation on **TS-IIIg** Performed at the MP2(full)/6-31G\* and mPW1PW91/6-311+G\*\* Level of Theories

	N <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>5</sub>	C <sub>5</sub> -H <sub>6</sub>	H <sub>6</sub> -O <sub>8</sub>	O <sub>8</sub> -H <sub>9</sub>	H <sub>9</sub> -O <sub>10</sub>	O <sub>10</sub> -H <sub>4</sub>	H <sub>4</sub> -O <sub>3</sub>	O <sub>3</sub> -C <sub>2</sub>	O <sub>3</sub> -H <sub>7</sub>
IRC <sup>a, b</sup>	1.357	1.365	1.894	0.995	1.663	0.987	1.792	0.984	3.110	0.968
Geomfreq <sup>a</sup>	1.383	1.357	2.185	0.985	1.789	0.987	1.823	0.984	3.318	0.969
IRC <sup>c,d</sup> (maxpoints=5)	1.295	1.445	1.170	1.635	1.385	1.072	1.666	0.992	3.033	0.956
Geomfreq <sup>c</sup>	1.369	1.352	2.185	0.975	1.764	0.977	1.788	0.977	3.393	0.957

<sup>a</sup> MP2(full)/6-31G\* <sup>b</sup> The IRC runs were normally terminated within fifteen optimization steps in this case. <sup>c</sup> mPW1PW91/6-311+G\*\*

(See computational section for further details) <sup>d</sup> The IRC runs were normally terminated within five optimization steps in this case.

**Table S51.** Computed Activation Parameters (in kcal mol<sup>-1</sup>)<sup>a</sup> with Respect to the Pre-Reacting Complexes for the Carbinolamine Formation (Step-I) and the Dehydration (step-II) Steps Obtained at the mPW1PW91/6-311+G\*\* Level of Theory

	$\Delta E^\ddagger$	$\Delta H^\ddagger$	$\Delta G^\ddagger$		$\Delta E^\ddagger$	$\Delta H^\ddagger$	$\Delta G^\ddagger$
<b>TS-I</b>	27.9	26.0	32.6	<b>TS-II</b>	47.4	43.0	42.7
<b>TS-Ia</b>	22.0	20.2	28.1	<b>TS-IIa</b>	42.1	38.6	40.0
<b>TS-Ib</b>	22.4	20.7	26.3	<b>TS-IIb</b>	35.8	31.9	33.2
<b>TS-Ic</b>	15.1	11.9	19.9	<b>TS-IIc</b>	44.2	38.5	40.8
<b>TS-Id</b>	11.4	9.0	16.2	<b>TS-IId</b>	35.3	31.9	32.1
<b>TS-Ie</b>	23.8	22.1	27.9	<b>TS-IIe</b>	40.0	37.3	39.2
<b>TS-If</b>	19.5	16.8	15.5	<b>TS-IIf</b>	25.7	21.7	23.5
<b>TS-Ig</b>	9.6	7.2	17.1	<b>TS-IIg</b>	21.5	18.8	21.9
<b>TS-Ih</b>	6.5	2.9	11.0	<b>TS-IIIg</b>	1.6	0.05	1.9
<b>TS-Ii</b>	23.1	21.4	27.8	<b>TS-IIh</b>			
<b>TS-Ij</b>	22.7	20.7	24.9	<b>TS-IIi</b>	28.9	25.6	27.2
<b>TS-Ik</b>	8.0	6.2	11.8	—	—	—	—
<b>TS-IIl</b>	12.3	9.5	19.0	—	—	—	—
<b>TS-Im</b>	4.0	0.4	2.3	—	—	—	—

**Table S52.** The mPW1PW91/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Transition States for Carbinolamine Formation (**Step-I**)

TS-I			TS-Ia				TS-Ib				
Et = -328.1754406 NImag = 1(-1525.2)			Et = -463.3202378 NImag= 1(-1532.5)				Et = -443.8848394 NImag= 1(-1540.1)				
6	-0.313868	0.736043	-0.445833	6	1.093368	0.250350	0.876554	6	-0.675067	0.267303	-0.850450
6	-1.586762	0.258456	0.239882	6	0.924922	1.567186	0.134146	6	-0.630756	1.566384	-0.063799
1	-0.377260	0.469219	-1.526932	1	2.022486	0.304005	1.481759	1	-1.532870	0.302637	-1.549447
1	-1.481764	0.359689	1.324852	1	0.120992	1.477640	-0.603074	1	0.129330	1.506044	0.720267
6	-2.037251	-1.144497	-0.149837	6	2.204003	2.103269	-0.499843	6	-1.980653	2.009061	0.490280
1	-1.324364	-1.912497	0.170545	1	2.583198	1.444997	-1.289052	1	-2.369067	1.314911	1.243306
1	-3.002234	-1.390958	0.302171	1	2.037670	3.085514	-0.950983	1	-1.904346	2.990638	0.965898
1	-2.149628	-1.235175	-1.235653	1	2.998773	2.213322	0.245863	1	-2.730421	2.085163	-0.304851
8	0.109090	1.972484	-0.160153	8	0.011980	-0.225535	1.546144	8	0.492223	-0.142623	-1.436485
7	1.028188	0.001168	0.001639	7	1.304191	-1.020987	-0.014576	7	-0.904529	-1.040204	-0.036198
6	1.075624	-0.437803	1.394779	6	0.719694	-0.986372	-1.359725	6	-0.410010	-1.040302	1.346029
1	0.683397	0.369364	2.014945	1	-0.309610	-0.618918	-1.291903	1	0.604147	-0.632674	1.355525
1	0.490818	-1.348902	1.553245	1	1.306599	-0.352278	-2.031433	1	-1.061437	-0.455907	2.002590
1	2.113628	-0.628945	1.679304	1	0.708219	-2.003580	-1.759821	1	-0.383880	-2.072438	1.704256
6	1.642083	-0.934609	-0.935408	6	2.625385	-1.643221	0.033166	6	-2.198566	-1.699791	-0.195903
1	1.104764	-1.888239	-0.949160	1	3.355225	-1.063611	-0.541299	1	-2.983337	-1.166188	0.349933
1	1.621619	-0.500741	-1.937053	1	2.956691	-1.706250	1.071619	1	-2.458835	-1.732840	-1.255616
1	2.680760	-1.118966	-0.648877	1	2.569360	-2.651578	-0.383878	1	-2.135458	-2.721372	0.185858
1	1.240617	1.183229	-0.048273	1	0.460774	-1.287055	0.822116	1	0.020468	-1.244198	-0.814851
1	-2.349343	0.989336	-0.050859	1	0.563131	2.272570	0.890466	1	1.795408	0.241677	-0.382754
7	-2.344783	-0.016311	-0.205687	1	-1.639414	0.019538	0.538202	8	2.386933	0.368625	0.402786
				7	-2.344783	-0.016311	-0.205687	6	3.649875	-0.159976	0.102614

	6 -3.174367 -1.188287 -0.022964 1 -3.822371 -1.331791 -0.896276 1 -2.541921 -2.075912 0.072890 1 -3.827633 -1.141619 0.867363 6 -3.120536 1.205133 -0.220219 1 -2.451249 2.068313 -0.281547 1 -3.771791 1.225861 -1.102504 1 -3.765639 1.337852 0.667492	1 4.138997 0.364850 -0.731548 1 4.284139 -0.044863 0.986760 1 3.617504 -1.231415 -0.150064 1 -0.260827 2.313315 -0.774902
<b>TS-Ic</b> Et = -463.3363045 Nmag=1( -1191.3)	<b>TS-Id</b> Et = -443.9062179 Nmag = 1( -872.9)	<b>TS-Ie</b> Et =-598.4607337 Nmag=1(-1549.4)
6 -0.798898 -0.759549 0.157861 6 -2.261421 -0.991974 -0.249495 1 -0.741018 -0.801512 1.276705 1 -2.346431 -0.841922 -1.331422 6 -3.350451 -0.226823 0.495397 1 -3.416306 0.821348 0.188047 1 -4.332997 -0.672339 0.310085 1 -3.184713 -0.245297 1.578617 8 0.024739 -1.560320 -0.496105 7 -0.317979 0.742279 -0.074621 6 -0.513096 1.156171 -1.458607 1 -0.256067 0.300925 -2.088169 1 -1.550922 1.453738 -1.652699 1 0.138912 2.002166 -1.701791 6 -0.745126 1.747555 0.888719 1 -1.771969 2.085911 0.717679 1 -0.683052 1.328779 1.897113 1 -0.085671 2.621550 0.834038 1 0.972715 0.487299 0.073921 1 1.370726 -1.059991 -0.112200 7 2.044985 -0.208076 0.128377	6 0.408638 -0.728280 -0.137323 6 1.870302 -1.071610 0.129745 1 0.207942 -0.778124 -1.228904 1 2.070607 -0.937378 1.197906 6 2.934692 -0.387204 -0.720933 1 3.100080 0.656003 -0.434913 1 3.895446 -0.898466 -0.611859 1 2.675441 -0.406351 -1.785148 8 -0.405756 -1.459559 0.626155 7 0.048120 0.795564 0.141722 6 0.396971 1.204307 1.508517 1 0.115243 0.384495 2.169961 1 1.467668 1.407218 1.588664 1 -0.165194 2.101357 1.776205 6 0.429311 1.774776 -0.880868 1 1.493289 2.007086 -0.829573 1 0.197079 1.368411 -1.867202 1 -0.144347 2.693075 -0.732248 1 -1.056671 0.666928 0.127428 1 -1.491907 -0.951775 0.500919 8 -2.319733 -0.075511 0.328673	6 -0.178476 0.831069 -0.394853 6 0.878622 1.635386 -1.133369 1 -1.176162 1.228383 -0.651691 1 1.873661 1.384397 -0.754148 6 0.638623 3.141628 -1.121802 1 0.678322 3.560923 -0.111069 1 1.391292 3.663376 -1.719451 1 -0.343571 3.387072 -1.539662 8 -0.088700 -0.539475 -0.510845 7 -0.125368 0.861941 1.151927 6 1.142156 1.239375 1.784187 1 1.955747 0.667728 1.327540 1 1.333239 2.312906 1.690915 1 1.084343 0.986918 2.845809 6 -1.312749 1.423794 1.800589 1 -1.335554 2.514260 1.700523 1 -2.198953 0.982511 1.334724 1 -1.294435 1.168774 2.863023 1 -0.157569 -0.321761 0.800850 1 0.845475 1.265107 -2.163994 1 1.822857 -1.093958 -0.392679

6 2.652858 -0.300425 1.446155	6 -3.144480 -0.331754 -0.768105	7 2.788838 -1.181359 -0.064992			
1 3.406299 -1.096891 1.484996	1 -3.886128 -1.110160 -0.536166	6 2.904489 -2.347580 0.785431			
1 3.137898 0.643254 1.720956	1 -3.702042 0.572093 -1.051827	1 3.890211 -2.365368 1.265493			
1 1.880660 -0.524173 2.186193	1 -2.593037 -0.671337 -1.663524	1 2.149671 -2.304428 1.576324			
1 -2.400172 -2.066913 -0.094447	1 1.910994 -2.152871 -0.036583	1 2.780953 -3.307179 0.251371			
6 2.993100 0.040952 -0.945771		6 3.692105 -1.238736 -1.195093			
1 2.464892 0.002995 -1.900799		1 3.518734 -0.381190 -1.851616			
1 3.462057 1.025631 -0.837659		1 4.730605 -1.186920 -0.846992			
1 3.786410 -0.716854 -0.962157		1 3.593800 -2.157354 -1.801551			
		1 -2.040485 -0.941058 -0.502115			
		7 -3.022960 -0.850689 -0.229299			
		6 -3.842169 -0.628742 -1.402490			
		1 -3.887163 -1.493205 -2.089529			
		1 -4.870862 -0.397405 -1.101401			
		1 -3.459891 0.228403 -1.964443			
		6 -3.427874 -2.031689 0.504356			
		1 -3.465689 -2.950798 -0.108257			
		1 -2.734284 -2.207709 1.331821			
		1 -4.426629 -1.882915 0.931768			
<b>TS-If</b>		<b>TS-Ig</b>		<b>TS-Ih</b>	
Et = -559.5866287 NIImg=1(-1555.0)		Et = -598.4854992 NIImg=1(-466.0)		Et = -559.6177063 NIImg=1(-658.3)	
6 0.040441 -0.657138 -0.540695	6 -1.080266 -0.686322 0.316022	6 0.921872 -0.344468 -0.630971			
6 -1.206581 -1.148239 -1.251522	6 -2.372580 -1.533793 0.469760	6 2.392035 -0.535409 -1.001916			
1 0.916893 -1.198717 -0.926373	1 -0.543013 -0.770666 1.301000	1 0.370817 -0.029938 -1.535646			
1 -2.102320 -0.718361 -0.795350	1 -2.050302 -2.466221 0.949624	1 2.363531 -1.256280 -1.826197			
6 -1.297029 -2.667420 -1.354726	6 -3.046790 -1.891178 -0.849396	6 3.286269 -1.095311 0.098576			
1 -1.372407 -3.147943 -0.373828	1 -2.273985 -2.184636 -1.563743	1 2.797191 -1.945951 0.577927			
1 -2.177878 -2.965020 -1.929911	1 -3.750973 -2.719836 -0.721257	1 4.236809 -1.436556 -0.321200			
1 -0.417538 -3.083026 -1.857737	1 -3.603247 -1.054214 -1.281363	1 3.522329 -0.355755 0.869192			
8 0.234911 0.725985 -0.543822	8 -0.357662 -0.975217 -0.744185	8 0.401980 -1.426226 -0.038118			
7 0.098815 -0.805823 0.987135	7 -1.370057 0.856565 0.341560	7 0.668933 0.911011 0.290253			

6 -1.169838 -0.959900 1.705361	6 -2.158884 1.296533 -0.801192	6 0.970094 0.683768 1.714902
1 -1.862180 -0.183335 1.373012	1 -1.810119 0.739381 -1.672685	1 0.712456 -0.351076 1.937553
1 -1.605330 -1.951636 1.551176	1 -3.231208 1.109349 -0.656772	1 2.025884 0.863176 1.921391
1 -0.975873 -0.824933 2.771890	1 -2.024826 2.372042 -0.970763	1 0.355545 1.359110 2.313080
6 1.185321 -1.653181 1.483608	6 -1.899976 1.363269 1.595967	6 1.236491 2.164999 -0.219343
1 0.977208 -2.712434 1.299162	1 -2.948205 1.074768 1.755559	1 2.319878 2.178580 -0.086795
1 2.107638 -1.356607 0.979370	1 -1.307280 0.967471 2.426853	1 0.998216 2.261851 -1.280708
1 1.295854 -1.497446 2.559139	1 -1.847168 2.458218 1.619553	1 0.796319 3.006001 0.320895
1 0.353710 0.391141 0.712631	1 -0.020593 1.260200 0.118955	1 -0.425241 1.017935 0.245065
1 -1.359302 1.481332 -0.327077	1 1.241503 -1.292738 -0.160260	1 -0.707461 -1.440453 -0.212559
8 -2.269459 1.663621 0.000418	7 2.213247 -1.106324 0.184419	8 -1.989506 -1.267817 -0.403156
6 -2.423283 3.048761 0.164421	6 3.167687 -1.537565 -0.820219	6 -2.746138 -2.142195 0.382293
1 -2.317313 3.599050 -0.781956	1 2.891166 -1.120445 -1.792166	1 -2.490310 -2.093549 1.454468
1 -3.431731 3.230823 0.546098	1 4.175980 -1.185362 -0.569336	1 -3.818496 -1.918892 0.291297
1 -1.708538 3.475497 0.884622	1 3.216549 -2.633995 -0.926675	1 -2.598884 -3.181315 0.056961
1 -1.148627 -0.715131 -2.256091	1 -3.080633 -1.069694 1.170311	1 2.811208 0.385067 -1.424908
1 2.010475 0.734881 -0.726918	1 1.637885 0.589133 0.097139	1 -2.070713 -0.050358 -0.007364
8 2.936222 0.430603 -0.596622	7 1.128023 1.485050 -0.148384	8 -1.921382 1.036350 0.289340
6 3.714447 1.538250 -0.227137	6 1.678540 2.614375 0.600378	6 -2.618410 1.861979 -0.603605
1 3.361929 2.020553 0.697864	1 1.122309 3.525713 0.365189	1 -2.377305 2.914629 -0.407647
1 4.735048 1.186553 -0.052497	1 1.593544 2.415169 1.670522	1 -2.382132 1.650796 -1.658541
1 3.754330 2.307051 -1.012827	1 2.733032 2.773420 0.353413	1 -3.704187 1.747277 -0.482182
	6 2.449855 -1.743663 1.466026	
	1 1.688299 -1.428311 2.184151	
	1 2.430728 -2.844854 1.412511	
	1 3.431133 -1.451160 1.860098	
	6 1.214564 1.634724 -1.606482	
	1 0.752327 0.744025 -2.035011	
	1 0.669725 2.528337 -1.922193	
	1 2.257280 1.721327 -1.927529	
<b>TS-Ii</b>	<b>TS-Ij</b>	<b>TS-Ik</b>

Et = -598.4590292 NIImg=1(-1520.83)				Et = -559.587708 NIImg=1(-1535.98)				Et = -559.6134955 NIImg=1(-608.22)			
6	1.789665	-0.957557	0.197104	6	1.318026	-0.887918	0.002022	6	1.470904	0.661238	-0.108324
6	1.357565	-0.314558	1.506352	6	0.709370	-0.595020	1.362637	6	2.859271	0.212034	-0.549410
1	2.726829	-1.523835	0.374726	1	2.228453	-1.498610	0.144468	1	1.518247	1.086932	0.916873
1	0.554970	0.405139	1.318481	1	-0.094460	0.141954	1.278090	1	2.767402	-0.336613	-1.492555
6	2.494068	0.306809	2.311156	6	1.727436	-0.184571	2.421858	6	3.711202	-0.554727	0.456347
1	2.965830	1.144355	1.786920	1	2.217520	0.764511	2.181242	1	3.384296	-1.589965	0.589437
1	2.133077	0.688689	3.270294	1	1.245120	-0.059302	3.394972	1	4.751725	-0.593820	0.121723
1	3.276152	-0.430420	2.523042	1	2.511536	-0.941226	2.536161	1	3.703842	-0.072788	1.440026
8	0.840283	-1.644944	-0.493831	8	0.479160	-1.392556	-0.963369	8	0.881064	1.423838	-1.021623
7	2.146255	0.029589	-0.966138	7	1.787197	0.332504	-0.835598	7	0.472097	-0.567671	0.158936
6	1.636849	1.403262	-0.895737	6	1.205420	1.644064	-0.526742	6	0.296091	-1.414339	-1.034892
1	0.584357	1.406935	-0.590767	1	0.124795	1.558706	-0.383726	1	0.288036	-0.747342	-1.897554
1	2.223781	2.006545	-0.195989	1	1.657081	2.074363	0.372224	1	1.120458	-2.125932	-1.108918
1	1.718390	1.850396	-1.890206	1	1.402412	2.311154	-1.369714	1	-0.660548	-1.930553	-0.951749
6	3.522454	-0.050423	-1.452305	6	3.221745	0.391759	-1.111753	6	0.615883	-1.339140	1.403618
1	4.215505	0.428800	-0.753162	1	3.781299	0.703187	-0.223712	1	1.413246	-2.075208	1.309600
1	3.800278	-1.099503	-1.571810	1	3.569242	-0.593359	-1.429019	1	0.847325	-0.654494	2.221660
1	3.597146	0.449540	-2.420986	1	3.406807	1.108769	-1.914794	1	-0.332090	-1.841129	1.606101
1	1.338574	-0.773287	-1.397673	1	1.070299	-0.359145	-1.561126	1	-0.405933	0.001135	0.251714
1	0.906179	-1.130558	2.082051	1	-1.142061	-1.210338	-0.856271	1	-0.288111	1.571766	-0.652719
1	-1.014205	-1.488199	-0.169523	8	-2.125811	-1.042476	-0.782787	8	-1.342642	1.397540	-0.142284
7	-2.031408	-1.364006	-0.083717	6	-2.707351	-2.120177	-0.092271	6	-1.641016	2.397067	0.791450
6	-2.668698	-1.877772	-1.280150	1	-2.329421	-2.220977	0.935667	1	-2.166438	3.243391	0.324966
1	-3.739427	-1.641681	-1.268571	1	-3.785894	-1.948588	-0.040482	1	-2.291293	2.000908	1.583057
1	-2.229140	-1.403495	-2.162108	1	-2.537490	-3.071265	-0.613231	1	-0.736663	2.800698	1.273230
1	-2.570747	-2.971198	-1.398575	1	0.231018	-1.533826	1.664813	1	3.358036	1.151488	-0.808069
6	-2.498572	-2.036979	1.111593	1	-2.122235	0.501182	-0.045530	1	-2.364457	-0.005312	-0.063221
1	-1.944379	-1.671861	1.981176	8	-1.941921	1.383513	0.360988	8	-2.630207	-0.929032	0.158228
1	-3.560324	-1.818466	1.276324	6	-3.021989	2.234384	0.081056	6	-3.918631	-1.173346	-0.342881
1	-2.388350	-3.135173	1.073670	1	-3.192395	2.363586	-0.997955	1	-4.178265	-2.210416	-0.111973

1 -1.888087 0.662611 -0.005307	1 -3.962105 1.882018 0.531014	1 -4.678763 -0.526553 0.119237
7 -1.666513 1.667744 -0.007218	1 -2.797268 3.216701 0.506604	1 -3.982673 -1.043978 -1.433427
6 -2.262097 2.285869 -1.173522		
1 -3.367287 2.300870 -1.158202		
1 -1.924699 3.325772 -1.263688		
1 -1.946054 1.753496 -2.075607		
6 -2.134695 2.269839 1.223634		
1 -1.725053 1.726589 2.080261		
1 -1.787825 3.308178 1.291212		
1 -3.235327 2.285083 1.325431		
<b>TS-II</b>		<b>TS-Im</b>
Et = -598.479191 NIImg=1(-1101.58)	Et = -559.6090286 NIImg=1(-1005.97)	
6 -0.206667 0.731226 -0.281242	6 0.093187 -0.375178 -0.270116	
6 0.519166 2.046029 0.034318	6 -0.640447 -1.691848 -0.051947	
1 -0.325629 0.663173 -1.391173	1 0.250016 -0.214801 -1.353956	
1 0.542692 2.178631 1.121972	1 -0.724442 -1.873567 1.024821	
6 0.038173 3.316922 -0.659042	6 -0.110544 -2.923563 -0.777792	
1 -0.890429 3.712295 -0.235151	1 0.807511 -3.321567 -0.334067	
1 0.788276 4.108819 -0.569488	1 -0.851187 -3.727273 -0.742998	
1 -0.129262 3.150553 -1.729385	1 0.089369 -2.714042 -1.834165	
8 0.392270 -0.313879 0.293304	8 -0.565050 0.644287 0.343425	
7 -1.716589 0.715862 0.165219	7 1.551518 -0.334610 0.268649	
6 -1.861806 1.027725 1.583099	6 1.641596 -0.726072 1.682889	
1 -1.053549 0.517956 2.111883	1 0.824745 -0.235888 2.212495	
1 -1.797352 2.106085 1.771652	1 1.565087 -1.810844 1.790810	
1 -2.828436 0.670115 1.953542	1 2.595789 -0.385137 2.089277	
6 -2.668686 1.434953 -0.672254	6 2.575410 -0.965926 -0.571474	
1 -2.641311 2.516738 -0.509342	1 2.532326 -2.053681 -0.504288	
1 -2.445032 1.237947 -1.724286	1 2.424196 -0.663513 -1.609219	
1 -3.685288 1.084487 -0.460797	1 3.561088 -0.626626 -0.244262	
1 -1.898770 -0.607569 0.028621	1 1.688791 0.804598 0.243795	

1	-0.560745	-1.487580	0.010134	1	0.193436	1.564828	0.326617
7	-1.595759	-1.828312	-0.086944	8	1.280154	2.141674	0.325285
6	-1.889896	-2.408948	-1.389780	6	1.463156	2.953907	-0.800571
1	-1.394800	-3.378996	-1.515117	1	0.896048	3.889229	-0.702831
1	-2.968292	-2.553012	-1.514600	1	2.522073	3.222732	-0.912134
1	-1.532764	-1.736708	-2.173181	1	1.140131	2.474849	-1.740817
1	1.556272	1.844941	-0.255656	1	-1.658202	-1.474468	-0.393570
6	-1.987490	-2.662030	1.041184	1	-2.251050	0.676696	-0.257422
1	-1.653665	-2.186172	1.965204	8	-3.147818	0.472038	-0.597155
1	-3.075130	-2.784800	1.075255	6	-4.037369	0.561917	0.482761
1	-1.528804	-3.655899	0.978780	1	-5.032011	0.285237	0.121007
1	2.288186	-0.294650	0.082141	1	-3.779092	-0.118039	1.309385
7	3.294641	-0.199525	-0.090263	1	-4.103484	1.580131	0.896043
6	4.019025	-0.338967	1.150593				
1	3.992469	-1.358824	1.582602				
1	5.075611	-0.079354	1.004643				
1	3.607414	0.349963	1.894058				
6	3.712388	-1.159896	-1.083148				
1	3.669679	-2.214473	-0.745299				
1	3.081221	-1.067482	-1.972373				
1	4.747983	-0.963409	-1.389516				

**Table S53.** The mPW1PW91/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Transition States for Dehydration of Carbinaolamine (**Step-II**)

TS-II				TS-IIa				TS-IIb			
Et = -328.1410795 NImag=1(-1337.4)				Et = -463.2911122 NImag=1( -637.9)				HF= -443.8622054 NImag=1(-406.1)			
6	.223289	-.046226	.516977	6	1.820759	0.359330	-0.156200	6	1.280445	0.401922	-0.372819
6	1.372778	-.399330	-.271991	6	1.905204	-0.998539	0.323652	6	1.899232	-0.544666	0.532581

1 .374812 .588726 1.383848	1 2.317213 0.586708 -1.093798	1 1.486348 0.278307 -1.430672
1 1.239729 -1.252199 -.936897	1 1.571637 -1.145385 1.351086	1 1.861288 -0.259484 1.584631
6 2.720489 -.356978 .423290	6 3.173341 -1.760099 -0.023372	6 3.265650 -1.054814 0.097485
1 2.881819 -1.201637 1.103710	1 4.037619 -1.435692 0.566176	1 4.047655 -0.291419 0.167807
1 3.528622 -.369803 -.313244	1 3.031878 -2.828800 0.156875	1 3.565946 -1.897752 0.724660
1 2.832157 .564721 1.005072	1 3.423550 -1.641157 -1.082711	1 3.231665 -1.416085 -0.935243
8 .110400 1.689598 -.854911	8 0.035211 -0.581463 -1.420177	8 -0.179406 -1.635461 -0.612613
7 -1.026222 -.475188 .363555	7 1.126396 1.348136 0.349760	7 0.408748 1.325869 -0.088299
6 -1.386061 -1.220534 -.830737	6 0.308376 1.196049 1.547786	6 -0.100442 1.564013 1.257417
1 -1.354424 -.564505 -1.707503	1 -0.661519 0.740917 1.284455	1 -1.003093 0.950634 1.374112
1 -.700637 -2.056113 -.974007	1 0.830801 0.574447 2.274484	1 0.651399 1.306701 2.000548
1 -2.393952 -1.619636 -.706515	1 0.155178 2.184750 1.984961	1 -0.346988 2.623540 1.350903
6 -2.054019 .435267 .838895	6 0.681146 2.369122 -0.586762	6 -0.411369 1.909596 -1.144830
1 -3.024749 -.063180 .844261	1 0.302357 3.235495 -0.044392	1 -0.502448 2.986132 -0.983516
1 -1.818888 .758152 1.855443	1 1.512746 2.678779 -1.222827	1 0.050434 1.723139 -2.114122
1 -2.050197 1.312248 .175590	1 -0.096871 1.909124 -1.210951	1 -1.392459 1.423369 -1.095847
1 .402700 2.578154 -.606660	1 -0.164886 -0.897391 -2.311319	1 -0.449549 -2.424297 -1.097999
1 1.124508 .661414 -.887294	1 1.008949 -1.283726 -0.417849	1 1.083627 -1.363900 0.317796
	1 -1.467986 -0.456783 -0.499998	1 -1.364833 -0.914522 -0.209532
	7 -2.262403 -0.338491 0.164234	8 -2.162115 -0.286449 0.087792
	6 -3.334832 0.390688 -0.471772	6 -3.292790 -1.070174 0.304863
	1 -2.950633 1.329689 -0.883313	1 -3.655669 -1.564335 -0.613372
	1 -3.827826 -0.159231 -1.296503	1 -3.126797 -1.862998 1.053707
	1 -4.116027 0.642265 0.257655	1 -4.109954 -0.438097 0.674618
	6 -2.690990 -1.635229 0.636112	
	1 -1.829324 -2.187072 1.023781	
	1 -3.416963 -1.529027 1.453047	
	1 -3.167551 -2.261651 -0.142062	
<b>TS-IIc</b>		<b>TS-IId</b>
Et =-463.280821 NIImag=1(-1231.2)		Et =-443.8645012 NIImag=1(-116.9)
6 -1.054862 .692591 -.319680		6 .998650 .796812 .031817
		<b>TS-IIe</b>
Et =-598.4379001 NIImag=1(-189.4)		
6 -0.352593 1.304343 0.415439		

6	-.039400	1.279570	.491758	6	-.103893	1.370492	-.731244	6	0.104610	2.167857	-0.680918
1	-1.093123	.958319	-1.366759	1	1.366687	1.302559	.916382	1	-1.361336	0.903799	0.366626
6	.509032	2.612189	-.004679	1	.124979	1.361931	-1.804674	1	1.052196	2.668222	-0.471251
1	-.187473	3.445692	.145435	6	-.543831	2.738837	-.232973	6	-0.966368	3.148850	-1.154763
1	1.438661	2.861662	.515714	1	.230775	3.504232	-.353642	1	-1.210606	3.899976	-0.396960
1	.741387	2.562838	-1.073660	1	-1.428080	3.071449	-.781611	1	-0.619301	3.674036	-2.047948
8	.043253	-.967923	-1.481156	1	-.813555	2.676474	.824523	1	-1.885237	2.618770	-1.420939
7	-2.127026	.022017	.117532	8	-.508493	.072435	1.903393	8	-0.119482	-0.408970	-1.319190
6	-2.220088	-.448365	1.482167	7	1.600379	-.315136	-.281001	7	0.309556	0.976977	1.483566
1	-1.551026	-1.301216	1.658643	6	1.095969	-1.172545	-1.355422	6	1.706047	1.328160	1.723120
1	-1.966223	.348475	2.182385	1	1.109809	-.626718	-2.301581	1	2.332232	0.600631	1.179090
1	-3.247056	-.762676	1.678553	1	1.747929	-2.041620	-1.439711	1	1.906917	2.340590	1.375050
6	-2.928708	-.709999	-.841605	1	.053859	-1.450582	-1.096253	1	1.891525	1.281158	2.797338
1	-3.987210	-.633889	-.576049	6	2.545626	-.920091	.640180	6	-0.242635	-0.028847	2.382599
1	-2.771485	-.301742	-1.838559	1	3.420239	-1.279365	.093866	1	-0.275464	0.367026	3.401020
1	-2.640571	-1.767561	-.864386	1	2.857634	-.189510	1.385680	1	-1.241139	-0.306271	2.040907
1	1.139164	-.872168	-.758250	1	2.063414	-1.761503	1.146655	1	0.403694	-0.910537	2.360656
1	-.290331	-1.857439	-1.302346	1	-.339641	-.625289	2.546996	1	-1.740685	-0.768977	-0.621749
7	1.944088	-.523221	.039433	1	-1.030148	-.400609	1.140329	1	0.265658	1.377630	-1.457287
1	.957223	.465715	.376148	8	-1.547262	-.928953	-.166915	1	1.528224	-0.716335	-0.726700
1	-.252169	1.277230	1.563183	6	-2.876988	-1.288522	-.186792	7	2.501391	-0.907163	-0.394874
6	3.168526	-.016949	-.534506	1	-3.515332	-.642939	.449090	6	2.612270	-2.302993	-0.031221
1	3.770322	.535024	.202660	1	-3.316058	-1.247033	-1.203049	1	1.826853	-2.561618	0.686514
1	3.803545	-.821715	-.939131	1	-3.048207	-2.324577	.171189	1	2.521867	-2.997363	-0.887739
1	2.928840	.661719	-1.358149	1	-.934109	.581299	-.612406	1	3.580472	-2.503898	0.445182
6	2.154479	-1.468159	1.108014					6	3.431829	-0.551539	-1.444853
1	2.713652	-2.359658	.780342					1	3.262679	0.485216	-1.751042
1	2.710290	-1.024271	1.947069					1	4.466400	-0.631965	-1.087134
1	1.184247	-1.807790	1.488838					1	3.347994	-1.184310	-2.347684
								1	-0.154355	-1.271014	-1.758113
								7	-2.582228	-0.954677	-0.036277

			6 -3.787578 -0.594862 -0.750971 1 -3.710709 0.434857 -1.114207 1 -4.000542 -1.242050 -1.621454 1 -4.658672 -0.648926 -0.085634 6 -2.580343 -2.347153 0.358289 1 -1.602043 -2.606002 0.774900 1 -3.338849 -2.534245 1.129281 1 -2.784382 -3.045494 -0.474429
<b>TS-IIf</b> Et =-559.5807507 NImag=1 (-25.0)	<b>TS-IIg</b> Et =-559.578852 NImag=1(-61.7)	<b>TS-IIIg</b> Et =-559.5786109 NImag=1(-130.07)	
6 1.258917 -0.748800 0.425721 6 1.833421 -0.935485 -0.898331 1 1.550507 0.153732 0.960245 1 1.735761 -1.947683 -1.297346 6 3.235955 -0.361346 -1.053167 1 3.987843 -0.936481 -0.503500 1 3.523645 -0.356671 -2.107148 1 3.260647 0.672525 -0.697394 8 -0.265809 0.828489 -1.425797 7 0.270399 -1.398607 0.950718 6 -0.379703 -2.546110 0.327006 1 -1.259747 -2.164820 -0.206234 1 0.304625 -3.050689 -0.351430 1 -0.685579 -3.238764 1.113595 6 -0.454797 -0.842821 2.092387 1 -0.489696 -1.577882 2.899954 1 0.034782 0.072828 2.418940 1 -1.461989 -0.604153 1.736671 1 -0.488574 1.385829 -2.180021 1 -1.496812 0.189546 -0.834926 8 -2.278469 -0.333041 -0.403728	6 1.704044 -0.414847 0.048249 6 1.935471 1.030708 -0.171372 1 2.050778 -0.880665 0.959884 1 2.421405 1.179001 -1.145682 6 2.726656 1.674067 0.959245 1 3.731789 1.249472 1.050620 1 2.832410 2.747003 0.783814 1 2.192436 1.528882 1.900690 8 0.184086 -0.156026 2.093094 7 1.084100 -1.176710 -0.787284 6 0.552913 -0.671798 -2.056897 1 1.384821 -0.377157 -2.702121 1 -0.005767 -1.473946 -2.534297 1 -0.113981 0.178993 -1.874483 6 0.654754 -2.515663 -0.395550 1 0.823790 -3.211901 -1.218560 1 1.212403 -2.836220 0.483968 1 -0.412306 -2.399227 -0.149906 1 0.105728 -0.782685 2.821886 1 -0.609156 -0.388428 1.471717 8 -1.595442 -0.781291 0.394099	6 -2.642154 1.254232 -1.529438 6 -1.880004 1.002800 -0.235378 6 -1.544767 -0.405099 -0.012649 7 -1.041980 -0.868403 1.084325 6 -0.502249 -2.223505 1.148784 6 -0.758411 -0.000529 2.228659 8 0.847113 1.602085 0.341387 6 1.706184 2.674855 0.175675 8 1.662046 -0.590552 -0.285411 6 3.047211 -0.683476 -0.421118 8 0.061511 -1.859094 -1.971310 1 -1.557970 -1.102044 -0.850041 1 -2.385454 1.439485 0.633899 1 -3.649615 0.826647 -1.509692 1 -2.738350 2.327725 -1.707427 1 -2.107945 0.824243 -2.381653 1 -0.384719 -0.616261 3.045204 1 -0.007011 0.739504 1.899020 1 -1.672637 0.504429 2.548410 1 -0.913571 -2.735678 2.021287 1 -0.745475 -2.758459 0.232408	

6 -3.474417 0.113167 -0.968618	6 -2.880550 -0.999731 0.858322	1 0.584298 -2.132117 1.214177
1 -3.498472 -0.006387 -2.064288	1 -3.242155 -0.211257 1.547323	1 0.271304 -1.613067 -2.878803
1 -4.304766 -0.471984 -0.557102	1 -3.622341 -1.055016 0.039088	1 0.739164 -1.379417 -1.411527
1 -3.679262 1.174107 -0.749799	1 -2.973214 -1.953296 1.414297	1 3.441855 -0.076111 -1.253548
1 1.073308 -0.266806 -1.449766	1 0.930790 1.483285 -0.261331	1 3.575417 -0.361925 0.490904
1 0.333460 1.666037 -0.274775	1 -1.423707 0.576644 -0.252469	1 3.336699 -1.725345 -0.614603
8 0.787976 2.046896 0.562048	8 -1.141554 1.448935 -0.732294	1 -0.851932 1.486992 -0.230492
6 0.228271 3.289690 0.864611	6 -2.192826 2.370404 -0.701805	1 1.347944 0.471832 -0.030404
1 0.397053 4.036738 0.071697	1 -2.463708 2.665648 0.323343	1 2.019358 2.826878 -0.875103
1 -0.858467 3.237402 1.040878	1 -1.884642 3.275841 -1.236767	1 1.234627 3.618814 0.498489
1 0.693476 3.675299 1.778894	1 -3.103567 1.990216 -1.190368	1 2.637644 2.577513 0.764692
<b>TS-IIh</b> Et = -598.4293531 NImag=1 (-726.40)	<b>TS-IIi</b> Et = -559.5767101 NImag=1(-61.65)	

6	2.628261	-0.340826	0.294640					
6	2.753302	0.400368	-0.935898					
1	3.154225	0.051855	1.158519					
1	2.351130	-0.092977	-1.820575					
6	4.081141	1.099423	-1.172749	6	1.696287	-0.026367	0.612523	
1	4.882583	0.406564	-1.451600	6	0.651870	-0.754152	1.350747	
1	3.982860	1.832826	-1.977236	1	2.682243	-0.469001	0.523888	
1	4.403413	1.642593	-0.277899	6	1.188286	-1.984699	2.070216	
8	1.031455	1.395364	0.751815	1	1.914201	-1.730233	2.849431	
7	1.871273	-1.378323	0.546174	1	0.367318	-2.526652	2.544286	
6	1.058128	-2.050891	-0.457514	1	1.670434	-2.666723	1.362954	
1	0.020946	-1.677215	-0.453102	8	1.405600	-1.096677	-1.564084	
1	1.499601	-1.914896	-1.443227	7	1.573889	1.154586	0.089829	
1	1.049631	-3.119500	-0.226700	6	0.291631	1.843985	-0.022246	
6	1.439787	-1.554463	1.925623	1	-0.222951	1.464166	-0.914083	
1	0.996663	-2.542189	2.052918	1	-0.358871	1.618073	0.822555	
1	2.293080	-1.453733	2.599517	1	0.480265	2.916121	-0.089145	
1	0.714826	-0.759844	2.142009	6	2.636641	1.684659	-0.753801	
1	1.220842	2.207138	1.242317	1	2.774990	2.746453	-0.540950	
1	1.928512	1.163741	-0.493910	1	3.565660	1.148876	-0.564178	
1	-0.681166	1.528108	0.439553	1	2.356087	1.544913	-1.800152	
7	-1.697758	1.646790	0.231111	1	1.436216	-2.042648	-1.748712	
6	-2.379281	2.088819	1.428593	1	0.399983	-0.892656	-1.447875	
1	-2.169227	1.394320	2.247683	8	-1.043151	-0.619093	-1.037365	
1	-2.083065	3.101555	1.761052	6	-1.880261	-1.453857	-1.759717	
1	-3.465386	2.105024	1.272400	1	-2.264575	-0.984266	-2.685289	
6	-1.840656	2.594732	-0.853261	1	-1.381955	-2.390711	-2.080676	
1	-1.234189	2.270677	-1.703973	1	-2.767691	-1.765078	-1.179354	
1	-2.885509	2.649644	-1.184316	1	0.116387	-0.083069	2.030930	
1	-1.527109	3.621638	-0.588257	1	-0.109801	-1.023377	0.580216	
1	-2.064731	-0.250884	-0.274606	8	-2.291898	0.464050	1.012422	
7	-2.184219	-1.246788	-0.518845	1	-1.880802	0.041682	0.197551	
6	-2.980193	-1.897596	0.499312	6	-3.430646	1.171604	0.614159	
1	-3.008927	-2.980514	0.323905	1	-4.216830	0.517726	0.205641	
1	-2.529443	-1.730624	1.482361	1	-3.846844	1.679242	1.491075	
1	-4.027863	-1.546988	0.543974	1	-3.217943	1.941782	-0.145981	
6	-2.788541	-1.350184	-1.829828					
1	-2.196402	-0.782932	-2.553943					

**Table 54.** The mPW1PW91/6-311+G\*\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Pre-reacting Complexes, Transition States and Final Products for Carbinolamine Formation (**Step-I**)

Pre-reacting complex Et = -328.3212375 NImag = 0				TS-I Et = -328.276655 NImag=1 (-1494.04)				Carbinolamine Et = -328.3339205 NImag = 0			
6 1.906909	0.933770	0.023053		6 -0.301926	0.756115	-0.380673		6 -0.233320	0.615908	-0.484897	
6 2.116932	-0.469997	-0.456149		6 -1.587233	0.246657	0.250900		6 -1.492940	0.216647	0.278244	
1 2.586413	1.255889	0.842290		1 -0.352385	0.574930	-1.474992		1 -0.380026	0.380243	-1.549203	
1 1.480258	-0.647587	-1.324049		1 -1.493036	0.247095	1.339869		1 -1.350609	0.449942	1.337276	
6 1.827287	-1.476338	0.660234		6 -2.062350	-1.103272	-0.271419		6 -1.898428	-1.239177	0.097941	
1 0.768695	-1.447104	0.924697		1 -1.362772	-1.910844	-0.037371		1 -1.170474	-1.925519	0.535209	
1 2.073238	-2.487509	0.332260		1 -3.026231	-1.376681	0.162709		1 -2.858698	-1.433949	0.580157	
1 2.420442	-1.264697	1.554013		1 -2.186471	-1.082621	-1.357692		1 -2.005224	-1.497705	-0.959455	
8 1.070627	1.694359	-0.393629		8 0.119005	1.980059	-0.017070		8 -0.111808	2.015710	-0.310309	
7 -1.579785	-0.098832	0.023242		7 1.024661	-0.000690	0.045823		7 1.018024	-0.016477	-0.115350	
6 -2.361906	-0.662657	-1.057289		6 1.027415	-0.654825	1.352244		6 1.299682	-0.086036	1.302278	
1 -1.701926	-0.990082	-1.863209		1 0.600379	0.024949	2.088112		1 1.034903	0.860307	1.775311	
1 -2.906007	-1.541523	-0.698587		1 0.457639	-1.587126	1.338622		1 0.762761	-0.898359	1.818732	
1 -3.103307	0.034697	-1.483116		1 2.056925	-0.875530	1.639830		1 2.370251	-0.248668	1.451794	
6 -2.399575	0.423166	1.097368		6 1.700425	-0.770563	-0.994388		6 1.388711	-1.212296	-0.837135	
1 -2.940304	-0.396552	1.579932		1 1.181566	-1.713322	-1.187522		1 0.873054	-2.124173	-0.497370	
1 -1.766210	0.892351	1.852647		1 1.724905	-0.183940	-1.912771		1 1.181250	-1.083474	-1.901564	
1 -3.146575	1.165024	0.767890		1 2.724599	-0.988209	-0.686215		1 2.463509	-1.382562	-0.725798	
1 -0.973669	0.631433	-0.331766		1 1.221205	1.174130	0.142213		1 0.758929	2.248816	-0.642820	
1 3.164550	-0.555058	-0.769969		1 -2.328976	1.016862	0.021023		1 -2.293546	0.874485	-0.070928	
Pre-reacting complex Et = -463.4945295 NImag = 0				TS-Ia Et = -463.4594453 NImag=1 (-1521.23)				Carbinolamine + amine Et = -463.5075705 NImag = 0			
6 0.40242	1.20613	0.73524		6 1.118579	0.249967	0.870852		6 -0.865942	-0.202545	-0.254708	
6 0.03795	1.60143	-0.6625		6 0.939926	1.565412	0.133076		6 -0.601114	1.193028	0.298874	

1	1.25914	1.76028	1.17072	1	2.038006	0.309102	1.484541	1	-0.726780	-0.179864	-1.344499
1	0.86494	1.24988	-1.2913	1	0.136940	1.471781	-0.602287	1	-0.738870	1.173753	1.383885
6	-0.10569	3.11544	-0.80619	6	2.214309	2.112285	-0.498219	6	-1.459107	2.280707	-0.332086
1	0.79845	3.63684	-0.48052	1	2.602450	1.458280	-1.283947	1	-2.518059	2.162832	-0.092740
1	-0.28555	3.3855	-1.84776	1	2.039099	3.090114	-0.951361	1	-1.152189	3.265856	0.024869
1	-0.94345	3.49278	-0.2156	1	3.004335	2.233659	0.248224	1	-1.362523	2.283888	-1.421526
8	-0.16503	0.36649	1.39332	8	0.034610	-0.235370	1.534298	8	0.118625	-1.046679	0.333634
7	2.70834	-0.72716	0.11776	7	1.337553	-1.017682	-0.017097	7	-2.169062	-0.795503	-0.036041
6	2.60277	-1.62999	-1.01149	6	0.768734	-0.978276	-1.367435	6	-2.708853	-0.663224	1.301229
1	1.55625	-1.73891	-1.30256	1	-0.258392	-0.610739	-1.311466	1	-1.929617	-0.870661	2.035627
1	3.14384	-1.21235	-1.86547	1	1.360948	-0.343151	-2.030976	1	-3.128921	0.333828	1.509083
1	3.01331	-2.63469	-0.81808	1	0.758313	-1.992287	-1.771168	1	-3.506582	-1.396705	1.442791
6	4.06549	-0.58863	0.60781	6	2.657307	-1.639729	0.046528	6	-3.156120	-0.602211	-1.075389
1	4.68347	-0.11064	-0.1575	1	3.395085	-1.059542	-0.514301	1	-3.632106	0.390418	-1.065271
1	4.07765	0.05298	1.49095	1	2.974003	-1.707146	1.087528	1	-2.697853	-0.748438	-2.055623
1	4.54394	-1.5464	0.87092	1	2.607383	-2.645334	-0.373853	1	-3.947720	-1.348460	-0.963420
1	2.10229	-1.04154	0.86486	1	0.489716	-1.282688	0.803615	1	-0.170064	-1.946542	0.157083
1	-0.86974	1.0714	-0.95948	1	0.573575	2.264137	0.890909	1	0.457571	1.406251	0.126422
1	-2.00094	-0.4824	0.51663	1	-1.705423	0.006600	0.550461	1	2.143896	-0.378089	0.096893
7	-2.76875	-0.66058	-0.1221	7	-2.405576	-0.021376	-0.193104	7	3.004965	0.117760	-0.107157
6	-2.78016	-2.05456	-0.50995	6	-3.237137	-1.195804	-0.036205	6	3.821385	0.210936	1.083237
1	-3.50881	-2.21066	-1.31142	1	-3.879863	-1.322869	-0.913695	1	4.668749	0.879527	0.901440
1	-1.7997	-2.34046	-0.89678	1	-2.610411	-2.086538	0.047887	1	3.236262	0.635080	1.901611
1	-3.03903	-2.74523	0.31128	1	-3.892135	-1.159870	0.851213	1	4.231782	-0.757040	1.421319
6	-4.01738	-0.23161	0.47093	6	-3.175859	1.203675	-0.206159	6	3.691635	-0.512436	-1.212864
1	-3.93343	0.80527	0.80269	1	-2.505769	2.064678	-0.256666	1	3.014167	-0.610074	-2.063841
1	-4.81704	-0.27643	-0.27488	1	-3.820337	1.233309	-1.090925	1	4.533011	0.110503	-1.532229
1	-4.33495	-0.84214	1.33388	1	-3.823397	1.329680	0.678666	1	4.094223	-1.513965	-0.978318
Pre-reacting Complex				<b>TS-Ib</b>				Carbinolamine + Methanol			
Et = -444.0597423 NIImag = 0				Et = -444.0240264 NIImag=1 (-1538.82)				Et = -444.0728003 NIImag = 0			
6	0.200783	1.320982	0.957181	6	-0.617727	0.262481	-0.830241	6	0.674790	0.144865	0.789995

6	0.246601	1.882882	-0.434066	6	-0.387444	1.544041	-0.053133	6	0.295637	1.397263	0.007238
1	1.117617	1.454708	1.563097	1	-1.408018	0.434515	-1.582297	1	1.309810	0.435741	1.636993
1	-0.362911	1.249254	-1.082498	1	0.294462	1.358903	0.779743	1	-0.345034	1.112604	-0.831855
6	1.654565	2.084181	-0.970828	6	-1.666069	2.234933	0.403955	6	1.492778	2.202420	-0.477233
1	2.178300	1.129961	-1.037258	1	-2.234664	1.629733	1.115331	1	2.082621	1.654141	-1.214469
1	1.630955	2.535458	-1.963948	1	-1.441950	3.183036	0.896493	1	1.164939	3.130917	-0.948735
1	2.237349	2.744634	-0.323013	1	-2.324086	2.452525	-0.442090	1	2.157814	2.470830	0.348617
8	-0.782428	0.823691	1.461634	8	0.491607	-0.358378	-1.341640	8	-0.552950	-0.385475	1.296260
7	1.390328	-1.162139	0.271113	7	-1.115926	-0.968550	-0.024022	7	1.383184	-0.907356	0.100530
6	0.859357	-1.723530	-0.959777	6	-0.732032	-1.021245	1.390426	6	0.900466	-1.247179	-1.224199
1	-0.193319	-1.455750	-1.064823	1	0.329913	-0.793841	1.484618	1	-0.189378	-1.285097	-1.232427
1	1.406710	-1.313681	-1.814114	1	-1.319343	-0.321428	1.989811	1	1.230107	-0.541083	-2.002568
1	0.945230	-2.820827	-1.008541	1	-0.905808	-2.033007	1.759581	1	1.270851	-2.238424	-1.496574
6	2.745821	-1.592066	0.555365	6	-2.487157	-1.405226	-0.273365	6	2.825899	-0.896886	0.203376
1	3.420545	-1.209527	-0.215842	1	-3.208158	-0.736895	0.205154	1	3.318199	-0.168132	-0.458828
1	3.074053	-1.185886	1.514301	1	-2.671918	-1.418793	-1.347562	1	3.125521	-0.678713	1.230552
1	2.864989	-2.687136	0.584061	1	-2.625097	-2.412694	0.121560	1	3.211922	-1.887383	-0.052530
1	0.781923	-1.409797	1.041273	1	-0.194289	-1.338978	-0.730748	1	-0.345902	-1.273201	1.603944
1	-2.022531	0.036735	0.292473	1	1.859786	-0.252260	-0.293424	1	-2.057581	-0.439759	0.188816
8	-2.427905	-0.443845	-0.444592	8	2.468057	-0.239696	0.479207	8	-2.741876	-0.540824	-0.488685
6	-3.774618	-0.711559	-0.136815	6	3.783238	-0.027672	0.038280	6	-3.898188	0.144726	-0.076517
1	-4.357221	0.206078	0.013280	1	3.896595	0.927652	-0.491556	1	-3.719791	1.218789	0.064458
1	-4.206028	-1.250887	-0.981291	1	4.435861	-0.005878	0.913663	1	-4.648940	0.028163	-0.859573
1	-3.880374	-1.338194	0.757632	1	4.135030	-0.828399	-0.625541	1	-4.314748	-0.259880	0.854885
1	-0.279978	2.845724	-0.375276	1	0.158996	2.196375	-0.740647	1	-0.322386	2.011120	0.669028
Pre-reacting complex				<b>TS-Ic</b>				Carbinolamine + Amine			
Et = -463.5023385 NImag = 0				Et = -463.4782552 NImag=1 (-1148.42)				Et = -463.5171733 NImag = 0			
6	-1.180082	-1.435080	0.175521	6	-0.815616	-0.764695	0.192931	6	0.916476	-0.616256	-0.204294
6	-2.587758	-1.235355	-0.316903	6	-2.261234	-0.995119	-0.263048	6	2.315375	-1.113227	0.158940
1	-1.001629	-1.171827	1.236638	1	-0.796683	-0.797581	1.308895	1	0.795645	-0.688402	-1.297364
1	-2.533525	-0.858355	-1.341197	1	-2.302761	-0.875969	-1.349782	1	2.434628	-1.051413	1.244613

6 -3.433636 -0.344569 0.578521	6 -3.366503 -0.196775 0.418356	6 3.467947 -0.413779 -0.548120
1 -2.991882 0.649912 0.654413	1 -3.391689 0.848793 0.101377	1 3.594006 0.618220 -0.215412
1 -4.447330 -0.244686 0.186739	1 -4.346350 -0.620043 0.183894	1 4.408762 -0.932880 -0.351442
1 -3.510985 -0.755765 1.588630	1 -3.260247 -0.211551 1.507305	1 3.324515 -0.398114 -1.632502
8 -0.296321 -1.916223 -0.493892	8 0.031679 -1.590566 -0.405514	8 0.028246 -1.476202 0.453317
7 -0.359149 1.325134 0.005616	7 -0.320077 0.723531 -0.049905	7 0.586963 0.777447 0.119057
6 -0.594873 1.707449 -1.370972	6 -0.557611 1.170796 -1.418054	6 0.900554 1.174564 1.476590
1 -0.443729 0.845075 -2.023949	1 -0.310138 0.349705 -2.092118	1 0.579540 0.391793 2.164889
1 -1.628982 2.045896 -1.495568	1 -1.601567 1.461185 -1.574149	1 1.973137 1.367547 1.640674
1 0.061057 2.521406 -1.722934	1 0.076425 2.031234 -1.650679	1 0.359049 2.091854 1.725157
6 -0.469670 2.440511 0.922825	6 -0.710537 1.719230 0.940964	6 0.966356 1.772251 -0.861717
1 -1.495864 2.822199 0.930386	1 -1.749315 2.039171 0.828865	1 2.033779 2.039397 -0.850022
1 -0.231004 2.113326 1.937041	1 -0.584958 1.303114 1.942237	1 0.720594 1.416649 -1.865263
1 0.192402 3.286580 0.672428	1 -0.070283 2.602388 0.850765	1 0.399519 2.691852 -0.684553
1 0.567084 0.900924 0.085433	1 0.959218 0.476725 0.058240	1 -1.732624 0.585772 -0.064675
1 1.668834 -1.125099 -0.113120	1 1.379915 -1.047601 -0.131042	1 -0.884346 -1.198655 0.226614
7 2.305604 -0.360130 0.090133	7 2.056153 -0.197413 0.089553	7 -2.421323 -0.161804 -0.113513
6 2.982621 -0.602859 1.349305	6 2.681279 -0.305744 1.397484	6 -3.083816 -0.158649 -1.404388
1 3.680929 -1.455098 1.317421	1 3.441882 -1.094412 1.414636	1 -3.703620 -1.053930 -1.501394
1 3.556063 0.282840 1.638398	1 3.159822 0.636045 1.684903	1 -3.732756 0.717134 -1.561601
1 2.248898 -0.794378 2.134847	1 1.924026 -0.552023 2.143722	1 -2.339799 -0.182546 -2.202742
1 -3.025695 -2.239394 -0.390627	1 -2.418092 -2.062026 -0.083499	1 2.325893 -2.179859 -0.081018
6 3.227058 -0.179810 -1.015571	6 2.992588 0.064936 -0.990711	6 -3.344765 -0.070205 1.002791
1 2.669864 -0.067299 -1.947306	1 2.458618 0.060323 -1.941709	1 -2.786989 -0.037234 1.940149
1 3.813068 0.731612 -0.864615	1 3.476535 1.039080 -0.865439	1 -4.001062 0.812841 0.956073
1 3.935845 -1.014838 -1.138526	1 3.775483 -0.700622 -1.037382	1 -3.982086 -0.958104 1.025664
Pre-reacting Complex Et = -444.0658042 NImag = 0		TS-Id Et = -444.0475136 NImag=1 (-788.84)
Carbinolamine + methanol Et = -444.0791438 NImag = 0		
6 0.723172 -1.393912 -0.214365	6 0.442611 -0.727630 -0.189351	6 0.598878 -0.641886 -0.247248
6 2.143041 -1.412154 0.272277	6 1.888511 -1.086326 0.128467	6 2.091768 -0.905436 -0.063201
1 0.569974 -1.066042 -1.258652	1 0.287930 -0.744923 -1.287211	1 0.372160 -0.625779 -1.324554

1 2.139042 -1.164642 1.336573	1 2.040225 -0.996564 1.207642	1 2.312419 -0.923371 1.007853
6 3.084205 -0.524481 -0.526701	6 2.989480 -0.372784 -0.646248	6 3.034059 0.043296 -0.791382
1 2.773528 0.519034 -0.465777	1 3.137699 0.659559 -0.320677	1 3.042549 1.042718 -0.352929
1 4.106153 -0.604525 -0.152498	1 3.943692 -0.884739 -0.505799	1 4.058146 -0.333694 -0.748199
1 3.097055 -0.808706 -1.582145	1 2.784015 -0.359801 -1.720474	1 2.768778 0.144376 -1.847716
8 -0.213905 -1.788489 0.446347	8 -0.411806 -1.484063 0.504008	8 -0.047027 -1.714484 0.382429
7 0.118178 1.363274 0.015727	7 0.076236 0.784166 0.126145	7 0.056907 0.627905 0.270908
6 0.211873 1.650867 1.432832	6 0.426053 1.175981 1.498310	6 0.423646 0.916830 1.648531
1 -0.083615 0.770064 2.006514	1 0.132612 0.363977 2.161673	1 0.287674 0.019380 2.251937
1 1.246268 1.894378 1.695951	1 1.497656 1.363189 1.581549	1 1.462255 1.263555 1.752392
1 -0.417888 2.496573 1.754108	1 -0.123085 2.078391 1.768395	1 -0.232756 1.696143 2.042869
6 0.433901 2.507825 -0.815330	6 0.467394 1.778547 -0.879101	6 0.209512 1.781082 -0.599944
1 1.481238 2.793848 -0.676460	1 1.536060 1.981119 -0.839620	1 1.223247 2.201714 -0.609714
1 0.294710 2.251765 -1.867406	1 0.208889 1.404785 -1.869734	1 -0.056715 1.510683 -1.624091
1 -0.181134 3.395703 -0.594681	1 -0.078964 2.705730 -0.698424	1 -0.471607 2.571371 -0.272005
1 -0.817778 1.028815 -0.199402	1 -1.015793 0.671342 0.093615	1 -1.760675 0.186316 0.260992
1 -1.801120 -1.036455 -0.157189	1 -1.487278 -0.949264 0.394339	1 -1.004544 -1.592555 0.289425
8 -2.383981 -0.343255 -0.505983	8 -2.296658 -0.068128 0.272526	8 -2.538070 -0.413227 0.260497
6 -3.709315 -0.590084 -0.097620	6 -3.336864 -0.292256 -0.631703	6 -3.478600 -0.006693 -0.705645
1 -3.811071 -0.600619 0.994329	1 -4.082129 -0.983284 -0.216251	1 -4.290855 -0.734372 -0.705699
1 -4.331841 0.214557 -0.490827	1 -3.855640 0.646178 -0.863049	1 -3.904204 0.976957 -0.474073
1 -4.090520 -1.539437 -0.492157	1 -2.988710 -0.721917 -1.584556	1 -3.052211 0.026930 -1.716283
1 2.461577 -2.461652 0.210154	1 1.933776 -2.158603 -0.078946	1 2.253190 -1.927168 -0.416631
Pre-reacting complex Et = -598.6767673 NImag = 0	TS-Ie Et = -598.63878 NImag=1 (-1546.61)	Carbinolamine + amine + amine Et = -598.684752 NImag = 0
6 0.097213 1.093386 -1.345451	6 -0.199108 0.825434 -0.385831	6 0.074294 1.171364 -0.056984
6 1.039498 2.173253 -0.893428	6 0.824259 1.620033 -1.175475	6 -0.198168 0.916286 1.420187
1 -0.887875 1.432266 -1.716386	1 -1.210966 1.179859 -0.644940	1 1.048324 1.666908 -0.152057
1 1.558547 1.814065 -0.000803	1 1.828966 1.409610 -0.801683	1 -1.169832 0.425043 1.522367
6 0.377165 3.523446 -0.674885	6 0.547145 3.117546 -1.226740	6 -0.136867 2.174313 2.274896
1 -0.380587 3.457416 0.106649	1 0.589205 3.582406 -0.238185	1 -0.916925 2.889148 2.005361

1	1.111613	4.274821	-0.380035	1	1.278267	3.629631	-1.855508	1	-0.269994	1.929277	3.330512
1	-0.110246	3.880404	-1.586242	1	-0.443819	3.320757	-1.642103	1	0.828379	2.677923	2.173911
8	0.399840	-0.079719	-1.404014	8	-0.072957	-0.544414	-0.431706	8	0.150568	-0.120607	-0.675219
7	-1.440285	1.039886	0.975033	7	-0.127750	0.932747	1.157305	7	-0.867678	1.978000	-0.796292
6	-0.501488	0.866527	2.065694	6	1.142604	1.360095	1.748085	6	-2.273772	1.738716	-0.531003
1	0.351714	0.270148	1.736015	1	1.958446	0.787326	1.302633	1	-2.463140	0.669808	-0.426074
1	-0.118732	1.841007	2.385977	1	1.312690	2.430197	1.604350	1	-2.635054	2.243235	0.379180
1	-0.942141	0.380372	2.951734	1	1.112105	1.153178	2.819072	1	-2.866377	2.108615	-1.371725
6	-2.613134	1.797282	1.362745	6	-1.310913	1.510266	1.796949	6	-0.544859	3.379349	-0.953404
1	-2.329295	2.819495	1.632915	1	-1.343837	2.594479	1.655716	1	-0.763499	3.991088	-0.064180
1	-3.312072	1.856714	0.525729	1	-2.200368	1.050855	1.360915	1	0.513799	3.495662	-1.193749
1	-3.148995	1.367426	2.225282	1	-1.281262	1.296767	2.866690	1	-1.122988	3.790423	-1.785659
1	-1.728011	0.127046	0.617302	1	-0.137694	-0.256114	0.865402	1	0.049404	0.052827	-1.616417
1	1.807115	2.243294	-1.675788	1	0.786142	1.202989	-2.186076	1	0.553108	0.200359	1.764578
1	2.162512	-0.746557	-0.283120	1	1.882779	-1.129201	-0.352263	1	-1.375827	-1.606774	-0.154167
7	2.925196	-0.852435	0.377805	7	2.857235	-1.193214	-0.055835	7	-2.263793	-2.074895	-0.006549
6	2.843564	-2.140602	1.032155	6	3.024050	-2.320175	0.837608	6	-2.689078	-2.728918	-1.225459
1	3.579019	-2.192612	1.840933	1	4.025879	-2.304743	1.278999	1	-3.711861	-3.100314	-1.109678
1	1.855765	-2.269490	1.479434	1	2.301456	-2.257903	1.654530	1	-2.692421	-2.013201	-2.050560
1	3.030031	-2.996682	0.360497	1	2.894453	-3.299460	0.345783	1	-2.057636	-3.586170	-1.517071
6	4.191452	-0.645832	-0.291963	6	3.726827	-1.270402	-1.210718	6	-2.172209	-2.983594	1.116269
1	4.183923	0.312812	-0.814862	1	3.517021	-0.442370	-1.891121	1	-1.791304	-2.454795	1.992380
1	4.999510	-0.612411	0.445327	1	4.773032	-1.186434	-0.899225	1	-3.167249	-3.363270	1.367864
1	4.443700	-1.432696	-1.023944	1	3.625465	-2.210686	-1.779395	1	-1.521631	-3.856193	0.932745
1	-1.239091	-1.445919	-0.988523	1	-2.062525	-1.023607	-0.447723	1	2.212710	-0.710553	-0.251991
7	-2.075800	-1.695776	-0.469786	7	-3.050200	-0.923723	-0.211856	7	3.200525	-0.649443	-0.029892
6	-3.214903	-1.738127	-1.366708	6	-3.831368	-0.728193	-1.415325	6	3.612963	-1.802133	0.741787
1	-3.167200	-2.558310	-2.101412	1	-3.859552	-1.612334	-2.074986	1	3.587710	-2.751169	0.178268
1	-4.135667	-1.864821	-0.789844	1	-4.865463	-0.480412	-1.154784	1	4.637352	-1.660852	1.099689
1	-3.292753	-0.796529	-1.913890	1	-3.426381	0.106739	-1.991352	1	2.971456	-1.912045	1.618574
6	-1.869481	-2.948958	0.230950	6	-3.488416	-2.073792	0.551111	6	3.971459	-0.479112	-1.242189

1 -1.767972 -3.817481 -0.439866	1 -3.508671 -3.010958 -0.031098	1 3.967531 -1.361774 -1.906048
1 -0.969759 -2.886753 0.845576	1 -2.828055 -2.225298 1.407837	1 3.590835 0.373326 -1.809280
1 -2.714866 -3.143247 0.897438	1 -4.499131 -1.905495 0.936873	1 5.014641 -0.264927 -0.990496
Pre-reacting Complex Et = -559.803116 NImag = 0	TS-If Et = -559.7719551 NImag=1 (-1564.72)	Carbinolamine + methanol + methanol Et = -559.8132967 NImag = 0
6 0.764087 -0.074200 -0.858914	6 -0.068556 -0.594879 0.467079	6 0.824860 -0.602020 -0.133620
6 1.546121 -1.375562 -0.702014	6 1.091951 -0.813097 1.415141	6 0.660540 -0.237049 1.335545
1 1.278087 0.602443 -1.571337	1 -0.971359 -1.072251 0.873104	1 0.877219 -1.692646 -0.226692
1 1.092552 -1.965189 0.099332	1 2.019861 -0.449360 0.968970	1 0.603050 0.850669 1.430684
6 3.058557 -1.282662 -0.545679	6 1.222168 -2.250134 1.905915	6 1.766532 -0.799009 2.218052
1 3.364132 -0.951949 0.449993	1 1.436251 -2.949809 1.093911	1 2.742577 -0.378476 1.967728
1 3.517712 -2.260873 -0.703008	1 2.033271 -2.339982 2.630856	1 1.571925 -0.570447 3.267504
1 3.497840 -0.597331 -1.276549	1 0.303928 -2.585462 2.395719	1 1.836815 -1.886246 2.126777
8 -0.515062 -0.221693 -1.048454	8 -0.304244 0.726705 0.089434	8 -0.383367 -0.156544 -0.793666
7 0.944477 0.881826 0.524795	7 0.071465 -1.123537 -0.967740	7 1.949943 -0.071244 -0.855474
6 0.729883 0.139648 1.776775	6 1.426967 -1.354848 -1.474231	6 2.299742 1.313692 -0.597429
1 -0.152458 -0.492505 1.674448	1 2.047305 -0.483802 -1.263963	1 1.402982 1.932177 -0.549800
1 1.601277 -0.478754 1.990721	1 1.875424 -2.249550 -1.035510	1 2.868256 1.451352 0.335243
1 0.581731 0.841889 2.599826	1 1.370068 -1.485986 -2.555482	1 2.916110 1.683507 -1.420145
6 2.126476 1.753234 0.560127	6 -0.892174 -2.156306 -1.349980	6 3.098845 -0.940782 -0.997234
1 3.025605 1.166786 0.733779	1 -0.643374 -3.117769 -0.891758	1 3.733060 -0.990141 -0.099107
1 2.212343 2.273932 -0.393036	1 -1.887983 -1.845397 -1.033042	1 2.773652 -1.953971 -1.240921
1 2.020120 2.491290 1.357811	1 -0.883858 -2.269737 -2.434688	1 3.720794 -0.582873 -1.821894
1 0.120572 1.492147 0.373857	1 -0.259956 0.073933 -1.039473	1 -0.158686 -0.131512 -1.730529
1 -1.329024 -1.301769 -0.037236	1 1.215984 1.617968 -0.133396	1 -0.997213 1.599795 -0.348644
8 -1.699061 -1.838690 0.702927	8 2.131630 1.853731 -0.383548	8 -1.112321 2.544651 -0.180628
6 -2.661906 -2.729736 0.206855	6 2.359189 3.213363 -0.112942	6 -2.381573 2.762339 0.387698
1 -2.248221 -3.416394 -0.543969	1 2.226648 3.454221 0.949910	1 -2.511823 2.225906 1.336177
1 -3.034030 -3.328903 1.040867	1 3.391595 3.442292 -0.383744	1 -2.473052 3.830409 0.588779
1 -3.518768 -2.210903 -0.243715	1 1.702419 3.870422 -0.697714	1 -3.196508 2.474285 -0.288476
1 1.312757 -1.914222 -1.625189	1 0.893766 -0.151790 2.263641	1 -0.306766 -0.631251 1.659788

1 -1.191648 1.271588 -0.933059	1 -2.083148 0.797111 0.143710	1 -1.774717 -1.416228 -0.381966
8 -1.253671 2.196293 -0.563730	8 -3.007338 0.484024 0.091654	8 -2.335115 -2.146179 -0.088369
6 -2.590696 2.514395 -0.253185	6 -3.879182 1.552688 0.357957	6 -3.679015 -1.826783 -0.355253
1 -3.043000 1.778157 0.421813	1 -3.780929 2.364255 -0.374987	1 -3.871811 -1.687436 -1.426925
1 -2.604898 3.488862 0.238371	1 -4.901476 1.173629 0.304528	1 -4.290264 -2.661639 -0.010201
1 -3.206796 2.580924 -1.157031	1 -3.727259 1.975424 1.359635	1 -4.008351 -0.924280 0.175683
Pre-reacting complex Et = -598.6828608 NImag = 0	TS-Ig Et = -598.6618454 NImag=1 (-459.05)	Carbinolamine + amine + amine Et = -598.6622252 NImag = 0
6 1.774637 -0.962606 -0.886788	6 -1.102148 -0.689997 0.341028	6 -1.125278 -0.654473 0.358181
6 3.259258 -0.759621 -0.877435	6 -2.400184 -1.526055 0.484141	6 -2.406760 -1.526610 0.436738
1 1.225007 -0.360007 -1.632303	1 -0.588254 -0.760688 1.336373	1 -0.639219 -0.757289 1.363903
1 3.610014 -0.995196 -1.891699	1 -2.091749 -2.444572 0.994785	1 -2.097095 -2.450966 0.936289
6 4.002263 -1.566669 0.170903	6 -3.060073 -1.914242 -0.833014	6 -3.015675 -1.897061 -0.909771
1 3.828575 -2.635985 0.040880	1 -2.290348 -2.248415 -1.530634	1 -2.217708 -2.201917 -1.589016
1 5.076550 -1.383339 0.109630	1 -3.778767 -2.724553 -0.683707	1 -3.724153 -2.723186 -0.802356
1 3.667332 -1.303419 1.175269	1 -3.596942 -1.085619 -1.299680	1 -3.551888 -1.067333 -1.375015
8 1.187607 -1.745985 -0.177378	8 -0.349838 -1.011031 -0.690885	8 -0.329164 -0.953102 -0.660974
7 1.138144 1.702431 0.309330	7 -1.378639 0.850414 0.316928	7 -1.416209 0.860824 0.362051
6 1.355724 1.475863 1.722897	6 -2.160815 1.265671 -0.840384	6 -2.197938 1.293375 -0.785716
1 0.978944 0.489876 2.002074	1 -1.805844 0.703812 -1.704610	1 -1.828546 0.769473 -1.667920
1 2.427787 1.496325 1.945672	1 -3.231130 1.073834 -0.700632	1 -3.269107 1.078423 -0.668012
1 0.872902 2.226415 2.372131	1 -2.033844 2.338144 -1.023573	1 -2.093357 2.374189 -0.935214
6 1.582792 3.012396 -0.117558	6 -1.919865 1.389883 1.553313	6 -1.977188 1.361350 1.602381
1 2.669771 3.096099 -0.010757	1 -2.965900 1.099877 1.713576	1 -3.019260 1.046190 1.759456
1 1.341593 3.162231 -1.172290	1 -1.333354 1.025448 2.400372	1 -1.386189 0.999615 2.448082
1 1.134507 3.842837 0.454808	1 -1.875415 2.483785 1.543839	1 -1.960815 2.456433 1.612402
1 0.143477 1.592288 0.094944	1 -0.030971 1.249991 0.102375	1 0.132382 1.266877 0.081387
1 -0.888507 -1.844823 0.080938	1 1.274638 -1.284609 -0.157898	1 1.238961 -1.262816 -0.123348
7 -1.892126 -1.764690 0.226150	7 2.249754 -1.098593 0.170446	7 2.228313 -1.086244 0.190987
6 -2.204310 -2.089017 1.605846	6 3.191891 -1.540432 -0.841140	6 3.152855 -1.607074 -0.799859
1 -1.610625 -1.465082 2.276540	1 2.916699 -1.122972 -1.811614	1 2.879188 -1.239684 -1.790770

1 -3.260510 -1.885168 1.806354	1 4.205314 -1.201610 -0.599185	1 4.176526 -1.281294 -0.584300
1 -2.013919 -3.143667 1.862274	1 3.224028 -2.636053 -0.946144	1 3.155120 -2.706686 -0.841132
1 3.417417 0.317539 -0.760531	1 -3.115008 -1.038950 1.159406	1 -3.154422 -1.069395 1.097498
1 -1.992078 0.310268 -0.151948	1 1.631791 0.594454 0.080677	1 1.696546 0.541869 0.044783
7 -1.921261 1.314153 -0.341095	7 1.118903 1.488504 -0.146622	7 1.184936 1.454075 -0.190714
6 -2.227898 1.563397 -1.735876	6 1.655328 2.597752 0.640719	6 1.747546 2.578096 0.561012
1 -2.035480 2.612559 -1.981913	1 1.101815 3.513895 0.425181	1 1.201618 3.494626 0.331854
1 -1.586060 0.950886 -2.372788	1 1.557952 2.371343 1.702742	1 1.666775 2.375367 1.628661
1 -3.276596 1.349342 -2.002089	1 2.711316 2.766937 0.413799	1 2.799365 2.718712 0.305465
6 -2.587904 -2.622065 -0.715113	6 2.494068 -1.729252 1.454027	6 2.466712 -1.646409 1.508670
1 -2.275523 -2.385972 -1.734290	1 1.741572 -1.409440 2.177631	1 1.729030 -1.263667 2.216722
1 -2.412006 -3.696408 -0.543184	1 2.466789 -2.828953 1.404148	1 2.406073 -2.745138 1.521756
1 -3.666287 -2.449175 -0.649174	1 3.478101 -1.441283 1.840087	1 3.462157 -1.366157 1.870652
6 -2.799063 2.041907 0.554632	6 1.227621 1.684718 -1.596773	6 1.240712 1.614718 -1.651283
1 -2.574049 1.779113 1.590245	1 0.784513 0.811424 -2.074951	1 0.759309 0.737124 -2.082131
1 -2.639536 3.119060 0.443476	1 0.683439 2.583124 -1.894299	1 0.704717 2.517675 -1.947490
1 -3.869860 1.846518 0.377022	1 2.273201 1.789348 -1.897753	1 2.278120 1.687718 -1.982808
Pre-reacting Complex Et = -559.8125664 NIImag = 0	TS-Ih Et = -559.8021286 NIImag=1 (-519.93)	Carbinolamine + methanol +methanol Et = -559.8251292 NIImag = 0
6 1.320657 -0.865421 -0.880142	6 0.942197 -0.363754 -0.606835	6 1.049681 -0.351412 -0.589458
6 2.799699 -0.641432 -0.862902	6 2.410445 -0.568975 -0.973227	6 2.527497 -0.657825 -0.863912
1 0.760924 -0.293651 -1.638323	1 0.387616 -0.102936 -1.524016	1 0.568602 -0.198469 -1.566562
1 3.160474 -0.928728 -1.860658	1 2.377359 -1.306461 -1.780442	1 2.524485 -1.391533 -1.675835
6 3.541326 -1.388178 0.230311	6 3.309747 -1.104311 0.134198	6 3.335248 -1.228624 0.296914
1 3.380831 -2.464252 0.150767	1 2.825122 -1.940804 0.638840	1 2.805222 -2.063093 0.757315
1 4.613778 -1.195313 0.168702	1 4.253751 -1.458279 -0.285341	1 4.298391 -1.597386 -0.064174
1 3.194498 -1.079180 1.217391	1 3.555838 -0.349513 0.883795	1 3.541769 -0.490076 1.072441
8 0.750774 -1.669781 -0.172250	8 0.423013 -1.416079 0.038221	8 0.494855 -1.442781 0.065967
7 0.631165 1.669152 0.266991	7 0.686342 0.933310 0.248469	7 0.743136 0.901520 0.149971
6 0.984689 1.631578 1.672108	6 1.047664 0.802279 1.671283	6 1.172172 0.920903 1.543329
1 0.652498 0.689107 2.111145	1 0.793941 -0.207407 1.987118	1 0.952710 -0.044040 1.997386

1 2.072100 1.690825 1.785923	1 2.111837 0.984396 1.813605	1 2.242692 1.137070 1.656008
1 0.545830 2.455641 2.258066	1 0.470176 1.525505 2.247217	1 0.614586 1.692548 2.080873
6 0.994498 2.920451 -0.365850	6 1.215233 2.162340 -0.355848	6 1.178823 2.092796 -0.558828
1 2.083870 3.034354 -0.378184	1 2.300028 2.202050 -0.258739	1 2.270674 2.223569 -0.554430
1 0.647592 2.928827 -1.401541	1 0.942235 2.190425 -1.411090	1 0.843313 2.052884 -1.598155
1 0.579000 3.808282 0.139310	1 0.778401 3.027037 0.145082	1 0.739277 2.978047 -0.092399
1 -0.371252 1.516662 0.167633	1 -0.399989 1.026202 0.221061	1 -1.027718 1.075043 0.249562
1 -1.023480 -1.782316 -0.185528	1 -0.683184 -1.446462 -0.122478	1 -0.464505 -1.491805 -0.121154
8 -1.997833 -1.722097 -0.171962	8 -1.955800 -1.293708 -0.336042	8 -2.199401 -1.452247 -0.440760
6 -2.511083 -2.691142 0.718174	6 -2.789346 -2.209077 0.312493	6 -3.071675 -2.312807 0.260197
1 -2.150135 -2.539642 1.741470	1 -2.712100 -2.148266 1.409093	1 -2.958655 -2.215962 1.345888
1 -3.597802 -2.600794 0.718100	1 -3.839973 -2.038197 0.045224	1 -4.118069 -2.123912 -0.003170
1 -2.250370 -3.705510 0.398662	1 -2.540667 -3.236725 0.019879	1 -2.827858 -3.337328 -0.022378
1 2.951114 0.440580 -0.803001	1 2.828965 0.338387 -1.420053	1 3.013336 0.235045 -1.270175
1 -2.309317 0.010471 -0.026946	1 -2.063855 -0.050375 -0.006079	1 -2.357243 -0.524086 -0.171651
8 -2.321410 0.985116 0.029414	8 -1.907904 1.029024 0.245678	8 -2.019718 1.101842 0.316233
6 -3.411237 1.480916 -0.710063	6 -2.751688 1.873337 -0.490620	6 -2.527754 2.266377 -0.294202
1 -3.387081 2.570530 -0.653923	1 -2.437416 2.916045 -0.371649	1 -2.195652 3.172501 0.225277
1 -3.362766 1.190437 -1.766800	1 -2.744399 1.635697 -1.563064	1 -2.240495 2.341312 -1.349809
1 -4.372007 1.143062 -0.302627	1 -3.788052 1.801568 -0.138756	1 -3.616659 2.228069 -0.240427
Pre-reacting Complex Et = -598.6762355 NIImg = 0		TS-II Et = -598.6394245 NIImg=1 (-1515.74)
Carbinolamine + amine + amine Et = -598.6880329 NIImg = 0		
6 1.295960 -1.832725 0.599070	6 1.801485 -0.964337 0.193862	6 2.004528 -0.773567 -0.417554
6 1.028496 -0.866331 1.720048	6 1.413043 -0.314193 1.510382	6 1.727432 -0.994645 1.065599
1 2.335925 -2.204825 0.515378	1 2.715418 -1.567496 0.350096	1 2.826499 -1.435777 -0.722725
1 0.520614 0.004064 1.291084	1 0.631144 0.429459 1.338585	1 0.922051 -0.323392 1.375979
6 2.276961 -0.467110 2.489392	6 2.582062 0.267495 2.295667	6 2.952073 -0.810841 1.950854
1 2.999444 0.009438 1.824255	1 3.073914 1.086983 1.765225	1 3.316092 0.218248 1.933457
1 2.036502 0.237147 3.287529	1 2.249873 0.661494 3.258343	1 2.719163 -1.057040 2.988903
1 2.760529 -1.333684 2.948678	1 3.339868 -0.494955 2.497324	1 3.774313 -1.459664 1.635942
8 0.446569 -2.246073 -0.156942	8 0.812703 -1.619923 -0.479432	8 0.816333 -1.161511 -1.103750

7	2.470503	0.208147	-1.060213	7	2.162849	0.006850	-0.973860	7	2.380983	0.553325	-0.848281
6	2.319758	1.622977	-0.771007	6	1.695943	1.393744	-0.888268	6	1.646871	1.660029	-0.262625
1	1.358162	1.796793	-0.283139	1	0.651301	1.424751	-0.567596	1	0.578638	1.441084	-0.209058
1	3.113782	1.942117	-0.089234	1	2.310518	1.975985	-0.196711	1	1.997466	1.923202	0.748516
1	2.380082	2.261467	-1.667789	1	1.771595	1.843966	-1.879974	1	1.773188	2.543718	-0.893594
6	3.678555	-0.101359	-1.799427	6	3.525637	-0.112917	-1.486746	6	3.797586	0.812943	-0.981095
1	4.552901	0.127494	-1.183478	1	4.245718	0.345880	-0.803518	1	4.310317	1.004822	-0.025265
1	3.707848	-1.167007	-2.035477	1	3.772144	-1.167546	-1.610962	1	4.290431	-0.031781	-1.467151
1	3.779201	0.464104	-2.740222	1	3.595483	0.383087	-2.456038	1	3.944262	1.692894	-1.613595
1	1.662078	-0.122310	-1.571575	1	1.323701	-0.764940	-1.384543	1	0.889116	-0.764560	-1.976556
1	0.295615	-1.348796	2.378573	1	0.946481	-1.116328	2.089894	1	1.341613	-2.012882	1.171496
1	-1.522979	-1.512351	-0.409335	1	-1.088537	-1.519837	-0.169512	1	-1.188835	-1.429778	-0.451872
7	-2.411049	-1.033058	-0.533444	7	-2.099313	-1.378315	-0.083107	7	-2.179960	-1.438297	-0.226548
6	-2.809530	-1.106614	-1.926507	6	-2.756188	-1.884885	-1.271783	6	-2.937971	-1.864875	-1.386733
1	-3.692305	-0.482348	-2.094455	1	-3.819755	-1.624689	-1.256017	1	-4.008751	-1.749004	-1.194261
1	-2.007615	-0.726656	-2.562460	1	-2.314546	-1.430645	-2.161171	1	-2.687445	-1.238530	-2.245338
1	-3.054850	-2.127978	-2.260000	1	-2.682979	-2.979841	-1.379670	1	-2.761955	-2.916800	-1.666251
6	-3.401242	-1.607996	0.357233	6	-2.579406	-2.020920	1.123530	6	-2.413051	-2.281261	0.929770
1	-3.031080	-1.591661	1.384312	1	-2.016512	-1.659351	1.986881	1	-1.779790	-1.958566	1.758467
1	-4.319675	-1.014151	0.325652	1	-3.633751	-1.775583	1.288340	1	-3.454401	-2.189140	1.252635
1	-3.667949	-2.647520	0.106007	1	-2.494287	-3.120235	1.098999	1	-2.216451	-3.350128	0.743201
1	-1.705062	0.901281	0.062526	1	-1.893609	0.704532	-0.011295	1	-2.174843	0.684574	0.149047
7	-1.268074	1.782754	0.339841	7	-1.664572	1.703608	-0.004876	7	-2.014778	1.682788	0.289977
6	-1.498816	2.781526	-0.683031	6	-2.243179	2.339952	-1.169981	6	-2.640150	2.437131	-0.774096
1	-2.556498	3.081789	-0.780457	1	-3.346459	2.365142	-1.159578	1	-3.743867	2.395478	-0.763453
1	-0.922349	3.686059	-0.462869	1	-1.894426	3.375397	-1.247798	1	-2.353774	3.491784	-0.705140
1	-1.165007	2.406037	-1.652766	1	-1.928837	1.815389	-2.075121	1	-2.298167	2.066900	-1.743213
6	-1.770801	2.194449	1.633822	6	-2.122726	2.301719	1.231734	6	-2.481117	2.078782	1.600685
1	-1.633255	1.390880	2.360750	1	-1.722719	1.748167	2.084121	1	-2.027401	1.443606	2.364694
1	-1.212307	3.064534	1.994044	1	-1.763486	3.333480	1.308659	1	-2.181189	3.110933	1.809732
1	-2.840015	2.468874	1.629171	1	-3.221658	2.328171	1.331015	1	-3.577857	2.024997	1.720525

Pre-reacting Complex Et = -559.8104737 NIImag = 0			TS-Ij Et = -559.7743539 NIImag=1 (-1536.81)			Carbinolamine + methanol + methanol Et = NIImag = 0					
6	-0.849235	-1.701433	0.328619	6	1.314183	-0.710541	0.554241	6	1.439074	-0.862234	0.072527
6	-0.939148	-1.578652	-1.167359	6	0.856331	0.420841	1.454483	6	0.968017	-0.264058	1.392201
1	-1.802333	-1.814697	0.873439	1	2.189186	-1.203548	1.010026	1	2.220198	-1.604848	0.277866
1	-0.443542	-0.645008	-1.449310	1	0.100836	1.023986	0.945420	1	0.207969	0.494604	1.188066
6	-2.363398	-1.638266	-1.695460	6	1.994426	1.279431	1.992936	6	2.099985	0.317610	2.227427
1	-2.970547	-0.839271	-1.266062	1	2.529730	1.805880	1.198330	1	2.575475	1.167837	1.734417
1	-2.382445	-1.528800	-2.780997	1	1.617664	2.036533	2.683233	1	1.725609	0.667513	3.191405
1	-2.841237	-2.591072	-1.452484	1	2.724798	0.673363	2.536699	1	2.875128	-0.427885	2.426772
8	0.199571	-1.773744	0.938268	8	0.348431	-1.604130	0.145826	8	0.307786	-1.545655	-0.489579
7	-1.494315	0.921211	0.767259	7	1.764439	-0.327104	-0.877216	7	1.976979	0.025927	-0.927278
6	-2.606239	1.721059	0.293363	6	1.300812	0.955410	-1.417811	6	1.305139	1.301667	-1.103087
1	-2.660461	1.675064	-0.796189	1	0.235013	1.083940	-1.225812	1	0.221829	1.184629	-1.061182
1	-3.546642	1.329649	0.694022	1	1.856194	1.790724	-0.984029	1	1.598496	2.049251	-0.349631
1	-2.539701	2.782234	0.585221	1	1.463780	0.951143	-2.496680	1	1.560833	1.704677	-2.086130
6	-1.306355	1.019130	2.201443	6	3.161706	-0.614640	-1.194129	6	3.418822	0.124950	-0.997262
1	-2.191458	0.634514	2.717841	1	3.830760	0.110109	-0.721887	1	3.859905	0.769285	-0.220717
1	-0.453039	0.409419	2.503120	1	3.413577	-1.615593	-0.843503	1	3.868612	-0.866536	-0.913611
1	-1.139759	2.050290	2.552386	1	3.304183	-0.572755	-2.274748	1	3.703475	0.539380	-1.968133
1	-0.642852	1.207185	0.288035	1	0.931622	-1.220735	-0.981071	1	0.496907	-1.611668	-1.430684
1	1.767517	-1.224076	0.297553	1	-1.246707	-1.323391	0.393573	1	-1.411681	-1.322487	-0.001642
8	2.538988	-0.733974	-0.045970	8	-2.206365	-1.075854	0.466804	8	-2.333226	-1.106291	0.226496
6	3.579344	-0.776167	0.908553	6	-3.000359	-2.165398	0.062594	6	-3.185766	-2.127808	-0.242899
1	3.904391	-1.803954	1.100102	1	-2.812961	-3.050033	0.681517	1	-2.930539	-3.098504	0.195748
1	4.425350	-0.219767	0.503676	1	-4.049447	-1.885900	0.177152	1	-4.203419	-1.875037	0.056159
1	3.283136	-0.317818	1.858705	1	-2.829130	-2.435042	-0.987096	1	-3.160641	-2.216517	-1.335420
1	-0.325563	-2.384371	-1.586892	1	0.338691	-0.067278	2.285450	1	0.466542	-1.060426	1.949681
1	1.704898	0.735282	-0.575603	1	-2.154876	0.483518	-0.306641	1	-2.379117	0.639344	-0.246155
8	1.064337	1.429908	-0.822952	8	-1.936847	1.352325	-0.703442	8	-2.201390	1.559413	-0.505048
6	1.702737	2.401862	-1.616468	6	-2.932778	2.280489	-0.355240	6	-2.994796	2.414101	0.278989

1	2.504159	2.917708	-1.073370	1	-3.912939	2.012721	-0.770625	1	-4.068301	2.266795	0.101458
1	2.124817	1.971831	-2.532610	1	-3.039557	2.388424	0.731780	1	-2.805462	2.291879	1.353444
1	0.956108	3.144464	-1.902304	1	-2.649175	3.251381	-0.766543	1	-2.748882	3.442129	0.006906
Pre-reacting Complex Et = -559.8106867 NIImag = 0				TS-Ik Et = -559.7978817 NIImag=1 (-550.64)				Carbinolamine + methanol + methanol Et = -559.8192468 NIImag = 0			
6	1.092052	-1.328371	-0.069842	6	1.449593	0.687675	-0.172700	6	1.531223	0.062092	-0.707153
6	2.582020	-1.422837	0.104177	6	2.800825	0.259232	-0.727915	6	2.773824	-0.821396	-0.775286
1	0.728346	-0.987363	-1.054284	1	1.588269	1.220606	0.788931	1	1.815605	1.095485	-0.957941
1	2.845568	-0.820208	0.977417	1	2.633658	-0.330327	-1.633304	1	2.485662	-1.846942	-0.528478
6	3.371827	-1.004839	-1.125054	6	3.774900	-0.437170	0.214342	6	3.958940	-0.375561	0.070249
1	3.151358	0.028667	-1.396310	1	3.498339	-1.473461	0.421786	1	3.784070	-0.509519	1.139109
1	4.445377	-1.085174	-0.946467	1	4.773071	-0.463145	-0.227412	1	4.845235	-0.960269	-0.184663
1	3.134183	-1.636304	-1.985135	1	3.857924	0.086774	1.170831	1	4.203494	0.676882	-0.099371
8	0.307773	-1.705787	0.779187	8	0.728113	1.343752	-1.078759	8	0.652112	-0.459264	-1.669786
7	0.955071	1.355349	0.217846	7	0.550460	-0.539742	0.315410	7	0.828541	0.163677	0.585684
6	1.039496	1.499667	1.657145	6	0.378918	-1.569764	-0.725669	6	0.554757	-1.121043	1.219105
1	0.482820	0.695658	2.142512	1	0.250167	-1.058345	-1.678201	1	0.169998	-1.815721	0.473018
1	2.083938	1.427766	1.977892	1	1.260090	-2.210803	-0.754351	1	1.446782	-1.557680	1.688993
1	0.649307	2.461941	2.025201	1	-0.516930	-2.146482	-0.501343	1	-0.210970	-0.992311	1.986339
6	1.670991	2.396409	-0.493070	6	0.844461	-1.106190	1.641886	6	1.374252	1.135597	1.521881
1	2.743631	2.323282	-0.287193	1	1.737334	-1.725243	1.604279	1	2.295718	0.803462	2.015011
1	1.524700	2.279396	-1.568712	1	0.995514	-0.292644	2.350949	1	1.582237	2.074535	1.004342
1	1.352383	3.414478	-0.215628	1	-0.006536	-1.707991	1.961440	1	0.634001	1.334310	2.301074
1	-0.023617	1.365718	-0.068252	1	-0.357278	-0.024000	0.403130	1	-0.736893	0.801477	0.053464
1	-1.434641	-1.500737	0.546967	1	-0.384818	1.472110	-0.618780	1	-0.169873	0.049320	-1.644341
8	-2.359117	-1.266162	0.334100	8	-1.396876	1.303451	-0.008535	8	-1.545972	1.005497	-0.485946
6	-3.019953	-2.390740	-0.203743	6	-1.823606	2.424422	0.714782	6	-1.838393	2.388865	-0.442462
1	-3.034451	-3.224208	0.506380	1	-2.370897	3.130601	0.076490	1	-2.687947	2.571570	-1.100587
1	-4.050685	-2.103517	-0.414187	1	-2.493658	2.124600	1.529412	1	-2.109618	2.713565	0.567576
1	-2.559293	-2.732009	-1.138150	1	-0.981044	2.971185	1.162219	1	-0.995173	2.992876	-0.795686
1	2.797064	-2.460451	0.383786	1	3.238106	1.199407	-1.074102	1	3.061007	-0.839319	-1.829907

1 -2.212624 0.348285 -0.363492	1 -2.376881 -0.103386 0.009913	1 -2.837693 -0.105821 0.249843
8 -1.947857 1.236788 -0.669089	8 -2.672066 -1.031619 0.141514	8 -3.450725 -0.678839 0.734945
6 -2.989400 2.145974 -0.401486	6 -3.889491 -1.238082 -0.529074	6 -4.127811 -1.497123 -0.185499
1 -2.654839 3.139008 -0.706144	1 -4.184069 -2.279701 -0.385486	1 -4.800252 -2.145362 0.378921
1 -3.897684 1.906881 -0.967945	1 -4.693441 -0.603933 -0.133993	1 -4.734307 -0.918037 -0.894487
1 -3.244917 2.181169 0.664471	1 -3.807110 -1.053041 -1.607952	1 -3.444948 -2.135977 -0.760718
Pre-reacting Complex Et = -598.6774209 NIImag = 0	TS-II Et = -598.6577677 NIImag=1 (-1082.87)	Carbinolamine + aimne + amine Et = -598.6926595 NIImag = 0
6 0.283103 1.077478 -1.008179	6 -0.296352 0.768197 -0.395744	6 0.478630 -0.923739 -0.333757
6 1.072370 2.128789 -0.293538	6 0.374540 2.106428 -0.067462	6 -0.305488 -2.213297 -0.095837
1 -0.602153 1.446065 -1.559581	1 -0.519737 0.756199 -1.487560	1 0.589105 -0.779441 -1.419884
1 0.426951 2.479267 0.519767	1 0.518644 2.166369 1.015718	1 -0.430970 -2.349040 0.982699
6 1.417289 3.299849 -1.212786	6 -0.271502 3.379366 -0.602050	6 0.293012 -3.464440 -0.724018
1 0.520732 3.736435 -1.660791	1 -1.179207 3.656731 -0.060431	1 1.228329 -3.761795 -0.246002
1 1.923418 4.087433 -0.652596	1 0.417822 4.222506 -0.514540	1 -0.398718 -4.304697 -0.632655
1 2.081817 2.988242 -2.021721	1 -0.531651 3.283467 -1.660605	1 0.493883 -3.322457 -1.789867
8 0.564496 -0.100564 -1.036972	8 0.429798 -0.269983 0.029270	8 -0.299797 0.107263 0.222993
7 -2.158365 1.063405 0.805561	7 -1.743867 0.628653 0.198722	7 1.840610 -0.846275 0.200552
6 -1.840738 0.992662 2.216416	6 -1.791042 0.933857 1.625396	6 1.976270 -1.257167 1.583292
1 -0.952130 0.375789 2.367028	1 -0.921313 0.478185 2.100124	1 1.169019 -0.819692 2.171969
1 -1.619393 1.993288 2.602387	1 -1.777328 2.012660 1.810827	1 1.956830 -2.350317 1.720311
1 -2.653983 0.576106 2.835014	1 -2.701631 0.520801 2.068406	1 2.926484 -0.891272 1.982565
6 -3.367848 1.815233 0.544229	6 -2.820951 1.272413 -0.545314	6 2.892512 -1.364720 -0.648499
1 -3.226218 2.863891 0.825119	1 -2.846442 2.354485 -0.396915	1 2.967270 -2.462248 -0.661723
1 -3.600246 1.787870 -0.522690	1 -2.694985 1.074410 -1.611270	1 2.740878 -1.026694 -1.676380
1 -4.249820 1.443747 1.093573	1 -3.784504 0.861793 -0.228231	1 3.857664 -0.976867 -0.307635
1 -2.245902 0.119889 0.424270	1 -1.847531 -0.687871 0.077111	1 2.093284 1.551131 0.079624
1 -1.127460 -1.459299 -0.921435	1 -0.483887 -1.489591 -0.072048	1 0.179012 0.957129 0.089689
7 -2.023120 -1.781971 -0.568201	7 -1.495347 -1.900482 -0.072167	7 1.425204 2.308555 -0.037575
6 -2.915918 -2.067787 -1.674830	6 -1.853069 -2.487436 -1.355283	6 1.650541 2.990770 -1.299584
1 -2.601799 -2.931216 -2.283725	1 -1.312478 -3.423377 -1.531442	1 0.835867 3.695220 -1.485857

1 -3.919760 -2.279481 -1.295171	1 -2.925846 -2.696235 -1.402366	1 2.595623 3.554275 -1.327984
1 -2.985740 -1.197541 -2.330463	1 -1.597408 -1.792255 -2.156221	1 1.656867 2.266587 -2.116143
1 1.964508 1.674115 0.142437	1 1.380025 2.003971 -0.484593	1 -1.308659 -2.041042 -0.495376
6 -1.822699 -2.927588 0.299180	6 -1.739472 -2.772719 1.066978	6 1.470289 3.199622 1.108888
1 -1.093647 -2.682988 1.073799	1 -1.386918 -2.285874 1.976650	1 1.337637 2.625131 2.027043
1 -2.763082 -3.185263 0.795167	1 -2.807333 -2.985754 1.173092	1 2.411221 3.765660 1.183514
1 -1.469715 -3.826003 -0.232759	1 -1.208740 -3.724892 0.961048	1 0.650862 3.920055 1.044759
1 2.469268 -0.671107 -0.077856	1 2.360185 -0.165155 -0.042165	1 -2.392550 0.099318 0.000806
7 3.356173 -0.627793 0.412509	7 3.376243 -0.073688 -0.115518	7 -3.389832 0.012716 -0.170670
6 3.267164 -1.344756 1.666390	6 3.977940 -0.153031 1.194305	6 -4.097249 -0.149136 1.079736
1 3.159338 -2.437388 1.550327	1 3.900130 -1.151532 1.664145	1 -4.083105 0.749418 1.722600
1 4.168866 -1.166210 2.260251	1 5.043517 0.096708 1.138779	1 -5.146384 -0.395117 0.886026
1 2.415301 -0.979128 2.243721	1 3.504438 0.568781 1.863518	1 -3.663940 -0.975898 1.646259
6 4.420834 -1.112782 -0.439390	6 3.897430 -1.063013 -1.028270	6 -3.860534 1.142167 -0.940144
1 4.368370 -2.195541 -0.647784	1 3.817650 -2.102195 -0.656909	1 -3.838565 2.100084 -0.389476
1 4.402424 -0.582823 -1.393844	1 3.364384 -1.005645 -1.979946	1 -3.253880 1.255806 -1.841114
1 5.389928 -0.915714 0.029295	1 4.957419 -0.872577 -1.230929	1 -4.894448 0.973320 -1.258321
Pre-reacting Complex Et == -559.8023626 NImag = 0	TS-Im Et = -559.7959323 NImag=1 (-814.85)	Carbinolamine + aimne + amine Et = -559.8193765 NImag = 0
6 0.660935 -0.055186 -0.812307	6 0.613054 -0.355560 -0.749425	6 -0.327712 0.698733 -0.697788
6 1.335921 -1.419330 -0.933558	6 0.484418 -1.869978 -0.824706	6 0.552205 1.944329 -0.743378
1 1.189322 0.694729 -1.437415	1 1.407069 -0.017293 -1.438019	1 -1.109681 0.785014 -1.465077
1 0.870985 -2.107748 -0.222914	1 -0.273332 -2.198735 -0.108996	1 1.338544 1.848870 0.010169
6 2.856348 -1.478925 -0.858873	6 1.764233 -2.685616 -0.688515	6 -0.181583 3.269857 -0.593567
1 3.235860 -1.379228 0.160889	1 2.146549 -2.706281 0.334769	1 -0.574949 3.416573 0.413930
1 3.215784 -2.440725 -1.230530	1 1.579924 -3.722989 -0.974373	1 0.496916 4.100804 -0.796877
1 3.323709 -0.700996 -1.470008	1 2.558998 -2.306138 -1.337317	1 -1.017144 3.351537 -1.294847
8 -0.635398 -0.078248 -0.932391	8 -0.581519 0.245496 -0.999011	8 0.527339 -0.382589 -1.012031
7 0.993524 0.636366 0.688787	7 1.120540 0.185443 0.617549	7 -1.043218 0.409381 0.553031
6 0.698329 -0.270931 1.809250	6 0.426109 -0.397123 1.779116	6 -0.235652 0.528683 1.760979
1 -0.246364 -0.780345 1.615506	1 -0.644469 -0.431958 1.578201	1 0.726433 0.035813 1.620441

1	1.497715	-1.005721	1.903866	1	0.796306	-1.404072	1.978293	1	-0.055884	1.573712	2.050016
1	0.624555	0.300360	2.736470	1	0.609756	0.233481	2.649520	1	-0.753801	0.035934	2.586987
6	2.280036	1.332634	0.825318	6	2.579536	0.210206	0.782291	6	-2.339171	1.056061	0.687709
1	3.092962	0.616031	0.910020	1	2.983606	-0.793246	0.905313	1	-2.279800	2.126042	0.924933
1	2.442057	1.957810	-0.052670	1	3.032632	0.676531	-0.092273	1	-2.909953	0.942224	-0.236433
1	2.266286	1.965554	1.714944	1	2.824731	0.803730	1.664072	1	-2.898729	0.571095	1.492113
1	0.258018	1.363268	0.667223	1	0.767385	1.250992	0.507529	1	-1.398650	-1.418453	0.293767
1	-1.239409	1.364946	-0.465486	1	-0.458274	1.355717	-0.643882	1	0.011090	-1.206451	-0.965641
8	-1.247147	2.195189	0.089068	8	-0.053598	2.307692	0.034045	8	-1.253702	-2.288121	-0.137985
6	-1.694196	3.302470	-0.654493	6	0.363251	3.463253	-0.632728	6	-2.480759	-2.895481	-0.473327
1	-2.744053	3.191934	-0.949023	1	-0.497825	4.047964	-0.979880	1	-2.258410	-3.827225	-0.994009
1	-1.611109	4.192530	-0.028013	1	0.946969	4.107474	0.036212	1	-3.071200	-3.136241	0.417995
1	-1.097506	3.462615	-1.561426	1	0.987917	3.246641	-1.513932	1	-3.088262	-2.268798	-1.137819
1	1.010445	-1.764177	-1.919386	1	0.045886	-2.045715	-1.810620	1	1.060982	1.914150	-1.710714
1	-1.431097	-1.377613	-0.161109	1	-1.989492	-0.515530	-0.227822	1	2.184657	-0.468384	-0.156725
8	-1.756419	-2.086955	0.439832	8	-2.603371	-0.982969	0.371793	8	2.948398	-0.417173	0.437557
6	-3.130504	-2.279100	0.231242	6	-3.894686	-0.448671	0.220745	6	3.826040	-1.477034	0.147564
1	-3.472049	-3.061612	0.912434	1	-4.556300	-0.967753	0.916796	1	4.671429	-1.404327	0.833565
1	-3.715709	-1.372670	0.437410	1	-3.931272	0.623700	0.451685	1	3.356543	-2.458836	0.290752
1	-3.354568	-2.603192	-0.793839	1	-4.288137	-0.595457	-0.793398	1	4.215910	-1.426555	-0.877218

**Table S55.** The mPW1PW91/6-311+G\*\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Pre-Reacting Complexes, Transition States and Final Products for the Dehydration step (**Step-II**) [Only in the case of **TS-IIIi**, geometry (in Cartesian coordinates), Total Electronic Energies (in hartree/particle) are at the mPW1PW91/6-311g\*\* level of theory]

Pre-reacting Complex Et = -328.3353946 NIImag = 0			TS-II Et = -328.2598271 NIImag=1 (-667.13)			Enamine Et = -328.3225422 NIImag = 0		
6 0.232998	-0.338721	-0.172224	6 0.212150	-0.150276	0.535579	6 -0.290655	-0.612194	-0.484364
6 1.368811	0.669492	-0.215463	6 1.362433	-0.379820	-0.295229	6 -1.372020	-0.487124	0.308401
1 0.385306	-1.074297	-0.973706	1 0.354285	0.397989	1.459672	1 -0.431517	-0.637531	-1.562984
1 1.205078	1.322374	-1.076706	1 1.229065	-1.145431	-1.058024	1 -1.251996	-0.452853	1.386934
6 2.735471	0.004118	-0.297167	6 2.704322	-0.444025	0.411588	6 -2.773756	-0.498223	-0.218881
1 2.831890	-0.594405	-1.207707	1 2.844332	-1.374612	0.969048	1 -3.318630	-1.395108	0.095984
1 3.532780	0.750367	-0.307371	1 3.515296	-0.367471	-0.314484	1 -3.351686	0.359695	0.139591
1 2.896827	-0.653493	0.558303	1 2.815512	0.390903	1.107615	1 -2.787722	-0.475029	-1.311409
8 0.339968	-1.007250	1.090208	8 0.214754	1.851443	-0.661375	8 0.035081	2.489380	0.145880
7 -1.058640	0.252380	-0.422832	7 -1.030002	-0.494013	0.282182	7 1.024947	-0.745645	-0.107800
6 -1.463752	1.283359	0.515731	6 -1.396587	-1.070177	-1.000912	6 1.344566	-0.657855	1.296726
1 -1.602166	0.904676	1.539293	1 -1.370836	-0.290847	-1.767746	1 1.178720	0.350108	1.703993
1 -0.727854	2.086606	0.542630	1 -0.708120	-1.869072	-1.268839	1 0.735634	-1.367817	1.860370
1 -2.408909	1.714282	0.178692	1 -2.400443	-1.485840	-0.925757	1 2.393445	-0.920313	1.440427
6 -2.103526	-0.730598	-0.616359	6 -2.073153	0.284919	0.926741	6 2.025307	-0.208273	-1.008862

1	-2.997288	-0.243626	-1.013021	1	-3.013914	-0.264393	0.911204	1	2.989074	-0.681294	-0.809092
1	-1.779758	-1.477048	-1.346183	1	-1.795090	0.491847	1.959159	1	1.745525	-0.433578	-2.039402
1	-2.400758	-1.253227	0.310178	1	-2.159519	1.235744	0.386695	1	2.135179	0.879819	-0.909499
1	-0.186333	-1.807607	1.063500	1	0.121267	2.795924	-0.804813	1	-0.615726	3.191527	0.129428
1	1.321906	1.290842	0.683144	1	1.205162	0.688075	-0.804608	1	-0.476224	1.668862	0.105101
Pre-reacting Complex Et = -463.5121862 NImag = 0				TS-IIa Et = -463.4450588 Nimag=1(-479.42)				Enamine + amine Et = -463.5011936 NImag = 0			
6	-1.261951	0.295139	-0.682981	6	1.728638	0.372387	-0.229590	6	-2.180027	0.263603	0.086072
6	-0.758468	1.557741	-0.002054	6	1.975471	-0.910897	0.383504	6	-2.114643	-0.931079	-0.536082
1	-1.957118	0.580938	-1.482850	1	2.132047	0.530128	-1.223155	1	-2.844920	0.370127	0.941303
1	0.020984	1.294902	0.718286	1	1.719462	-0.965871	1.440229	1	-1.453224	-1.061822	-1.386896
6	-1.863324	2.369119	0.656845	6	3.312450	-1.552105	0.047379	6	-3.020124	-2.075344	-0.193394
1	-2.358635	1.801531	1.446200	1	4.156214	-1.048626	0.527369	1	-3.741857	-2.275491	-0.993268
1	-1.459922	3.284950	1.094098	1	3.317669	-2.593530	0.372471	1	-2.465637	-3.006700	-0.037181
1	-2.629982	2.657101	-0.067986	1	3.482806	-1.550598	-1.032048	1	-3.592475	-1.872122	0.715569
8	-0.102950	-0.310238	-1.287319	8	0.054967	-1.057709	-1.387829	8	0.303736	-1.414295	1.511579
7	-1.998433	-0.579814	0.186762	7	1.005291	1.351571	0.232293	7	-1.530874	1.425976	-0.238623
6	-1.264679	-1.108273	1.321426	6	0.288884	1.294117	1.500528	6	-0.580468	1.421347	-1.328457
1	-0.483849	-1.827171	1.032329	1	-0.709139	0.867086	1.320590	1	0.352102	0.892548	-1.084105
1	-0.791315	-0.303747	1.882971	1	0.838674	0.686834	2.215080	1	-1.034363	0.958084	-2.207106
1	-1.964183	-1.615393	1.989840	1	0.201481	2.308131	1.891910	1	-0.332935	2.453573	-1.582695
6	-2.732312	-1.614673	-0.508809	6	0.558740	2.398554	-0.672015	6	-1.266933	2.369840	0.824835
1	-3.442812	-2.084520	0.175305	1	0.587763	3.363120	-0.163937	1	-1.155922	3.373010	0.407266
1	-3.302038	-1.178182	-1.332635	1	1.200274	2.427367	-1.550037	1	-2.107492	2.383055	1.520801
1	-2.093042	-2.419716	-0.914010	1	-0.463620	2.177257	-0.987829	1	-0.356365	2.127494	1.390432
1	-0.389908	-1.007790	-1.879320	1	-0.180754	-1.497423	-2.207169	1	0.136640	-2.278900	1.887746
1	-0.262021	2.151036	-0.774355	1	1.125734	-1.413140	-0.253871	1	-0.472722	-1.216864	0.962592
1	1.822780	-0.193509	-0.295671	1	-1.447834	-0.621121	-0.468562	1	1.953607	-0.664974	0.463466
7	2.656833	-0.029524	0.257532	7	-2.228186	-0.314337	0.143330	7	2.588728	-0.170551	-0.155401
6	3.326005	-1.281306	0.535164	6	-3.286090	0.253089	-0.663089	6	3.470958	0.677312	0.617094
1	2.625468	-1.985096	0.989604	1	-2.884596	1.038323	-1.308680	1	2.883824	1.324707	1.271668

1	3.765859	-1.762351	-0.356677	1	-3.789270	-0.484451	-1.313229	1	4.189156	0.120937	1.244449
1	4.137907	-1.117535	1.250640	1	-4.056869	0.704929	-0.027913	1	4.051259	1.320343	-0.052276
6	3.511463	0.927732	-0.410559	6	-2.690017	-1.437848	0.929611	6	3.303408	-1.113445	-0.988038
1	2.942858	1.828509	-0.649750	1	-1.848712	-1.890070	1.460106	1	2.594494	-1.764060	-1.504544
1	4.330873	1.220930	0.253219	1	-3.422212	-1.110771	1.677075	1	3.876563	-0.577498	-1.751201
1	3.962492	0.549508	-1.344938	1	-3.167037	-2.230322	0.326904	1	4.012368	-1.752477	-0.432666
Pre-reacting Complex Et = -444.0770958 NImag = 0				<b>TS-IIb</b> Et = -444.0200153 NImag=1(-296.21)				Enamine + methanol Et = -444.0667471 NImag = 0			
6	-0.805005	0.210353	-0.710464	6	1.269636	0.386580	-0.383183	6	1.501699	0.294949	-0.565320
6	-0.418240	1.573408	-0.161155	6	1.908073	-0.546908	0.520367	6	2.164078	-0.635679	0.155806
1	-1.434040	0.351412	-1.597981	1	1.449703	0.242666	-1.443480	1	1.390274	0.141022	-1.636609
1	0.297643	1.444042	0.655248	1	1.874959	-0.252910	1.568396	1	2.294342	-0.497258	1.225219
6	-1.612237	2.400750	0.289471	6	3.279498	-1.033872	0.076601	6	2.886047	-1.788680	-0.475475
1	-2.155436	1.908355	1.097467	1	4.045698	-0.256913	0.144260	1	3.973238	-1.679085	-0.393617
1	-1.289091	3.382718	0.641182	1	3.596260	-1.869685	0.701787	1	2.631435	-2.743766	-0.005133
1	-2.318067	2.558048	-0.530716	1	3.247965	-1.395642	-0.953915	1	2.646228	-1.872630	-1.538311
8	0.435562	-0.397026	-1.146049	8	-0.220793	-1.773195	-0.536761	8	-0.688969	-1.957892	0.478606
7	-1.566035	-0.593463	0.198216	7	0.408985	1.311829	-0.098160	7	0.953376	1.468673	-0.128595
6	-0.927946	-0.904875	1.465863	6	-0.059619	1.595598	1.252507	6	0.979903	1.765496	1.281144
1	-0.051684	-1.559954	1.362969	1	-0.991701	1.040518	1.398754	1	0.323759	1.103626	1.865124
1	-0.610257	0.007114	1.970266	1	0.685021	1.298630	1.985128	1	1.998782	1.670052	1.663436
1	-1.655101	-1.402913	2.110558	1	-0.241585	2.667218	1.336618	1	0.650909	2.793343	1.436476
6	-2.160756	-1.763286	-0.412662	6	-0.385825	1.934458	-1.151887	6	-0.146400	2.041478	-0.884155
1	-2.916106	-2.182834	0.255546	1	-0.402056	3.015119	-1.003441	1	-0.163895	3.123675	-0.735252
1	-2.658226	-1.483945	-1.344598	1	0.047155	1.701971	-2.122366	1	0.010631	1.851378	-1.947294
1	-1.437644	-2.569502	-0.629368	1	-1.395021	1.518071	-1.087887	1	-1.117381	1.622988	-0.592028
1	0.236787	-1.205200	-1.623180	1	-0.468452	-2.582323	-0.985764	1	-0.567372	-2.477289	1.274451
1	0.124245	2.089689	-0.957219	1	1.120421	-1.380305	0.337806	1	0.163827	-1.512647	0.325377
1	1.952780	-0.460323	-0.044666	1	-1.402812	-0.957586	-0.193026	1	-2.066196	-0.733675	0.360464
8	2.707190	-0.513258	0.558701	8	-2.154254	-0.288261	0.070279	8	-2.714273	-0.019513	0.258295
6	3.813795	0.106479	-0.047487	6	-3.340228	-0.991534	0.294427	6	-3.881541	-0.547984	-0.321263

1	4.118625	-0.394169	-0.975842	1	-3.702708	-1.501953	-0.610473	1	-3.692737	-0.996917	-1.304759
1	3.629793	1.165052	-0.273131	1	-3.233555	-1.751558	1.082305	1	-4.357604	-1.304468	0.315925
1	4.648330	0.051941	0.653342	1	-4.121023	-0.292396	0.611280	1	-4.588641	0.272694	-0.452938
Pre-reacting complex Et = -463.508619 NImag = 0				<b>TS-IIc</b> Et = -463.4381319 NImag=1(-501.39)				Enamine + amine + amine Et = -463.5028615 NImag = 0			
6	-1.430965	0.545005	-0.290657	6	-1.137863	0.781391	-0.312455	6	-1.501864	0.853197	-0.456056
6	-0.838141	1.486432	0.744083	6	-0.083471	1.390699	0.428032	6	-0.882987	1.762355	0.321637
1	-2.155917	1.098136	-0.901638	1	-1.171984	0.941244	-1.382944	1	-1.511382	1.007934	-1.533388
6	-0.426134	2.824521	0.145634	6	0.459087	2.692342	-0.145101	6	-0.305157	3.035302	-0.217507
1	-1.287076	3.357309	-0.268524	1	-0.217955	3.537448	0.009393	1	-0.856829	3.915111	0.132826
1	0.025662	3.466934	0.904241	1	1.413876	2.944168	0.320752	1	0.736260	3.179507	0.090586
1	0.301141	2.686392	-0.656236	1	0.638147	2.599202	-1.219277	1	-0.331110	3.050892	-1.310282
8	-0.338858	0.149156	-1.144530	8	-0.011778	-1.277482	-1.374792	8	0.753441	-2.712451	0.014745
7	-2.156106	-0.554772	0.286347	7	-2.092862	0.004570	0.147004	7	-2.192247	-0.266762	-0.067540
6	-1.394327	-1.419219	1.169260	6	-2.122151	-0.451088	1.522587	6	-2.198451	-0.620250	1.329721
1	-0.615544	-1.992472	0.644872	1	-1.460756	-1.312469	1.653729	1	-1.213035	-0.953614	1.685798
1	-0.917726	-0.838862	1.957980	1	-1.811120	0.345130	2.196159	1	-2.518592	0.235805	1.928237
1	-2.077540	-2.127392	1.643168	1	-3.140133	-0.743754	1.777505	1	-2.907854	-1.433288	1.488842
6	-2.910823	-1.315849	-0.686428	6	-2.854474	-0.790367	-0.808368	6	-2.262892	-1.378582	-0.997813
1	-3.604119	-1.984306	-0.171089	1	-3.781360	-1.125610	-0.343164	1	-3.157261	-1.970643	-0.788446
1	-3.500942	-0.640233	-1.310870	1	-3.094400	-0.179939	-1.678358	1	-2.347954	-0.991926	-2.015167
1	-2.283273	-1.942628	-1.344718	1	-2.217276	-1.621894	-1.126464	1	-1.383254	-2.030961	-0.934426
1	1.632208	-0.243063	-0.322648	1	1.179453	-0.968127	-0.611572	1	1.263768	-1.870265	0.014845
1	-0.694249	-0.246409	-1.941994	1	0.153100	-1.609693	-2.258487	1	1.399621	-3.407380	-0.108254
7	2.489486	-0.382818	0.200889	7	1.908639	-0.502282	0.085291	7	2.001697	-0.184479	0.021149
1	0.031814	1.007274	1.201587	1	0.843701	0.560159	0.325106	1	1.139851	0.358114	0.037716
1	-1.586000	1.632467	1.527645	1	-0.256185	1.436310	1.504253	1	-0.858832	1.627000	1.398715
6	3.477575	0.599316	-0.188811	6	3.102399	-0.061571	-0.600868	6	2.736644	0.114569	-1.196678
1	4.340514	0.543234	0.482061	1	3.725411	0.570270	0.043982	1	3.107125	1.149858	-1.237283
1	3.852759	0.472657	-1.219790	1	3.726345	-0.902907	-0.939898	1	3.599662	-0.551918	-1.278578
1	3.057956	1.603380	-0.101675	1	2.823520	0.520155	-1.482252	1	2.097665	-0.058457	-2.064075

6	2.956405	-1.742016	0.038745	6	2.182970	-1.330216	1.236332	6	2.768523	0.091754	1.224622
1	3.305556	-1.977319	-0.982503	1	2.733990	-2.246097	0.975259	1	3.631203	-0.578247	1.273534
1	3.791470	-1.931526	0.720328	1	2.775483	-0.789902	1.985590	1	3.142919	1.125393	1.273150
1	2.158974	-2.442836	0.294434	1	1.242942	-1.637002	1.702000	1	2.151453	-0.094690	2.104864
Pre-reacting Complex				<b>TS-IIId</b>				Enamine + methanol			
Et = -444.0768526 NIImag = 0				Et = -444.0205492 NIImag=(-139.37)				Et = -444.0638594 NIImag = 0			
6	-0.958788	0.577667	-0.333448	6	1.122150	0.664447	0.069924	6	-0.771674	-1.087235	0.493976
6	-0.380985	1.539250	0.690733	6	0.185395	1.430840	-0.760189	6	-0.000168	-1.811697	-0.345364
1	-1.562996	1.143501	-1.053316	1	1.514438	1.096445	0.982268	1	-0.592493	-1.163824	1.564594
1	-1.191150	1.826028	1.365860	1	0.534171	1.429298	-1.800501	1	-0.165820	-1.754313	-1.417020
6	0.242038	2.771893	0.049687	6	-0.067401	2.836696	-0.239847	6	0.983150	-2.836572	0.136015
1	-0.500049	3.345841	-0.512538	1	0.837396	3.451222	-0.241590	1	0.646734	-3.855824	-0.084799
1	0.663906	3.432671	0.809605	1	-0.810189	3.338795	-0.860962	1	1.962923	-2.723620	-0.339018
1	1.042523	2.492451	-0.636965	1	-0.458932	2.785620	0.777160	1	1.128952	-2.771593	1.217500
8	0.174592	0.033880	-1.056209	8	-0.641228	0.227668	1.811463	8	0.263659	2.992329	-0.056388
7	-1.826354	-0.414287	0.230211	7	1.523150	-0.530094	-0.212054	7	-1.814328	-0.261221	0.179682
6	-1.247385	-1.256851	1.263681	6	0.965359	-1.282799	-1.337261	6	-2.125738	-0.033549	-1.208767
1	-0.842954	-0.648015	2.071142	1	1.072558	-0.707145	-2.256913	1	-2.241427	-0.988517	-1.726488
1	-2.036349	-1.882493	1.686024	1	1.514592	-2.216877	-1.433696	1	-3.068215	0.510434	-1.278421
1	-0.447122	-1.913209	0.894091	1	-0.108352	-1.445620	-1.118108	1	-1.351754	0.552952	-1.724118
6	-2.533604	-1.191696	-0.765886	6	2.320490	-1.288035	0.738269	6	-2.147493	0.815846	1.094324
1	-3.341068	-1.751467	-0.289029	1	3.184076	-1.721193	0.231910	1	-3.211455	1.049711	1.008200
1	-2.983203	-0.525847	-1.507069	1	2.651130	-0.639025	1.545683	1	-1.957295	0.490420	2.118446
1	-1.896972	-1.924467	-1.291994	1	1.702751	-2.086429	1.153995	1	-1.564996	1.723402	0.896352
1	-0.143607	-0.419894	-1.838788	1	-0.882038	-0.206886	2.628466	1	0.416332	3.627189	-0.755891
1	1.621932	-0.755651	-0.159029	1	-1.173472	-0.253501	1.014277	1	0.868220	2.252680	-0.243361
8	2.343990	-1.157990	0.343841	8	-1.656446	-0.755727	-0.196324	8	1.849937	0.745938	-0.489575
6	3.567139	-0.723568	-0.195634	6	-3.002295	-1.064723	-0.232007	6	3.008809	0.536474	0.293075
1	3.678701	0.367800	-0.155777	1	-3.628242	-0.321096	0.296829	1	2.766141	0.363967	1.347075
1	4.367087	-1.165709	0.400263	1	-3.390784	-1.115572	-1.264468	1	3.598274	-0.307516	-0.079852
1	3.704655	-1.045208	-1.236511	1	-3.233388	-2.043421	0.230204	1	3.617734	1.437840	0.224549

1	0.372006	1.016381	1.286708	1	-0.748562	0.811970	-0.754615	1	1.258360	-0.020584	-0.397366
Carbinolamine Et = -598.6935384 NImag = 0				TS-IIe Et = -598.6297169 NImag=1 (-111.28)				Enamine + amine + amine Et = -598.6759049 NImag = 0			
6	-0.772246	-1.229440	-0.356470	6	-0.363159	1.236762	0.446420	6	-0.655403	1.863058	0.420857
6	-2.000822	-1.098137	-1.246904	6	0.137134	2.110877	-0.621508	6	-0.209789	2.444925	-0.714495
1	-0.197289	-2.104964	-0.688946	1	-1.370417	0.836249	0.358519	1	-1.702098	1.574341	0.487127
1	-2.521426	-0.167720	-1.001677	1	1.083924	2.588819	-0.369746	1	0.835078	2.725567	-0.805687
6	-2.948394	-2.285249	-1.170609	6	-0.901568	3.121254	-1.101489	6	-1.131820	2.880560	-1.814647
1	-3.341334	-2.416301	-0.161272	1	-1.148222	3.858197	-0.333187	1	-1.208332	3.972298	-1.872524
1	-3.790365	-2.156195	-1.854904	1	-0.520929	3.658898	-1.970938	1	-0.791645	2.543251	-2.799887
1	-2.439312	-3.214388	-1.442750	1	-1.822900	2.618993	-1.402037	1	-2.142720	2.493913	-1.661628
8	0.024877	-0.063939	-0.556956	8	-0.087618	-0.563688	-1.248527	8	0.018978	-0.591830	-1.552482
7	-1.106176	-1.484728	1.025611	7	0.272650	0.887059	1.515765	7	0.050225	1.586189	1.558045
6	-1.886822	-0.440960	1.669552	6	1.661478	1.242618	1.796164	6	1.467748	1.859130	1.602579
1	-1.362069	0.522737	1.723514	1	2.312060	0.564174	1.222709	1	2.052418	1.140718	1.010107
1	-2.828520	-0.287034	1.141036	1	1.851104	2.276156	1.514746	1	1.661521	2.870104	1.237642
1	-2.131899	-0.761406	2.684721	1	1.832387	1.131789	2.866063	1	1.804770	1.803840	2.639356
6	0.042808	-1.853759	1.822800	6	-0.307656	-0.123330	2.391587	6	-0.414894	0.522003	2.420151
1	-0.288374	-2.200494	2.804714	1	-0.314404	0.243536	3.419348	1	-0.196046	0.764425	3.463664
1	0.577110	-2.676689	1.340749	1	-1.318385	-0.349354	2.056250	1	-1.491164	0.397405	2.303212
1	0.752298	-1.023926	1.981007	1	0.301930	-1.027222	2.333595	1	0.062188	-0.438591	2.182886
1	2.923511	-0.421562	-1.741340	1	-1.824677	-0.845819	-0.622786	1	-1.808150	-1.267248	-0.481662
1	-1.631554	-0.968429	-2.267577	1	0.319718	1.348890	-1.408747	1	-0.045743	0.333896	-1.250265
1	-0.433687	1.934495	-0.026224	1	1.658388	-0.774702	-0.747924	1	1.964230	-1.074330	-0.738007
7	-0.676795	2.878007	0.260881	7	2.641538	-0.869559	-0.424398	7	2.878107	-1.080813	-0.296488
6	0.518158	3.651130	0.507420	6	2.895511	-2.246173	-0.058116	6	3.111841	-2.356917	0.345029
1	1.156903	3.130273	1.224299	1	2.146198	-2.584808	0.661738	1	2.287191	-2.589330	1.021973
1	1.115269	3.859285	-0.399821	1	2.870651	-2.941891	-0.915137	1	3.221423	-3.198435	-0.361021
1	0.253074	4.617624	0.948059	1	3.880572	-2.345646	0.412220	1	4.027294	-2.310387	0.943084
6	-1.545039	3.485707	-0.722630	6	3.538150	-0.411927	-1.464508	6	3.896869	-0.746815	-1.268491
1	-2.399833	2.834589	-0.915660	1	3.267383	0.601519	-1.770050	1	3.645728	0.194793	-1.761644

1 -1.933576 4.435621 -0.341356	1 4.571327 -0.386707 -1.099209	1 4.859313 -0.608947 -0.766004
1 -1.050980 3.694482 -1.688468	1 3.523807 -1.046077 -2.367670	1 4.040334 -1.514822 -2.048791
1 0.973870 -0.308135 -0.547016	1 -0.162099 -1.398487 -1.717002	1 -0.055359 -0.552077 -2.507140
7 2.826421 -0.584626 -0.745806	7 -2.723952 -0.893045 -0.110835	7 -2.681048 -1.347999 0.029764
6 3.368993 -1.896357 -0.422287	6 -3.810953 -0.462770 -0.964642	6 -3.795666 -1.269400 -0.891083
1 2.876209 -2.661018 -1.024851	1 -3.578697 0.510245 -1.403303	1 -3.715231 -0.364424 -1.497072
1 4.454176 -1.968247 -0.586416	1 -4.020143 -1.160495 -1.793355	1 -3.872513 -2.133325 -1.574009
1 3.173733 -2.119255 0.628816	1 -4.734525 -0.356178 -0.384992	1 -4.734968 -1.209461 -0.332869
6 3.493303 0.490863 -0.023249	6 -2.929335 -2.231894 0.399312	6 -2.686599 -2.569078 0.807935
1 3.087669 1.453329 -0.337032	1 -2.044437 -2.561543 0.948922	1 -1.798153 -2.610706 1.441182
1 3.300922 0.380320 1.046254	1 -3.781803 -2.255271 1.087561	1 -3.561905 -2.586472 1.464646
1 4.582679 0.501156 -0.172754	1 -3.126134 -2.977435 -0.390417	1 -2.713997 -3.487793 0.196925
Pre-reacting Complex HF=-559.8122648 NIImag= 0	TS-IIIf Et =-559.7774586 NIImag=1 (-143.57)	Enamine + methanol + methanol Et = -559.8050149 NIImag = 0
6 1.790985 2.647049 -0.549440	6 1.109585 -0.946720 0.400227	6 1.771723 0.081707 0.445496
6 2.229086 1.189421 -0.487375	6 1.609136 -1.052731 -0.944722	6 2.365915 0.184348 -0.766741
6 1.260400 0.299094 0.279842	1 1.517435 -0.145441 1.012817	1 1.562189 0.992635 1.002002
7 1.808813 -0.965754 0.639529	1 1.311828 -1.957874 -1.473808	1 2.581316 -0.712138 -1.340599
6 1.023479 -1.697123 1.617859	6 3.073669 -0.687348 -1.131140	6 2.930709 1.477528 -1.278933
6 2.244416 -1.817680 -0.452440	1 3.748568 -1.454372 -0.742099	1 4.026163 1.481554 -1.248763
8 -0.006693 0.208392 -0.454891	1 3.292719 -0.557766 -2.191925	1 2.650163 1.668599 -2.320115
8 -1.644527 -2.129611 -0.877047	1 3.299808 0.257143 -0.631940	1 2.585071 2.325262 -0.682202
6 -2.979174 -2.174258 -0.430143	8 -0.108694 1.035773 -1.466902	8 -0.566634 0.672044 -1.570873
8 -1.677086 2.409881 0.334284	7 0.081752 -1.552676 0.909509	7 1.388646 -1.052280 1.098725
6 -3.026722 2.068583 0.535053	6 -0.678678 -2.585278 0.216883	6 1.558088 -2.332983 0.457361
1 0.969215 0.797682 1.206999	1 -1.517031 -2.104137 -0.296024	1 0.841762 -2.489544 -0.360487
1 3.202640 1.106398 0.001957	1 -0.045142 -3.110950 -0.492666	1 2.573341 -2.421147 0.064539
1 1.708649 3.075700 0.451917	1 -1.050502 -3.293083 0.958119	1 1.406851 -3.122309 1.194865
1 2.516462 3.241495 -1.108291	6 -0.538447 -1.055309 2.132340	6 0.328355 -0.969319 2.084673
1 0.818802 2.764725 -1.030905	1 -0.628909 -1.866835 2.856622	1 0.508919 -1.695290 2.881846
1 1.412347 -2.211291 -1.055610	1 0.061427 -0.244946 2.539379	1 0.317177 0.029022 2.522153

1 2.937170 -1.285135 -1.104624	1 -1.525627 -0.670246 1.868222	1 -0.654563 -1.169788 1.641679
1 2.782697 -2.672209 -0.037771	1 -0.167975 1.558993 -2.267015	1 -0.534260 0.964998 -2.483399
1 1.633371 -2.499553 2.039429	1 -1.462033 0.409225 -0.949618	1 -1.537368 -0.862459 -1.019029
1 0.737977 -1.029231 2.433152	8 -2.253852 -0.062096 -0.535357	8 -1.902329 -1.658937 -0.609017
1 0.114526 -2.148644 1.196356	6 -3.423494 0.631279 -0.870080	6 -3.239702 -1.811751 -1.018358
1 0.190975 0.157355 -1.394535	1 -3.589524 0.671656 -1.955828	1 -3.332070 -1.939544 -2.104625
1 -1.219560 -1.331627 -0.539329	1 -4.278635 0.116520 -0.423034	1 -3.631057 -2.710816 -0.540461
1 -3.573087 -1.330062 -0.801727	1 -3.418899 1.663305 -0.492653	1 -3.868773 -0.965171 -0.714706
1 -3.421693 -3.093581 -0.815094	1 0.937038 -0.180792 -1.379322	1 0.362721 0.475999 -1.316772
1 -3.052342 -2.195098 0.664565	1 0.546449 1.729669 -0.176260	1 -0.934760 1.955918 -0.164364
1 2.360376 0.798847 -1.504081	8 0.992315 1.956769 0.695660	8 -0.952478 2.520972 0.618821
1 -1.195471 1.629324 0.030468	6 0.737377 3.294949 1.020995	6 -2.276307 2.600578 1.089798
1 -3.518537 1.741367 -0.390206	1 1.142408 3.990427 0.272854	1 -2.951777 3.065316 0.359998
1 -3.152458 1.282396 1.290827	1 -0.336622 3.501524 1.126597	1 -2.682408 1.617875 1.360981
1 -3.542122 2.961597 0.890903	1 1.217906 3.520085 1.976789	1 -2.270307 3.223698 1.985158
Pre-reacting complex Et = -559.8175044 NIImag = 0	<b>TS-IIg</b> Et = -559.7747494 NIImag=1 (-85.46)	Iminium ion + methanol + methanol Et = -559.7767279 NIImag = 0
6 -1.748110 0.295580 -0.346100	6 1.764907 -0.084557 0.066300	6 1.712535 -0.355725 0.050746
6 -1.024728 1.627486 -0.482890	6 1.654196 1.368289 -0.214127	6 1.897128 1.081067 -0.249073
1 -2.728799 0.370679 -0.832821	1 2.348762 -0.418899 0.912653	1 2.096002 -0.756746 0.980488
1 -1.566426 2.349877 0.134282	1 2.135043 1.563710 -1.181405	1 2.374650 1.184466 -1.230752
6 -0.965482 2.119612 -1.923787	6 2.287229 2.223444 0.873501	6 2.697193 1.802685 0.825886
1 -1.963181 2.199447 -2.367474	1 3.357361 2.025916 0.976831	1 3.713560 1.410158 0.913048
1 -0.503108 3.106768 -1.973695	1 2.166159 3.281909 0.640005	1 2.770638 2.865273 0.591702
1 -0.361545 1.460723 -2.554644	1 1.811487 2.031994 1.835935	1 2.206974 1.703967 1.795552
8 -1.018898 -0.757711 -1.060538	8 0.300213 -0.345032 1.901467	8 0.110889 -0.494206 2.108029
7 -1.990807 -0.097761 0.995945	7 1.331548 -1.013609 -0.718159	7 1.101133 -1.195482 -0.704714
6 -0.834500 -0.238694 1.865809	6 0.521581 -0.773003 -1.907916	6 0.430043 -0.840193 -1.950714
1 -1.182992 -0.306754 2.899065	1 0.969794 -1.311231 -2.745439	1 0.789248 -1.503603 -2.739462
1 -0.239098 -1.136776 1.648400	1 -0.483738 -1.140456 -1.694114	1 -0.639240 -0.974506 -1.775118
1 -0.181032 0.628723 1.789963	1 0.455550 0.287149 -2.126889	1 0.608877 0.198147 -2.206355

6 -2.901997 -1.218673 1.120930	6 1.402690 -2.412056 -0.316309	6 0.830827 -2.555177 -0.248860
1 -3.224119 -1.306276 2.161121	1 1.788041 -3.009907 -1.143685	1 1.110488 -3.260223 -1.032766
1 -3.788884 -1.044725 0.507302	1 2.045579 -2.514802 0.554403	1 1.386099 -2.756335 0.663378
1 -2.454336 -2.175950 0.817025	1 0.389713 -2.727480 -0.059263	1 -0.241183 -2.599999 -0.042677
1 -1.126528 -0.612737 -2.002935	1 -0.016592 0.343637 2.486767	1 -0.207777 0.079090 2.804521
1 0.679026 -1.218383 -0.639749	1 -0.551952 -0.634511 1.273490	1 -0.672352 -0.583573 1.427189
8 1.611037 -1.402953 -0.422624	8 -1.477281 -0.953142 0.359360	8 -1.610171 -0.698930 0.300090
6 2.179919 -2.198565 -1.438872	6 -2.605559 -1.595168 0.853390	6 -2.897551 -1.119728 0.598278
1 2.184673 -1.688082 -2.409544	1 -3.177718 -0.975757 1.566707	1 -3.413872 -0.460940 1.320281
1 3.212938 -2.407157 -1.159250	1 -3.303639 -1.867656 0.046127	1 -3.541164 -1.159521 -0.297329
1 1.654775 -3.154188 -1.544453	1 -2.355896 -2.529785 1.383841	1 -2.916616 -2.132028 1.039796
1 -0.009929 1.552371 -0.085356	1 0.590258 1.608536 -0.347333	1 0.885759 1.509536 -0.358670
1 2.225616 0.203448 0.158890	1 -1.608093 0.446326 -0.360481	1 -1.433924 0.677685 -0.348477
8 2.374244 1.111619 0.471546	8 -1.513000 1.335594 -0.828735	8 -1.163201 1.554423 -0.797375
6 3.389632 1.098572 1.443362	6 -2.620809 2.139992 -0.533255	6 -2.062280 2.563619 -0.433173
1 4.354262 0.769985 1.034558	1 -2.727107 2.330255 0.544353	1 -2.097118 2.723323 0.654288
1 3.512485 2.118414 1.811973	1 -2.496472 3.105240 -1.031617	1 -1.748640 3.502902 -0.898066
1 3.142383 0.455375 2.297939	1 -3.562240 1.700072 -0.890008	1 -3.085835 2.351718 -0.772068
Pre-reacting Complex Et = -559.776878 NIImag = 0		TS-IIIg Et = -559.7742756 NIImag=1 (-78.71)
Enamine + methanol + methanol Et = -559.8117115 NIImag = 0		
6 -1.457877 -0.426408 0.001724	6 1.535428 -0.465958 0.105765	6 1.521233 1.816171 1.915208
6 -2.010846 0.889570 -0.370665	6 1.884913 0.938715 0.196120	6 1.880441 1.021525 0.693989
1 -1.321946 -1.195903 -0.762004	1 1.520708 -1.081006 1.002581	6 1.529522 -0.275432 0.545682
1 -2.664103 1.271293 0.421092	1 2.391878 1.291802 -0.706961	7 1.943099 -1.143667 -0.429075
6 -2.712026 0.883979 -1.721917	6 2.612309 1.336144 1.470241	6 1.090996 -2.269898 -0.750557
1 -3.594559 0.240138 -1.720211	1 3.622145 0.920478 1.523485	6 2.789142 -0.660031 -1.487500
1 -3.035454 1.892374 -1.982631	1 2.698032 2.421950 1.529564	8 -0.861914 1.442225 -0.812814
1 -2.038720 0.534601 -2.506351	1 2.062031 1.003861 2.353129	6 -1.001277 2.840368 -0.975054
8 0.172730 -2.122567 -1.698624	8 -0.334745 -1.771440 2.086515	8 -2.753579 -0.218377 0.266251
7 -0.999863 -0.711298 1.167290	7 1.066063 -1.033859 -0.957675	6 -3.562588 -0.762961 -0.754078
6 -0.948410 0.271405 2.249321	6 0.864495 -0.283916 -2.196976	8 -1.181795 -1.852028 1.838900

1 -0.682953 -0.241853 3.170167	1 0.471976 -0.961813 -2.950914	1 0.851125 -0.730675 1.264573
1 -0.192626 1.020199 1.987398	1 0.155953 0.530747 -1.992963	1 2.555490 1.489086 -0.017301
1 -1.920033 0.749498 2.370730	1 1.814731 0.125370 -2.544399	1 2.396738 2.002102 2.547748
6 -0.320131 -1.981471 1.415771	6 0.531115 -2.389680 -0.917501	1 1.106305 2.798010 1.664723
1 -0.782919 -2.466244 2.277198	1 1.018867 -2.994448 -1.683936	1 0.784245 1.289214 2.525725
1 -0.378306 -2.604722 0.526512	1 0.687293 -2.815694 0.070372	1 3.150307 -1.505930 -2.073873
1 0.729624 -1.760243 1.608392	1 -0.542560 -2.333278 -1.101460	1 2.264991 0.031496 -2.165710
1 0.483742 -2.315219 -2.581831	1 -0.665994 -1.665456 2.977508	1 3.653787 -0.139227 -1.069789
1 0.848510 -1.456264 -1.268386	1 -0.959341 -1.268835 1.499065	1 1.701223 -3.116944 -1.074702
8 1.625974 -0.501132 -0.472305	8 -1.768436 -0.451361 0.305886	1 0.520948 -2.560218 0.131691
6 2.954196 -0.851733 -0.288602	6 -3.160222 -0.493991 0.163797	1 0.378160 -2.032161 -1.553440
1 3.606422 -0.529823 -1.120510	1 -3.673563 0.194539 0.850143	1 -1.599768 -1.993556 2.687920
1 3.382305 -0.408692 0.628217	1 -3.473284 -0.238121 -0.857721	1 -1.804870 -1.299208 1.328613
1 3.087333 -1.944523 -0.196895	1 -3.521986 -1.505521 0.377827	1 -4.169054 0.008248 -1.241637
1 -1.126492 1.554085 -0.372334	1 0.835530 1.423411 0.105499	1 -2.969469 -1.278818 -1.517473
1 1.262403 0.844081 -0.059102	1 -1.373130 0.511337 -0.000614	1 -4.236871 -1.486732 -0.294952
8 0.899585 1.762214 0.278457	8 -0.735839 1.633866 -0.433018	1 -0.007721 1.247474 -0.384037
6 1.777399 2.786446 -0.095356	6 -1.423790 2.827638 -0.275622	1 -2.122445 0.414257 -0.128727
1 1.982409 2.782911 -1.174897	1 -1.820135 2.965691 0.746189	1 -1.073857 3.357910 -0.012692
1 1.331419 3.754082 0.156410	1 -0.779794 3.698461 -0.481892	1 -0.166804 3.261305 -1.544488
1 2.742844 2.720470 0.426119	1 -2.285131 2.911303 -0.960776	1 -1.920670 3.017027 -1.533482
Carbinolamine Et = -598.6995998 NIImag = 0		<b>TS-IIh</b>
Et = -598.6229451 NIImag=1 (-490.14)		Enamine + amine + amine Et = -598.677986 NIImag =1(-10.42)
6 -1.841595 -0.128515 0.408607	6 2.519035 -0.474832 0.325457	6 -3.046990 -0.106285 0.148554
6 -2.398215 -1.497316 0.775056	6 2.891690 0.345418 -0.803928	6 -2.778785 -0.795526 -0.978882
1 -1.896542 0.516224 1.296812	1 2.949837 -0.203529 1.282044	1 -3.683441 -0.566525 0.902619
1 -3.484388 -1.410561 0.864792	1 2.573615 -0.033919 -1.773091	1 -2.136483 -0.360015 -1.737916
6 -1.798498 -2.044115 2.062649	6 4.329980 0.841562 -0.793193	6 -3.436563 -2.101557 -1.307499
1 -2.025232 -1.394452 2.913264	1 5.054791 0.047566 -0.993327	1 -4.138510 -2.003626 -2.143221
1 -2.194955 -3.036127 2.290808	1 4.462091 1.613046 -1.553252	1 -2.709596 -2.865681 -1.602335
1 -0.713035 -2.123943 1.980584	1 4.575545 1.293460 0.171144	1 -4.002539 -2.487745 -0.455310

8	-0.477881	-0.297875	0.050579	8	1.247523	1.658744	0.773590	8	-0.454222	-2.150008	0.784137
7	-2.640546	0.537015	-0.600618	7	1.661568	-1.451814	0.370401	7	-2.655384	1.164326	0.477716
6	-2.712169	-0.154000	-1.874518	6	0.922832	-1.965225	-0.774984	6	-1.803300	1.899798	-0.430121
1	-1.735152	-0.238765	-2.374475	1	-0.143008	-1.720472	-0.663495	1	-0.764806	1.538352	-0.452373
1	-3.121036	-1.156301	-1.745159	1	1.309580	-1.542772	-1.696538	1	-2.217772	1.848442	-1.439193
1	-3.388055	0.392940	-2.535877	1	1.038891	-3.051332	-0.802878	1	-1.789616	2.948028	-0.125285
6	-2.266103	1.924499	-0.779031	6	1.194436	-1.950821	1.654309	6	-2.517630	1.488708	1.879410
1	-3.006907	2.425393	-1.407157	1	1.174400	-3.041629	1.639041	1	-2.646020	2.563952	2.023237
1	-2.250877	2.430475	0.189551	1	1.853461	-1.605579	2.447527	1	-3.290284	0.974263	2.453624
1	-1.278429	2.055165	-1.251127	1	0.186564	-1.572595	1.835281	1	-1.538301	1.200188	2.286908
1	0.052402	0.499552	0.280575	1	1.368011	2.434959	1.325068	1	-0.821284	-3.032692	0.844681
1	-2.190914	-2.192578	-0.043657	1	2.189046	1.216238	-0.442322	1	-1.130280	-1.627366	0.322435
1	1.360336	-1.225725	-0.539731	1	-0.512514	1.674191	0.381755	1	1.525065	-1.657305	0.490857
7	2.367767	-1.135061	-0.640685	7	-1.525737	1.727572	0.154720	7	2.483894	-1.361871	0.328325
6	3.034613	-2.174466	0.120402	6	-2.225934	2.303673	1.284669	6	3.238649	-1.465001	1.561504
1	2.682072	-2.161981	1.153453	1	-2.003797	1.732334	2.188800	1	2.730776	-0.911670	2.353556
1	2.874268	-3.187003	-0.284360	1	-1.952837	3.355670	1.477033	1	3.380252	-2.503114	1.906153
1	4.113080	-1.991324	0.133325	1	-3.309886	2.272400	1.125222	1	4.231438	-1.023927	1.429645
6	2.722857	-1.157544	-2.047191	6	-1.693397	2.524911	-1.043438	6	3.058768	-2.150373	-0.743523
1	2.142131	-0.407832	-2.587730	1	-1.084573	2.112478	-1.851157	1	2.422413	-2.092180	-1.628738
1	3.782138	-0.911573	-2.166917	1	-2.739233	2.514333	-1.371506	1	4.042066	-1.753187	-1.013640
1	2.552177	-2.134473	-2.528046	1	-1.399792	3.579978	-0.909704	1	3.191344	-3.214733	-0.486009
1	2.088107	0.794198	0.260070	1	-2.078142	-0.190721	-0.170786	1	2.079853	0.659334	-0.262121
7	1.518741	1.555251	0.640252	7	-2.307698	-1.178980	-0.348958	7	1.840170	1.612957	-0.540062
6	1.803941	1.721480	2.054890	6	-3.108740	-1.699039	0.739000	6	2.286744	2.544682	0.472507
1	1.111047	2.446257	2.491705	1	-3.233009	-2.782905	0.637247	1	1.912269	3.549701	0.250420
1	1.664090	0.771350	2.573500	1	-2.611307	-1.509282	1.693017	1	1.889710	2.252994	1.447467
1	2.827145	2.076268	2.252672	1	-4.118641	-1.257642	0.795035	1	3.385435	2.616965	0.560320
6	1.746981	2.769107	-0.123577	6	-2.975791	-1.301450	-1.628007	6	2.400471	1.900544	-1.842350
1	1.579268	2.575409	-1.184399	1	-2.371758	-0.835071	-2.409622	1	2.086646	1.138135	-2.558671
1	1.043113	3.545162	0.189949	1	-3.103906	-2.357375	-1.890715	1	2.032415	2.865996	-2.205465

1	2.764583	3.172027	-0.003418	1	-3.975217	-0.834410	-1.650995	1	3.504076	1.945650	-1.854194
Carbinolamine Et = -559.8175047 NIImag = 0				TS-IIi Et = -559.7563776 NIImag=1(-76.14 )				Enamine + amine + amine Et = -559.8073767 NIImag = 0			
6	-1.748021	0.295140	-0.346219	6	1.716375	0.104061	-0.583495	6	2.138311	-0.033204	0.016465
6	-1.024426	1.626722	-0.485351	6	0.674678	0.849213	-1.310329	6	1.869561	1.014549	-0.797577
1	-2.729000	0.369805	-0.832409	1	2.682089	0.568484	-0.427593	1	2.688507	0.153248	0.936804
6	-0.965329	2.116455	-1.927077	6	1.190858	2.146453	-1.913739	6	2.461889	2.376646	-0.581492
1	-1.963090	2.195628	-2.370761	1	1.961350	1.976517	-2.670189	1	3.238658	2.603102	-1.320660
1	-0.502904	3.103498	-1.978712	1	0.372798	2.688703	-2.387858	1	1.715729	3.173662	-0.663420
1	-0.361546	1.456467	-2.556929	1	1.608783	2.791569	-1.137548	1	2.924237	2.456913	0.406079
8	-1.019544	-0.759404	-1.059550	8	1.321492	1.018810	1.616062	8	-1.510800	-1.411458	1.844695
7	-1.989968	-0.096172	0.996547	7	1.616804	-1.114010	-0.162640	7	1.833763	-1.346987	-0.171825
6	-0.833057	-0.237167	1.865634	6	0.358034	-1.852623	-0.159888	6	1.073912	-1.738255	-1.335116
1	-0.239208	-1.136515	1.649266	1	-0.198981	-1.570059	0.740838	1	0.024513	-1.418353	-1.286343
1	-0.178330	0.629118	1.787619	1	-0.267217	-1.573646	-1.005041	1	1.528366	-1.314364	-2.233914
1	-1.180682	-0.302929	2.899331	1	0.583018	-2.917806	-0.180102	1	1.095301	-2.825041	-1.422929
6	-2.901961	-1.216180	1.123740	6	2.670530	-1.677468	0.669657	6	1.757074	-2.227150	0.979456
1	-3.223178	-1.302279	2.164339	1	2.850441	-2.712300	0.377922	1	2.048430	-3.238511	0.685343
1	-3.789308	-1.042263	0.510769	1	3.583374	-1.098298	0.553544	1	2.457444	-1.883879	1.742695
1	-2.455332	-2.174184	0.820592	1	2.353811	-1.631515	1.712355	1	0.749927	-2.256191	1.412038
1	-1.127861	-0.615900	-2.002092	1	1.330409	1.940854	1.874026	1	-2.020913	-1.519693	1.032700
1	0.678594	-1.219596	-0.638312	1	0.312555	0.784971	1.475549	1	-1.227854	-0.492849	1.780226
8	1.610771	-1.403634	-0.421494	8	-1.065554	0.470363	1.113142	8	-0.860936	1.253134	0.642915
6	2.179740	-2.198966	-1.437909	6	-1.926490	1.120906	1.985403	6	-1.050677	2.566883	1.138358
1	1.655356	-3.155062	-1.543002	1	-2.371613	0.444226	2.735933	1	-2.032558	2.600822	1.610199
1	2.183497	-1.688671	-2.408685	1	-1.422001	1.920373	2.559609	1	-0.297457	2.823878	1.888960
1	3.213097	-2.406636	-1.158843	1	-2.769267	1.605671	1.463692	1	-1.022599	3.310087	0.335093
1	-1.565905	2.350206	0.130722	1	0.198813	0.210183	-2.059761	1	1.336244	0.849861	-1.729154
1	-0.009610	1.552139	-0.087810	1	-0.121935	1.040815	-0.566662	1	0.038726	1.165318	0.270032
8	2.372881	1.111601	0.471851	8	-2.239363	-0.397085	-1.064039	8	-2.495303	-0.547520	-0.756316
1	2.224922	0.203092	0.159832	1	-1.861453	-0.059106	-0.201488	1	-2.039294	0.225586	-0.388718

6	3.389403	1.100355	1.442501	6	-3.478724	-0.996463	-0.814303	6	-3.731507	-0.151208	-1.306087
1	4.353948	0.772653	1.032792	1	-4.223140	-0.284288	-0.430520	1	-3.605325	0.568215	-2.123829
1	3.511474	2.120576	1.810320	1	-3.866210	-1.400744	-1.753718	1	-4.213421	-1.041979	-1.709770
1	3.143886	0.457413	2.297768	1	-3.417421	-1.827706	-0.095668	1	-4.398051	0.286250	-0.553056

**Table S56.** The MP2(full)/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Transition States for Carbinolamine Formation (**Step-I**)

TS-I				TS-Ia				TS-Ib			
Et = -327.1671155	NImag=1	(-1535.61)		Et = -461.8653952	NImag=1	(-1529.85)		Et = -442.5482354	Nmag = 1	(-1535.63)	
6	-0.311110	0.721665	-0.478092	6	1.079650	0.266468	0.882826	6	0.678960	0.264523	0.857976
6	-1.575369	0.270482	0.232335	6	0.822659	1.554633	0.122626	6	0.641007	1.557881	0.067859
1	-0.385893	0.434126	-1.552479	1	2.005133	0.385177	1.484283	1	1.531798	0.296996	1.563712
1	-1.460256	0.425270	1.308882	1	0.008121	1.400467	-0.589948	1	-0.124695	1.496725	-0.709383
6	-2.003725	-1.157288	-0.089540	6	2.062145	2.134978	-0.551003	6	1.995850	1.969828	-0.499427
1	-1.281648	-1.893285	0.276785	1	2.449351	1.475945	-1.333448	1	2.360819	1.259631	-1.247024
1	-2.969168	-1.392193	0.366424	1	1.840251	3.099097	-1.015959	1	1.933820	2.948461	-0.982031
1	-2.103649	-1.299007	-1.170070	1	2.863195	2.293539	0.177657	1	2.748008	2.036719	0.292851
8	0.117425	1.978208	-0.226368	8	0.021029	-0.263486	1.575836	8	-0.504568	-0.138350	1.446383
7	1.021776	-0.001046	-0.022119	7	1.354738	-0.998276	0.008329	7	0.902297	-1.039885	0.045559
6	1.079548	-0.334614	1.406637	6	0.747126	-1.012156	-1.334109	6	0.386518	-1.032763	-1.335612
1	0.716717	0.533034	1.957675	1	-0.291864	-0.683089	-1.255027	1	-0.624327	-0.622092	-1.325513
1	0.474731	-1.215116	1.637552	1	1.301992	-0.367432	-2.020919	1	1.033202	-0.446805	-1.993570
1	2.118389	-0.528623	1.683476	1	0.777246	-2.038070	-1.708987	1	0.357512	-2.065149	-1.691310
6	1.589444	-1.030674	-0.897070	6	2.724369	-1.523247	0.032591	6	2.214067	-1.683459	0.176471
1	1.020844	-1.961649	-0.819414	1	3.393837	-0.885047	-0.551496	1	2.976107	-1.125809	-0.375575
1	1.558409	-0.672836	-1.927360	1	3.070698	-1.563738	1.066561	1	2.486610	-1.724496	1.232209
1	2.627081	-1.218903	-0.611822	1	2.730676	-2.530510	-0.389233	1	2.155219	-2.699145	-0.219857

1 1.268118 1.177008 -0.139047	1 0.537244 -1.322365 0.860734	1 -0.021081 -1.261381 0.832177			
1 -2.348234 0.976401 -0.090442	1 0.443989 2.256916 0.873706	1 -1.807389 0.303655 0.371563			
	1 -1.619026 -0.027730 0.533160	8 -2.412566 0.443662 -0.405235			
	7 -2.314104 -0.038601 -0.223623	6 -3.638504 -0.202135 -0.107880			
	6 -3.127536 -1.238135 -0.090978	1 -4.142439 0.247126 0.757364			
	1 -3.778517 -1.343247 -0.965486	1 -4.288479 -0.091436 -0.978314			
	1 -2.475216 -2.114441 -0.044883	1 -3.509352 -1.274716 0.091750			
	1 -3.768709 -1.241108 0.806566	1 0.288270 2.315164 0.776534			
	6 -3.127524 1.165823 -0.156710				
	1 -2.478309 2.045047 -0.170073				
	1 -3.784703 1.216203 -1.031392				
	1 -3.763394 1.220230 0.743106				
<b>TS-Ic</b>		<b>TS-Id</b>		<b>TS-Ie</b>	
Et =-461.884261 NImag=1(-1173.07)		Et =-442.5711418 NImag=1 (-985.43)		Et =-596.5623004 NImag=1 (-1533.26)	
6 0.796431 -0.753677 -0.220822	6 0.388108 -0.725215 -0.128432	6 -0.196489 0.771236 -0.397460			
6 2.258502 -1.016622 0.152011	6 1.846666 -1.083619 0.109911	6 0.854461 1.581825 -1.130231			
1 0.721468 -0.721384 -1.339560	1 0.156104 -0.789129 -1.212979	1 -1.200001 1.139162 -0.675032			
1 2.337900 -0.980371 1.243324	1 2.058452 -0.960708 1.176425	1 1.846866 1.336573 -0.743733			
6 3.334550 -0.159613 -0.507882	6 2.897538 -0.387619 -0.749532	6 0.591946 3.084759 -1.108458			
1 3.387528 0.844449 -0.080480	1 3.081081 0.642224 -0.434270	1 0.625550 3.492107 -0.094270			
1 4.321344 -0.614095 -0.378452	1 3.852327 -0.915479 -0.680085	1 1.337496 3.620063 -1.702272			
1 3.158535 -0.059673 -1.583949	1 2.606335 -0.373926 -1.804473	1 -0.393592 3.312813 -1.525814			
8 -0.022232 -1.607597 0.394851	8 -0.417531 -1.455244 0.670478	8 -0.074356 -0.613476 -0.501483			
7 0.326857 0.719634 0.125364	7 0.052369 0.789269 0.153194	7 -0.162770 0.819635 1.144978			
6 0.539946 1.020463 1.541164	6 0.433177 1.190761 1.519223	6 1.106762 1.208255 1.781706			
1 0.279688 0.117236 2.096408	1 0.148545 0.372459 2.179995	1 1.921364 0.639371 1.327793			
1 1.581491 1.295252 1.745014	1 1.507654 1.377306 1.574925	1 1.285650 2.282358 1.682789			
1 -0.105794 1.848960 1.851093	1 -0.112536 2.096383 1.791036	1 1.037685 0.958827 2.843031			
6 0.752036 1.802611 -0.761148	6 0.431758 1.771974 -0.875701	6 -1.351826 1.419479 1.770380			
1 1.773646 2.135561 -0.559768	1 1.494095 2.005516 -0.823415	1 -1.347127 2.506344 1.639869			
1 0.692284 1.457909 -1.796992	1 0.194531 1.362530 -1.859131	1 -2.235277 0.978691 1.302878			

1 0.080435 2.659625 -0.637133	1 -0.147108 2.685114 -0.718867	1 -1.341176 1.188834 2.838040
1 -0.978145 0.484390 -0.036918	1 -1.055722 0.681548 0.155288	1 -0.185566 -0.383035 0.819360
1 -1.404712 -1.074596 0.011952	1 -1.512125 -0.935806 0.545814	1 0.827400 1.216076 -2.162829
7 -2.048594 -0.194808 -0.146096	8 -2.336841 -0.048967 0.349019	1 1.866033 -1.051190 -0.381563
6 -2.676815 -0.151712 -1.463848	6 -3.089282 -0.327579 -0.813665	7 2.839292 -1.089336 -0.059143
1 -3.439814 -0.931623 -1.564691	1 -3.804847 -1.139848 -0.633227	6 2.996686 -2.246924 0.809473
1 -3.148652 0.821719 -1.631396	1 -3.661204 0.558831 -1.113787	1 3.988405 -2.228189 1.273352
1 -1.912046 -0.311349 -2.227179	1 -2.462736 -0.627928 -1.670443	1 2.248278 -2.206897 1.605651
1 2.407325 -2.067231 -0.117908	1 1.877759 -2.162503 -0.071960	1 2.889458 -3.211658 0.285693
6 -2.983060 -0.031594 0.964898		6 3.730126 -1.159925 -1.207842
1 -2.436577 -0.174131 1.898890		1 3.524714 -0.322728 -1.879745
1 -3.426113 0.969233 0.953355		1 4.769277 -1.078612 -0.872407
1 -3.789317 -0.772024 0.914472		1 3.636268 -2.096239 -1.783348
		1 -2.035141 -0.956893 -0.497717
		7 -3.017441 -0.830247 -0.230075
		6 -3.824607 -0.644267 -1.426939
		1 -3.863938 -1.533742 -2.077967
		1 -4.852055 -0.395633 -1.141528
		1 -3.424129 0.189143 -2.010093
		6 -3.448073 -1.995821 0.528705
		1 -3.486398 -2.923392 -0.066926
		1 -2.763618 -2.155928 1.365996
		1 -4.449067 -1.820491 0.936333
TS-If Et=-557.9252496 NImag=1(-1541.11)	Ts-Ig Et=-596.5893588 NImag=1 (-630.66)	TS-Ih Et=-557.9523427 NImag=1 (-696.20)
6 0.242719 0.236080 0.387730	6 -1.029333 -0.679305 0.270782	6 0.897183 -0.333510 -0.637172
6 -0.807256 0.528206 1.438146	6 -2.246844 -1.605232 0.489945	6 2.354265 -0.517982 -1.041370
1 1.246080 0.365743 0.819692	1 -0.431112 -0.724623 1.224004	1 0.319679 0.000949 -1.518595
1 -1.799786 0.518698 0.983502	1 -1.821845 -2.539739 0.876789	1 2.308270 -1.244765 -1.859244
6 -0.540319 1.812422 2.217406	6 -3.017930 -1.927562 -0.784117	6 3.267439 -1.067809 0.048394
1 -0.574545 2.697263 1.576326	1 -2.296918 -2.147024 -1.573020	1 2.779293 -1.905062 0.549260

1	-1.284801	1.949212	3.005763	1	-3.668914	-2.795114	-0.638126	1	4.204055	-1.423723	-0.388832
1	0.445602	1.781917	2.691067	1	-3.647073	-1.098186	-1.114237	1	3.526530	-0.314657	0.795946
8	0.112061	-1.005062	-0.269209	8	-0.342959	-0.929493	-0.836728	8	0.391218	-1.452023	-0.065665
7	0.222847	1.081135	-0.890483	7	-1.403937	0.838939	0.303359	7	0.667616	0.872435	0.330129
6	-1.029164	1.779978	-1.226193	6	-2.184149	1.250539	-0.863069	6	0.982156	0.591104	1.747882
1	-1.859684	1.077035	-1.154525	1	-1.806775	0.679844	-1.712626	1	0.710324	-0.445554	1.937411
1	-1.194079	2.638918	-0.570509	1	-3.254144	1.052932	-0.727301	1	2.041415	0.752165	1.945162
1	-0.946542	2.130959	-2.256670	1	-2.055486	2.324591	-1.042392	1	0.380579	1.259792	2.366245
6	1.435084	1.885314	-1.110455	6	-1.993003	1.306617	1.553264	6	1.244317	2.144806	-0.138357
1	1.462728	2.739423	-0.426350	1	-3.030849	0.971131	1.672933	1	2.327887	2.140741	-0.012443
1	2.301094	1.240692	-0.952481	1	-1.403497	0.922740	2.391468	1	0.994454	2.281098	-1.192324
1	1.431386	2.250183	-2.139349	1	-1.981943	2.401925	1.585932	1	0.810755	2.961783	0.442029
1	0.217829	-0.133669	-1.252993	1	-0.082768	1.281312	0.136368	1	-0.424158	0.997533	0.300382
1	-1.644537	-1.245590	-0.585601	1	1.276469	-1.272792	-0.209739	1	-0.716725	-1.448795	-0.251455
8	-2.602803	-1.101015	-0.779250	7	2.228185	-1.087810	0.179354	8	-2.016486	-1.236076	-0.429751
6	-3.343211	-2.016047	0.012640	6	3.217904	-1.429796	-0.835803	6	-2.747901	-2.100689	0.416173
1	-3.170981	-1.871860	1.087632	1	2.955791	-0.937484	-1.775327	1	-2.232131	-2.290142	1.370686
1	-4.400950	-1.841714	-0.192057	1	4.210761	-1.084708	-0.526530	1	-3.731176	-1.672619	0.648855
1	-3.110293	-3.058469	-0.237337	1	3.281421	-2.512954	-1.024213	1	-2.909860	-3.069180	-0.072532
1	-0.775287	-0.329161	2.119982	1	-2.909880	-1.225287	1.278813	1	2.760931	0.402886	-1.474526
1	1.878256	-1.333526	-0.462960	1	1.600355	0.636485	0.158581	1	-2.076991	-0.013637	0.011483
8	2.845552	-1.137802	-0.506114	7	1.087063	1.525258	-0.079788	8	-1.928598	1.070501	0.322439
6	3.453814	-1.782567	0.601733	6	1.593525	2.646058	0.720294	6	-2.532474	1.876068	-0.677019
1	3.336687	-2.872425	0.560225	1	1.020898	3.548092	0.491315	1	-2.235093	2.920690	-0.534683
1	4.519607	-1.550188	0.567960	1	1.478329	2.409161	1.779611	1	-2.244895	1.567019	-1.691897
1	3.053811	-1.430677	1.562620	1	2.650469	2.832378	0.508002	1	-3.625430	1.825293	-0.609201
				6	2.442313	-1.845869	1.405756				
				1	1.653635	-1.609335	2.123562				
				1	2.445332	-2.935032	1.242201				
				1	3.406482	-1.572803	1.848999				
				6	1.223606	1.720075	-1.533268				

	1 0.793427 0.832475 -1.997574 1 0.670497 2.612695 -1.835860 1 2.275298 1.837405 -1.810995	
<b>TS-Ii</b> Et =-596.559578 NIImag=1(-1512.58)	<b>Ts-Ij</b> Et =-557.9241477 NIImag=1 (-1533.24)	<b>TS-Ik</b> Et=-557.9505096 NIImag=1 (-739.17)
6 1.734337 -0.956688 0.309857 6 1.163742 -0.187117 1.487200 1 2.650815 -1.488156 0.637469 1 0.371541 0.479363 1.136432 6 2.209310 0.554439 2.314339 1 2.709870 1.337239 1.738325 1 1.751089 1.032090 3.184486 1 2.977655 -0.134501 2.679307 8 0.849099 -1.741120 -0.392430 7 2.182767 -0.091826 -0.913282 6 1.722681 1.304042 -1.008895 1 0.665142 1.374077 -0.741308 1 2.314164 1.952826 -0.357083 1 1.859390 1.629083 -2.043471 6 3.593428 -0.256215 -1.284129 1 4.243700 0.258676 -0.570653 1 3.831163 -1.321216 -1.294901 1 3.754085 0.159590 -2.281122 1 1.397243 -0.927704 -1.340862 1 0.677776 -0.948602 2.108142 1 -1.010953 -1.507234 -0.123732 7 -2.023701 -1.334515 -0.049554 6 -2.669808 -1.876927 -1.237134 1 -3.731038 -1.606286 -1.239534 1 -2.205105 -1.446805 -2.128062 1 -2.601101 -2.974813 -1.308886	6 1.320002 -0.889224 -0.023857 6 0.674602 -0.613357 1.319745 1 2.219461 -1.514462 0.130067 1 -0.130994 0.117085 1.215074 6 1.670999 -0.195256 2.397137 1 2.151239 0.758651 2.162322 1 1.170881 -0.079176 3.361844 1 2.458165 -0.946363 2.516910 8 0.493278 -1.372778 -1.027869 7 1.818590 0.341356 -0.821766 6 1.193309 1.640832 -0.518562 1 0.113688 1.523564 -0.417509 1 1.602245 2.064673 0.402310 1 1.411504 2.317508 -1.347892 6 3.272106 0.431866 -1.003229 1 3.761321 0.725948 -0.069899 1 3.651275 -0.539560 -1.324424 1 3.489984 1.175532 -1.772329 1 1.137465 -0.336753 -1.603682 1 -1.157530 -1.188745 -0.912030 8 -2.143588 -1.048428 -0.798796 6 -2.641289 -2.157258 -0.063148 1 -2.206845 -2.218358 0.942709 1 -3.721145 -2.031604 0.033583 1 -2.443854 -3.099799 -0.585333 1 0.200757 -1.558654 1.607895	6 1.434085 0.657932 -0.126217 6 2.825255 0.195422 -0.527344 1 1.462631 1.123706 0.881897 1 2.749750 -0.315450 -1.492114 6 3.611507 -0.634171 0.482860 1 3.256946 -1.665579 0.543525 1 4.665909 -0.676751 0.197615 1 3.559877 -0.197410 1.485027 8 0.871676 1.406148 -1.089756 7 0.434219 -0.543916 0.145937 6 0.303487 -1.437396 -1.023746 1 0.292814 -0.799072 -1.906812 1 1.147947 -2.127354 -1.054145 1 -0.637623 -1.977739 -0.929568 6 0.529365 -1.273908 1.427698 1 1.317280 -2.022740 1.382134 1 0.744321 -0.558900 2.223534 1 -0.437262 -1.746527 1.608083 1 -0.450559 0.021205 0.190268 1 -0.300400 1.590939 -0.723477 8 -1.362216 1.453794 -0.187499 6 -1.539100 2.455005 0.797441 1 -2.066050 3.327228 0.389155 1 -2.133137 2.064291 1.632748 1 -0.577377 2.806918 1.198226 1 3.356885 1.130253 -0.731122

6 -2.521654 -1.967459 1.163524	1 -2.136218 0.505318 -0.010129	1 -2.372931 0.041995 0.046841	
1 -1.959458 -1.594506 2.023665	8 -1.968308 1.389819 0.402531	8 -2.604646 -0.887308 0.301370	
1 -3.576379 -1.711247 1.309413	6 -3.048324 2.238736 0.047222	6 -3.766770 -1.267820 -0.420223	
1 -2.440810 -3.066879 1.147990	1 -3.154821 2.342086 -1.040042	1 -3.987741 -2.304841 -0.160763	
1 -1.801778 0.677894 -0.068907	1 -4.003254 1.882563 0.454285	1 -4.635016 -0.653593 -0.152150	
7 -1.547611 1.675342 -0.117846	1 -2.842939 3.224124 0.469850	1 -3.621275 -1.204619 -1.506184	
6 -2.132482 2.244604 -1.323607			
1 -3.235554 2.263829 -1.313934			
1 -1.784665 3.275145 -1.454153			
1 -1.809322 1.664307 -2.192213			
6 -2.040232 2.344951 1.077220			
1 -1.646417 1.841372 1.964143			
1 -1.689071 3.382372 1.092268			
1 -3.140891 2.364271 1.151150			
<b>TS-II</b>		<b>Ts-Im</b>	
Et = -596.5791395 NImag=1(-1100.26)		Et = -557.9489014 NImag=1(-957.65)	

6	-0.161103	0.716110	-0.226333					
6	0.560550	2.028830	0.085866					
1	-0.189149	0.589686	-1.337783					
1	0.552143	2.164324	1.172710					
6	0.089067	3.292086	-0.628548	6	0.822490	0.032509	-0.766056	
1	-0.843260	3.685862	-0.216022	6	1.679108	-1.217816	-0.870546	
1	0.838866	4.083163	-0.536072	1	1.296002	0.860797	-1.326597	
1	-0.063499	3.111057	-1.697608	1	1.207415	-2.010454	-0.281582	
8	0.382868	-0.312271	0.454297	6	3.157650	-1.073925	-0.524011	
7	-1.691408	0.741495	0.102212	1	3.327722	-0.975805	0.550793	
6	-1.928116	1.115518	1.498060	1	3.708246	-1.958526	-0.853931	
1	-1.168719	0.607784	2.095046	1	3.601621	-0.205660	-1.020899	
1	-1.852749	2.198972	1.644925	8	-0.451425	-0.235434	-1.199387	
1	-2.926926	0.789862	1.806563	7	0.722700	0.618339	0.665241	
6	-2.573148	1.444265	-0.831911	6	0.443253	-0.395301	1.706005	
1	-2.555011	2.528129	-0.693980	1	-0.332790	-1.070770	1.342886	
1	-2.263734	1.214378	-1.854774	1	1.352079	-0.952149	1.943622	
1	-3.601623	1.095185	-0.688465	1	0.092383	0.124024	2.600223	
1	-1.889793	-0.587582	-0.001227	6	1.806972	1.541281	1.049748	
1	-0.571957	-1.515048	0.091864	1	2.738133	1.004204	1.226875	
7	-1.604968	-1.816171	-0.055174	1	1.950825	2.273626	0.253815	
6	-1.851821	-2.450703	-1.349178	1	1.509417	2.060080	1.963381	
1	-1.378402	-3.436850	-1.401766	1	-0.231218	1.224044	0.537082	
1	-2.926870	-2.568125	-1.514376	1	-1.112332	0.661977	-0.806782	
1	-1.436910	-1.820071	-2.138272	8	-1.494958	1.578832	-0.030773	
1	1.602255	1.822358	-0.180924	6	-1.566474	2.831401	-0.683762	
6	-2.082366	-2.588546	1.091502	1	-2.438717	2.874296	-1.347111	
1	-1.769345	-2.078289	2.003879	1	-1.666498	3.637592	0.052779	
1	-3.173471	-2.664755	1.073241	1	-0.675245	3.044591	-1.297309	
1	-1.658534	-3.598465	1.089347	1	1.574737	-1.522431	-1.916713	
1	2.270378	-0.294587	0.124327	1	-1.280547	-1.693145	-0.500596	
7	3.264229	-0.217655	-0.125518	8	-1.746427	-2.273921	0.144841	
6	4.064364	-0.319105	1.081528	6	-3.018644	-1.668205	0.359384	
1	4.026689	-1.313498	1.562449	1	-3.460201	-2.140773	1.238926	
1	5.114507	-0.104821	0.852464	1	-2.931501	-0.589997	0.534602	
1	3.717542	0.422161	1.806114	1	-3.692078	-1.829382	-0.492179	
6	3.591947	-1.265979	-1.073960					
1	3.536677	-2.286655	-0.652570					

**Table S57.** The MP2(full)/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Transition States for Dehydration step (**Step-II**)

TS-II Et = -327.1273192 NIImag=1(-1072.23)			TS-IIa Et = -461.830923 NIImag=1 (-618.18)				TS-IIb Et = -442.5211865 NIImag=1(-456.07)			
6 0.234933 -0.118506 0.550479	6 1.868441 0.335319 -0.120473		6 1.287999 0.426185 -0.375645				6 1.908470 -0.523540 0.520416			
6 1.372134 -0.377735 -0.286154	6 1.840227 -1.042108 0.302586		6 1.476389 0.296272 -1.438492				1 1.472719 -1.204774 1.315828	1 1.902027 -0.229656 1.570481		
1 0.384982 0.462615 1.456323	1 2.391353 0.560196 -1.046358		6 3.258835 -1.043517 0.049136				6 3.064289 -1.870697 -0.047532	1 4.046174 -0.284579 0.090055		
1 1.260965 -1.219182 -0.969499	1 3.929487 -1.629710 0.577605		1 3.570955 -1.883674 0.673593				1 2.846528 -2.933779 0.079092	1 3.184928 -1.411708 -0.978201		
6 2.724765 -0.315556 0.401708	1 3.345830 -1.717704 -1.093781		8 -0.186430 -1.713058 -0.537648				8 0.002201 -0.419091 -1.468181	7 0.390385 1.321812 -0.085851		
1 2.909344 -1.172026 1.058178	7 1.177484 1.325378 0.374444		7 0.390385 1.321812 -0.085851				7 0.328789 1.177004 1.559577	6 -0.100045 1.563975 1.273798		
1 3.525670 -0.286994 -0.341344	6 -0.635891 0.736159 1.268406		6 -0.100045 1.563975 1.273798				1 -0.635891 0.736159 1.268406	1 -0.986601 0.935510 1.402265		
1 2.804379 0.597288 0.999798	1 0.834577 0.547760 2.290367		1 -0.986601 0.935510 1.402265				1 0.834577 0.547760 2.290367	1 0.674203 1.326299 1.998916		
8 0.070452 1.686035 -0.767559	1 0.183317 2.169002 1.989652		1 0.674203 1.326299 1.998916				1 0.183317 2.169002 1.989652	1 -0.361409 2.620214 1.352930		
7 -1.008412 -0.526927 0.353408	6 0.781437 2.376549 -0.562841		1 -0.361409 2.620214 1.352930				6 0.781437 2.376549 -0.562841	6 -0.430298 1.924485 -1.141735		
6 -1.362048 -1.110015 -0.938383	1 0.422693 3.245734 -0.012601		6 -0.430298 1.924485 -1.141735				1 0.422693 3.245734 -0.012601	1 -0.486710 3.002337 -0.978429		
1 -1.264964 -0.329602 -1.699018	1 1.636828 2.657424 -1.178796		1 -0.486710 3.002337 -0.978429				1 1.636828 2.657424 -1.178796	1 0.022873 1.717693 -2.110563		
1 -0.704272 -1.947844 -1.165817	1 0.007011 1.920823 -1.194053		1 0.022873 1.717693 -2.110563				1 0.007011 1.920823 -1.194053	1 -1.416262 1.456456 -1.072871		
1 -2.388387 -1.473661 -0.885232	1 -0.263439 -0.762320 -2.338309		1 -1.416262 1.456456 -1.072871				1 -0.263439 -0.762320 -2.338309	1 -0.483274 -2.598314 -0.801707		
6 -2.036249 0.346420 0.908024	1 0.942699 -1.218978 -0.467492		1 -0.483274 -2.598314 -0.801707				1 0.942699 -1.218978 -0.467492	1 1.074156 -1.337430 0.325686		
1 -3.005510 -0.152258 0.877556	1 -1.473132 -0.369990 -0.483534		1 1.074156 -1.337430 0.325686				1 -1.473132 -0.369990 -0.483534	1 -1.341540 -0.919141 -0.201597		
1 -1.788163 0.592256 1.941520	7 -2.264908 -0.301801 0.193085		1 -1.341540 -0.919141 -0.201597				7 -2.264908 -0.301801 0.193085	8 -2.141505 -0.262499 0.068786		
1 -2.013270 1.260489 0.297634	6 -3.368606 0.401714 -0.435772		8 -2.141505 -0.262499 0.068786				6 -3.368606 0.401714 -0.435772	6 -3.282879 -1.063624 0.265175		
1 0.042315 2.657296 -0.839737	1 -3.016214 1.367330 -0.810004		6 -3.282879 -1.063624 0.265175				1 -3.016214 1.367330 -0.810004	1 -3.620744 -1.549726 -0.663314		
1 1.130968 0.664187 -0.877791	1 -3.819841 -0.146524 -1.282160		1 -3.620744 -1.549726 -0.663314				1 -3.819841 -0.146524 -1.282160	1 -3.113139 -1.856781 1.008855		

	1 -4.165094 0.590620 0.293596 6 -2.648591 -1.644483 0.592531 1 -1.766772 -2.175846 0.961556 1 -3.387178 -1.605448 1.401857 1 -3.087036 -2.242062 -0.226594	1 -4.103720 -0.435782 0.627376
<b>TS-IIc</b> Et = -461.8203221 NImag=1(-1402.65)	<b>TS-IId</b> Et = -442.5294246 NIMag=1(-136.36)	<b>TS-IIe</b> Et = -596.5387742 NImag = 1 (-208.0)
6 -1.047421 0.718147 -0.278835 6 -0.023576 1.246167 0.550278 1 -1.111404 1.068675 -1.301787 6 0.564267 2.572834 0.087907 1 -0.104279 3.423869 0.260351 1 1.503782 2.779875 0.609921 1 0.790156 2.537540 -0.982716 8 -0.057661 -0.910528 -1.463219 7 -2.140736 0.064347 0.145995 6 -2.148652 -0.565838 1.453391 1 -1.448993 -1.411722 1.479649 1 -1.872466 0.151394 2.226319 1 -3.157040 -0.927988 1.660235 6 -2.968481 -0.595897 -0.851107 1 -4.012815 -0.569003 -0.529237 1 -2.864205 -0.081006 -1.804583 1 -2.653674 -1.634930 -0.990251 1 1.165626 -0.849651 -0.780438 1 -0.395103 -1.802779 -1.267214 7 1.938471 -0.524828 -0.004966 1 0.985580 0.412887 0.390030 1 -0.230848 1.213153 1.621111 6 3.164285 0.011218 -0.571435 1 3.758215 0.531553 0.190505	6 1.148077 0.601303 0.081771 6 0.320129 1.444704 -0.808246 1 1.563871 1.016288 0.991617 1 0.779163 1.484551 -1.805785 6 0.101180 2.838667 -0.235727 1 1.040934 3.388721 -0.124425 1 -0.548048 3.416520 -0.897295 1 -0.382699 2.750896 0.737867 8 -0.627731 0.432145 1.718602 7 1.453080 -0.628193 -0.187367 6 0.904250 -1.336019 -1.356208 1 1.054060 -0.723982 -2.245549 1 1.451312 -2.272057 -1.464501 1 -0.175480 -1.475894 -1.152878 6 2.051670 -1.469440 0.845362 1 2.858893 -2.062170 0.413452 1 2.432013 -0.844458 1.651766 1 1.266739 -2.124788 1.229694 1 -0.753152 -0.096325 2.522412 1 -1.141337 -0.115608 0.946426 8 -1.611617 -0.776178 -0.217188 6 -2.993618 -0.934476 -0.197524 1 -3.503838 -0.172376 0.422497 1 -3.441193 -0.858820 -1.205604	6 -0.502090 1.455762 0.511140 6 -0.394267 2.290043 -0.669294 1 -1.405527 0.856501 0.618978 1 0.457386 2.971975 -0.673171 6 -1.700427 2.967077 -1.066510 1 -2.002878 3.749835 -0.364392 1 -1.596225 3.422252 -2.054116 1 -2.503440 2.227655 -1.128744 8 -0.219518 -0.227358 -1.592263 7 0.425035 1.171586 1.376081 6 1.766305 1.753728 1.387073 1 2.423961 1.016533 0.916697 1 1.774944 2.696609 0.846423 1 2.051274 1.924736 2.427096 6 0.248060 0.042547 2.295327 1 0.314434 0.400156 3.325643 1 -0.715917 -0.425055 2.092631 1 1.053764 -0.663987 2.086626 1 -1.424464 -0.982331 -0.530249 1 -0.202146 1.390257 -1.387934 1 1.284373 -0.688230 -0.817009 7 2.232089 -0.863054 -0.403457 6 2.390397 -2.292257 -0.180021 1 1.594711 -2.650972 0.479197

1 3.792751 -0.776984 -1.010643	1 -3.316350 -1.916486 0.203470	1 2.353990 -2.888897 -1.108208
1 2.907647 0.722055 -1.360665	1 -0.631788 0.887176 -0.899473	1 3.351991 -2.498254 0.304850
6 2.159707 -1.532404 1.015485		6 3.199869 -0.389880 -1.383859
1 2.721237 -2.396574 0.632405		1 2.982798 0.653479 -1.629778
1 2.713807 -1.119755 1.867773		1 4.217272 -0.445720 -0.978837
1 1.188391 -1.888384 1.373676		1 3.185694 -0.965665 -2.325387
		1 -0.232451 -0.694786 -2.444226
		7 -2.123361 -1.273158 0.192329
		6 -3.456723 -1.097246 -0.363330
		1 -3.565002 -0.072334 -0.729515
		1 -3.676496 -1.780276 -1.201867
		1 -4.216578 -1.266794 0.408247
		6 -1.888408 -2.663648 0.549696
		1 -0.848949 -2.787284 0.865948
		1 -2.537470 -2.957649 1.382920
		1 -2.075545 -3.367272 -0.279735
TS-IIf Et =-557.9146889 NIImag=1 (-585.87)		TS-IIg Et =-557.9209705 NIImag=1 (-276.5)
TS-IIIg Et =-557.913067 NIImag=1(-438.80)		
6 1.536540 -0.234590 0.489469	6 -1.628030 -0.373089 -0.232614	6 1.430218 -0.640989 0.133377
6 2.149740 -0.126151 -0.798596	6 -1.859827 0.993353 0.312270	6 1.956406 0.694526 0.114539
1 1.523137 0.656175 1.113033	1 -2.122277 -0.662784 -1.153005	1 1.317546 -1.167108 1.079721
1 2.345092 -1.071032 -1.308295	1 -2.510495 0.900628 1.193151	1 2.474711 0.941924 -0.817079
6 3.292969 0.871701 -0.894239	6 -2.488067 1.922018 -0.717826	6 2.733161 1.098130 1.357312
1 4.211475 0.511626 -0.420488	1 -3.452597 1.542093 -1.069452	1 3.713678 0.615465 1.421128
1 3.518816 1.082065 -1.942504	1 -2.659843 2.907253 -0.278137	1 2.893677 2.179022 1.364416
1 3.012242 1.818467 -0.423635	1 -1.812469 2.027695 -1.566206	1 2.171239 0.845197 2.260989
8 -0.217944 0.865458 -1.534036	8 -0.036884 0.321074 -1.629600	8 -0.567168 -1.615320 2.234974
7 0.776871 -1.205351 0.923949	7 -1.112084 -1.346289 0.458317	7 0.870426 -1.228621 -0.890568
6 0.565157 -2.454101 0.192139	6 -0.474426 -1.184604 1.769357	6 0.776120 -0.553707 -2.190119
1 -0.333268 -2.336535 -0.418985	1 -0.977287 -1.852558 2.473358	1 0.245698 -1.211540 -2.876801
1 1.435679 -2.680434 -0.419787	1 0.575873 -1.447635 1.644536	1 0.231522 0.387158 -2.043463

1	0.420217	-3.251449	0.923195	1	-0.534544	-0.153456	2.102189	1	1.778602	-0.358330	-2.578282
6	-0.126781	-0.995382	2.058292	6	-0.851110	-2.639153	-0.174764	6	0.150060	-2.494353	-0.743196
1	0.056667	-1.761554	2.815142	1	-1.091941	-3.437428	0.529518	1	0.555618	-3.220666	-1.450945
1	0.036971	0.001270	2.462307	1	-1.466877	-2.738979	-1.068930	1	0.254981	-2.850024	0.279977
1	-1.145447	-1.065474	1.671032	1	0.212326	-2.639764	-0.427307	1	-0.904289	-2.299600	-0.940721
1	-0.405545	1.329964	-2.365533	1	-0.040075	-0.109720	-2.501556	1	-0.780263	-1.188949	3.078260
1	-1.314128	-0.164097	-0.994699	1	0.757804	-0.197369	-1.057943	1	-1.103784	-1.123651	1.561941
8	-1.950444	-0.834672	-0.570116	8	1.619238	-0.854179	-0.248245	8	-1.809713	-0.298510	0.168941
6	-3.169564	-0.753582	-1.284680	6	2.904651	-0.854511	-0.815471	6	-3.193399	0.004194	0.119686
1	-3.039563	-0.975387	-2.352924	1	2.936485	-0.315608	-1.778865	1	-3.485891	0.743581	0.877709
1	-3.858963	-1.490941	-0.866213	1	3.647670	-0.372335	-0.160025	1	-3.481864	0.395350	-0.863903
1	-3.635703	0.237187	-1.197656	1	3.268989	-1.876522	-1.009914	1	-3.756225	-0.914775	0.303834
1	1.144008	0.349096	-1.330082	1	-0.895001	1.380381	0.656690	1	0.909423	1.306877	-0.023894
1	-0.225101	1.760723	-0.147991	1	1.476353	0.482903	0.743977	1	-1.285035	0.567962	-0.095629
8	-0.232058	2.084883	0.805864	8	1.263237	1.320738	1.258035	8	-0.428945	1.701354	-0.548015
6	-1.596792	2.282267	1.137088	6	1.745941	2.399644	0.470270	6	-0.899703	2.983687	-0.239779
1	-2.022359	3.158770	0.628509	1	1.372122	2.348116	-0.558953	1	-1.277146	3.071168	0.795056
1	-2.203537	1.405316	0.882889	1	1.397045	3.329335	0.927208	1	-0.109726	3.744744	-0.352508
1	-1.662848	2.457380	2.214515	1	2.843812	2.426765	0.442597	1	-1.726016	3.287411	-0.903950
<b>TS-IIh</b>											
Et = -596.528754 NImag=1 (-364.52)											

6	-2.192662	-0.890912	-0.127177
6	-2.831846	0.409152	-0.000162
1	-2.418374	-1.479421	-1.012509
1	-2.834040	0.800901	1.018469
6	-4.199082	0.485126	-0.666180
1	-4.952763	-0.131368	-0.166368
1	-4.556436	1.517428	-0.663553
1	-4.130031	0.167101	-1.710628
8	-0.671460	0.647986	-1.489988
7	-1.303436	-1.406956	0.664833
6	-0.765724	-0.693255	1.826836
1	0.011346	-0.006272	1.478892
1	-1.561992	-0.150677	2.333212
1	-0.339021	-1.430447	2.506803
6	-0.565177	-2.619879	0.298810
1	-0.718589	-3.372019	1.076853
1	-0.935723	-2.989925	-0.656386
1	0.494160	-2.344422	0.225302
1	-0.515323	1.048206	-2.362618
1	-2.027634	0.951456	-0.642012
1	0.454940	1.425668	-0.417448
7	1.101780	1.812705	0.317304
6	2.247532	2.429802	-0.336703
1	2.731822	1.702431	-0.992984
1	1.979722	3.311404	-0.944578
1	2.980715	2.755940	0.410379
6	0.372000	2.801699	1.095864
1	-0.544332	2.355893	1.492886
1	0.978809	3.145072	1.942138
1	0.084186	3.692077	0.510621
1	1.982337	-0.163913	0.291487
7	2.254660	-1.092795	-0.044589
6	2.104487	-1.102420	-1.498826
1	2.160470	-2.134185	-1.866290
1	1.127548	-0.668710	-1.738274
1	2.891115	-0.526904	-2.016223
6	3.617045	-1.387331	0.372630
1	3.697340	-1.300714	1.459802

**Table S58.** The PCM-mPW1PW91/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies (in cm<sup>-1</sup>) of Transition States for Carbinolamine Formation (**Step-I**)

TS-I				TS-Ia				TS-Ib			
Et = -328.1850755 NIImag=1(-1553.29)				Et = -463.3252738 NIImag=1 (-1573.29)				Et = -443.8885164 NIImag=1(-1582.90)			
6	-0.294638	0.734533	-0.427230	6	1.096090	0.252715	0.866175	6	-0.251328	-0.048488	-0.310367
6	-1.580473	0.264927	0.239057	6	0.926965	1.567160	0.120671	6	-0.078664	1.336812	0.289167
1	-0.361528	0.503824	-1.513581	1	2.008581	0.317674	1.491703	1	-0.247534	0.037330	-1.413590
1	-1.482268	0.337294	1.327060	1	0.131389	1.472221	-0.625048	1	-0.250269	1.300245	1.369657
6	-2.049342	-1.122033	-0.186099	6	2.210160	2.106688	-0.502373	6	-0.929835	2.416135	-0.369905
1	-1.346583	-1.906700	0.113560	1	2.601143	1.446425	-1.283540	1	-2.002256	2.236352	-0.239270
1	-3.016789	-1.365378	0.262062	1	2.041771	3.085528	-0.959936	1	-0.711610	3.399556	0.055168
1	-2.164423	-1.183138	-1.273562	1	2.995840	2.224993	0.251407	1	-0.734638	2.470768	-1.446115
8	0.131738	1.980684	-0.118909	8	-0.001173	-0.224090	1.531091	8	0.582088	-1.025982	0.179739
7	1.020864	-0.000323	0.014667	7	1.317954	-1.014736	-0.004745	7	-1.558060	-0.805943	0.018678
6	1.048601	-0.508653	1.386919	6	0.758413	-0.990503	-1.361042	6	-2.225600	-0.451804	1.273650
1	0.657403	0.265003	2.048783	1	-0.271514	-0.624966	-1.317296	1	-1.482573	-0.421229	2.071073
1	0.457844	-1.423041	1.493096	1	1.356238	-0.361712	-2.027717	1	-2.736014	0.513002	1.203775
1	2.083072	-0.721035	1.666652	1	0.756945	-2.011032	-1.751535	1	-2.959794	-1.225089	1.509093
6	1.647643	-0.899233	-0.953323	6	2.641495	-1.633992	0.064822	6	-2.488352	-1.021120	-1.090146
1	1.102139	-1.845488	-1.022271	1	3.377177	-1.056586	-0.504002	1	-3.023654	-0.099690	-1.339769
1	1.656684	-0.419645	-1.933957	1	2.959498	-1.691172	1.107690	1	-1.931912	-1.361677	-1.965102
1	2.676107	-1.105466	-0.647993	1	2.590513	-2.644177	-0.347327	1	-3.213696	-1.787635	-0.809440
1	1.240610	1.192306	0.013514	1	0.451112	-1.276618	0.826357	1	-0.621378	-1.583056	0.233078
1	-2.332962	1.011010	-0.040690	1	0.555327	2.275602	0.869737	1	2.154450	-0.473685	0.565378
				1	-1.636709	0.011842	0.482451	8	3.048045	-0.061063	0.657693
				7	-2.370599	-0.015014	-0.233655	6	3.758645	-0.375900	-0.507837
				6	-3.181198	-1.199058	-0.041454	1	3.254925	-0.032109	-1.424684
				1	-3.870340	-1.325825	-0.885369	1	4.732703	0.121651	-0.459164

	1 -2.538401 -2.083527 -0.000965 1 -3.792422 -1.181332 0.879897 6 -3.156663 1.199277 -0.184783 1 -2.498362 2.069991 -0.258218 1 -3.849331 1.233205 -1.034611 1 -3.762127 1.306717 0.734301	1 3.943290 -1.456356 -0.618930 1 0.986121 1.565777 0.171262
<b>TS-Id</b> Et =-463.3463921 NImag=1(-1112.20)	<b>TS-Id</b> Et =-443.9165019 Nimag=1	<b>TS-Ie</b> Et =-598.4634916 NImag=1 (-1579.76)
6 -0.814632 -0.759195 0.168203 6 -2.285673 -0.971251 -0.231464 1 -0.761191 -0.786986 1.287734 1 -2.371514 -0.835183 -1.315666 6 -3.360593 -0.175196 0.501993 1 -3.410221 0.867321 0.174398 1 -4.350615 -0.609024 0.328233 1 -3.190728 -0.174993 1.584686 8 -0.009553 -1.600588 -0.467357 7 -0.312849 0.716898 -0.089769 6 -0.504552 1.120459 -1.477709 1 -0.253109 0.260582 -2.102862 1 -1.539226 1.426373 -1.676656 1 0.154716 1.958849 -1.725758 6 -0.719833 1.744992 0.860426 1 -1.741495 2.099067 0.689709 1 -0.657001 1.343878 1.875846 1 -0.046098 2.605857 0.784791 1 0.998666 0.454112 0.060943 1 1.428248 -1.079781 -0.087865 7 2.056454 -0.220787 0.126929 6 2.659558 -0.267155 1.453505 1 3.431619 -1.042894 1.512653	6 0.399401 -0.720731 -0.132947 6 1.858677 -1.077091 0.124460 1 0.187979 -0.779764 -1.219665 1 2.069246 -0.946413 1.191235 6 2.921885 -0.398248 -0.732307 1 3.095925 0.642974 -0.445573 1 3.878896 -0.916940 -0.627174 1 2.656475 -0.415380 -1.794762 8 -0.419202 -1.456719 0.638815 7 0.050741 0.793019 0.150505 6 0.448132 1.219351 1.501681 1 0.173607 0.420390 2.190356 1 1.523363 1.404183 1.544141 1 -0.087699 2.133437 1.764341 6 0.410291 1.763701 -0.894372 1 1.478451 1.977348 -0.879758 1 0.134854 1.357675 -1.869249 1 -0.142060 2.690554 -0.724329 1 -1.040104 0.682974 0.165359 1 -1.485897 -0.953467 0.520297 8 -2.350808 -0.083625 0.361330 6 -3.117535 -0.321073 -0.779980 1 -3.877424 -1.099543 -0.604645	6 -0.185479 0.831195 -0.389076 6 0.855208 1.619688 -1.165933 1 -1.189495 1.204135 -0.654175 1 1.856887 1.391740 -0.789471 6 0.600491 3.123119 -1.200537 1 0.647196 3.575691 -0.204838 1 1.342008 3.630756 -1.823604 1 -0.388289 3.345223 -1.615709 8 -0.081281 -0.546788 -0.462031 7 -0.121122 0.910156 1.149967 6 1.146605 1.322243 1.760823 1 1.963937 0.746135 1.318548 1 1.325578 2.393995 1.631743 1 1.097850 1.103476 2.830057 6 -1.306290 1.485674 1.792056 1 -1.333969 2.572814 1.663020 1 -2.194776 1.030765 1.345308 1 -1.278758 1.258869 2.860378 1 -0.142537 -0.291611 0.833216 1 0.815835 1.217190 -2.184437 1 1.842531 -1.072103 -0.331925 7 2.819115 -1.179723 -0.044291 6 2.935069 -2.324059 0.835878

1 3.117041 0.696182 1.699585	1 -3.656127 0.587854 -1.086376	1 3.942957 -2.366042 1.265901
1 1.887555 -0.488148 2.194097	1 -2.521854 -0.651600 -1.650540	1 2.224606 -2.228152 1.662357
1 -2.447557 -2.040950 -0.058061	1 1.892159 -2.158106 -0.047551	1 2.750032 -3.294188 0.339168
6 3.005523 0.035844 -0.949460		6 3.664176 -1.303384 -1.213828
1 2.481713 -0.019767 -1.905724		1 3.489679 -0.459815 -1.888023
1 3.447904 1.031236 -0.843367		1 4.719774 -1.280168 -0.917553
1 3.813707 -0.704798 -0.950941		1 3.505364 -2.235790 -1.786214
		1 -2.036764 -0.951083 -0.438982
		7 -3.031169 -0.872840 -0.210013
		6 -3.803272 -0.708380 -1.423895
		1 -3.801995 -1.596069 -2.083001
		1 -4.848859 -0.490629 -1.175145
		1 -3.415621 0.138161 -1.998307
		6 -3.443962 -2.035376 0.548249
		1 -3.434429 -2.977338 -0.030569
		1 -2.786780 -2.164487 1.413249
		1 -4.464751 -1.894635 0.923186
TS-If	TS-Ig	TS-Ih
Et =-559.5911508 NIImag=1(-1598.48)	Et =-598.4907174 NIImag=1 (-682.16)	Et =-559.6240534 NIImag=1 (-355.30)
6 -0.013820 -0.711446 -0.393912	6 -1.083972 -0.681591 0.275888	6 0.918698 -0.321966 -0.637506
6 -1.090939 -0.883700 -1.446253	6 -2.378510 -1.504113 0.516319	6 2.384758 -0.517357 -1.016241
1 0.779424 -1.457164 -0.554127	1 -0.507575 -0.752192 1.239220	1 0.370758 0.014921 -1.533942
1 -1.926050 -0.205871 -1.247346	1 -2.031413 -2.458968 0.931316	1 2.348156 -1.220229 -1.855767
6 -1.565775 -2.324161 -1.609204	6 -3.186093 -1.800152 -0.741436	6 3.287199 -1.100086 0.066095
1 -2.066048 -2.700968 -0.711423	1 -2.492689 -2.077613 -1.539660	1 2.803117 -1.956086 0.541432
1 -2.277622 -2.404456 -2.434795	1 -3.889025 -2.623949 -0.578633	1 4.229410 -1.440124 -0.372663
1 -0.728085 -2.994489 -1.827910	1 -3.766876 -0.938847 -1.083648	1 3.539237 -0.373143 0.842750
8 0.511619 0.578477 -0.266260	8 -0.410721 -1.017798 -0.804904	8 0.389385 -1.430840 -0.080914
7 -0.415557 -0.841360 1.074863	7 -1.343388 0.862276 0.275904	7 0.672041 0.892424 0.319456
6 -1.807822 -0.505790 1.400919	6 -2.081919 1.317823 -0.895043	6 0.993159 0.630121 1.736185
1 -2.067407 0.437437 0.915439	1 -1.739285 0.723641 -1.744203	1 0.717221 -0.401234 1.949784

1 -2.496300 -1.295056 1.085299	1 -3.165223 1.191568 -0.772813	1 2.055228 0.784792 1.925546
1 -1.885581 -0.383341 2.483242	1 -1.885827 2.380106 -1.082058	1 0.407506 1.311660 2.355583
6 0.079710 -2.021619 1.784460	6 -1.891072 1.397800 1.512461	6 1.238722 2.162825 -0.161565
1 -0.471284 -2.920157 1.489176	1 -2.954832 1.155219 1.638021	1 2.322742 2.168325 -0.038909
1 1.139282 -2.160818 1.562559	1 -1.340762 0.982743 2.362823	1 0.988832 2.291968 -1.216536
1 -0.041232 -1.869638 2.858792	1 -1.790522 2.488826 1.532016	1 0.807272 2.985602 0.411762
1 0.269216 0.214252 0.958836	1 -0.008362 1.253527 0.115703	1 -0.411981 1.002574 0.284578
1 -0.753781 1.778888 -0.503058	1 1.219648 -1.324940 -0.214059	1 -0.683835 -1.436329 -0.250009
8 -1.573999 2.324546 -0.473956	7 2.185007 -1.163087 0.151481	8 -2.035565 -1.274498 -0.435963
6 -1.294931 3.482289 0.272425	6 3.154256 -1.554880 -0.855050	6 -2.747096 -2.108433 0.426189
1 -0.532219 4.116156 -0.203342	1 2.906251 -1.082126 -1.809251	1 -2.380922 -2.076323 1.468177
1 -2.216884 4.066044 0.345209	1 4.160393 -1.229114 -0.564799	1 -3.814413 -1.838740 0.453757
1 -0.956914 3.260057 1.295793	1 3.194167 -2.645462 -1.017943	1 -2.689403 -3.158075 0.099141
1 -0.639776 -0.538023 -2.383034	1 -3.004675 -1.051128 1.296666	1 2.804141 0.409170 -1.423563
1 2.184363 0.415362 -0.732593	1 1.653317 0.572502 0.132274	1 -2.091323 -0.036423 -0.032358
8 3.107212 0.114762 -0.897732	7 1.168491 1.483894 -0.086540	8 -1.943297 1.030603 0.285541
6 3.856369 0.436247 0.242352	6 1.694730 2.561913 0.753141	6 -2.578886 1.878028 -0.634593
1 3.475333 -0.042999 1.158607	1 1.157217 3.490930 0.546622	1 -2.340900 2.923650 -0.404472
1 4.879670 0.081213 0.087099	1 1.558436 2.300873 1.804451	1 -2.277031 1.685339 -1.676155
1 3.905392 1.519898 0.432391	1 2.760567 2.723161 0.563292	1 -3.671608 1.770819 -0.585027
	6 2.396425 -1.858608 1.406934	
	1 1.629038 -1.565750 2.128331	
	1 2.368490 -2.956932 1.306163	
	1 3.374673 -1.593118 1.825893	
	6 1.330460 1.719218 -1.526203	
	1 0.885557 0.865023 -2.038083	
	1 0.810333 2.636019 -1.814864	
	1 2.388142 1.812347 -1.791518	
<b>TS-II</b>		<b>TS-Ij</b>
Et = -598.4628613 NIImg=1(-1563.68)		Et = -559.5930319 NIImg=1 (-1587.95)
6 1.832290 -0.922269 0.225077		6 1.337902 -0.857668 -0.197358
		<b>TS-Ik</b>
		Et = -559.619361 NIImg=1 (-561.23)
6 1.374661 0.629825 -0.358275		

6	1.362733	-0.263079	1.512958	6	0.791776	-0.882150	1.219719	6	2.664480	0.081324	-0.959228
1	2.784241	-1.451664	0.426942	1	2.257337	-1.467288	-0.235380	1	1.610418	1.372826	0.431561
1	0.531688	0.416618	1.300814	1	-0.032015	-0.170132	1.325382	1	2.413544	-0.736926	-1.642537
6	2.466807	0.431272	2.303826	6	1.852017	-0.664947	2.294962	6	3.789903	-0.318322	-0.010507
1	2.903642	1.272475	1.756492	1	2.306922	0.328625	2.233518	1	3.610466	-1.277897	0.482489
1	2.083054	0.824274	3.249546	1	1.416826	-0.760932	3.293301	1	4.728764	-0.420587	-0.561873
1	3.279299	-0.264214	2.540340	1	2.656931	-1.402868	2.211965	1	3.949737	0.435592	0.767747
8	0.908796	-1.676672	-0.449057	8	0.448467	-1.173353	-1.209818	8	0.525546	1.040096	-1.297427
7	2.149374	0.033287	-0.961148	7	1.733854	0.515877	-0.775658	7	0.583554	-0.457971	0.522659
6	1.599347	1.393158	-0.931042	6	1.138173	1.711797	-0.167679	6	0.256397	-1.670915	-0.251165
1	0.548463	1.377702	-0.624598	1	0.070508	1.558362	0.006929	1	0.018568	-1.347272	-1.264731
1	2.169877	2.034795	-0.252336	1	1.629463	1.961717	0.777472	1	1.111583	-2.348294	-0.255439
1	1.668166	1.809739	-1.939244	1	1.270356	2.546316	-0.860245	1	-0.617683	-2.149148	0.191319
6	3.529128	-0.013161	-1.446416	6	3.152333	0.685519	-1.094509	6	1.098583	-0.747050	1.872350
1	4.204294	0.511980	-0.763167	1	3.746888	0.827006	-0.186243	1	1.971493	-1.394366	1.815984
1	3.845141	-1.054500	-1.534931	1	3.511874	-0.197202	-1.626680	1	1.369984	0.190980	2.359781
1	3.583723	0.459745	-2.429512	1	3.274295	1.560735	-1.736067	1	0.318630	-1.243877	2.453070
1	1.362952	-0.818495	-1.368296	1	0.982448	-0.036534	-1.602233	1	-0.310750	0.079122	0.634126
1	0.943802	-1.079727	2.112122	1	-1.153976	-1.057574	-0.959693	1	-0.550037	1.291480	-0.710524
1	-0.958612	-1.497643	-0.145813	8	-2.140855	-0.944398	-0.823003	8	-1.442002	1.260898	0.041218
7	-1.979285	-1.398112	-0.068468	6	-2.648613	-2.131096	-0.261246	6	-1.696738	2.500972	0.641126
6	-2.597079	-1.940663	-1.262101	1	-2.210574	-2.356580	0.721323	1	-2.305184	3.149518	-0.006439
1	-3.673565	-1.732351	-1.258213	1	-3.727477	-2.011815	-0.131020	1	-2.247178	2.362216	1.579869
1	-2.166198	-1.464576	-2.147473	1	-2.477372	-2.994351	-0.917670	1	-0.769924	3.046337	0.875422
1	-2.472608	-3.033280	-1.368390	1	0.352261	-1.878995	1.340523	1	3.007931	0.899743	-1.600794
6	-2.437830	-2.065662	1.133047	1	-2.196671	0.451934	0.179797	1	-2.494899	-0.088126	0.226028
1	-1.898879	-1.674849	2.000927	8	-2.096263	1.269223	0.724291	8	-2.905655	-0.972218	0.376185
1	-3.505887	-1.871921	1.287519	6	-2.949212	2.249437	0.189686	6	-3.624329	-1.307407	-0.782540
1	-2.301380	-3.161871	1.111740	1	-2.725479	2.482325	-0.861892	1	-4.068540	-2.295813	-0.631642
1	-1.917357	0.641341	-0.015068	1	-4.009515	1.962620	0.252026	1	-4.442455	-0.601737	-0.991659
7	-1.731801	1.652670	-0.030015	1	-2.817062	3.166361	0.771287	1	-2.990200	-1.358734	-1.680739

6	-2.337795	2.235098	-1.208849		
1	-3.443457	2.214309	-1.202827		
1	-2.034205	3.284304	-1.310058		
1	-1.996335	1.702492	-2.101487		
6	-2.224308	2.256712	1.189813		
1	-1.799704	1.740746	2.056005		
1	-1.912633	3.307015	1.242568		
1	-3.325662	2.237576	1.288391		
<b>TS-Ij</b>					
Et = -559.6186291 NImag = 1(-773.28)					

6	0.829531	-0.003537	-0.756257
6	1.683138	-1.261901	-0.833261
1	1.298183	0.799213	-1.351843
1	1.230819	-2.036298	-0.204501
6	3.170454	-1.113957	-0.530806
1	3.371629	-0.961425	0.533557
1	3.705587	-2.020197	-0.826950
1	3.613363	-0.277345	-1.081253
8	-0.448273	-0.270927	-1.167489
7	0.744836	0.635063	0.652288
6	0.479543	-0.331653	1.734086
1	-0.314095	-1.011641	1.417043
1	1.383898	-0.895406	1.974190
1	0.155886	0.218772	2.619704
6	1.834518	1.567822	0.983251
1	2.772447	1.037869	1.149930
1	1.961042	2.279703	0.165901
1	1.565987	2.112479	1.890787
1	-0.208363	1.235217	0.510526
1	-1.079850	0.620912	-0.815053
8	-1.474379	1.573066	-0.054579
6	-1.581924	2.810990	-0.693720
1	-2.496160	2.865704	-1.303094
1	-1.633231	3.627939	0.040433
1	-0.734375	3.031552	-1.366909
1	1.555481	-1.606903	-1.864625
1	-1.301815	-1.635640	-0.425055
8	-1.802948	-2.231653	0.175269
6	-3.075589	-1.649323	0.350028
1	-3.555680	-2.134737	1.204918
1	-3.013876	-0.571502	0.547805
1	-3.723961	-1.798243	-0.527062

**Table S59.** The PCM-mPW1PW91/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Transition States for Dehydration Step (**Step-II**)

TS-II				TS-IIa				TS-IIb			
Et = -328.1487344 NImag=1 (-1230.89)				Et = -463.2950976 NImag=1 (-534.44)				Et = -443.8669675 NImag=1 (-288.80)			
6	0.211466	-0.059875	0.506806	6	1.829248	0.336154	-0.181369	6	1.381865	0.489886	-0.306137
6	1.365611	-0.403765	-0.283246	6	1.908014	-1.014874	0.324481	6	1.851462	-0.658462	0.445762
1	0.363257	0.571287	1.376806	1	2.308576	0.539131	-1.133908	1	1.745010	0.604837	-1.323705
1	1.222201	-1.229879	-0.979859	1	1.601446	-1.131798	1.364553	1	1.668386	-0.591180	1.519455
6	2.702733	-0.425308	0.435127	6	3.173059	-1.783299	-0.023309	6	3.258499	-1.129209	0.107802
1	2.829285	-1.304112	1.078121	1	4.043651	-1.440468	0.545579	1	4.027743	-0.443723	0.477039
1	3.522769	-0.426988	-0.288472	1	3.037445	-2.847300	0.187632	1	3.442529	-2.108554	0.556145
1	2.827025	0.464833	1.061705	1	3.408593	-1.689714	-1.088536	1	3.389982	-1.234775	-0.973885
8	0.175349	1.785591	-0.845074	8	-0.031021	-0.675329	-1.392462	8	-0.326553	-1.309448	-0.987461
7	-1.037534	-0.458417	0.332167	7	1.154583	1.337598	0.315803	7	0.471143	1.341807	0.052627
6	-1.410374	-1.225169	-0.844042	6	0.361634	1.227662	1.534685	6	-0.220389	1.260454	1.337449
1	-1.408774	-0.583130	-1.731929	1	-0.624901	0.800132	1.295486	1	-0.998731	0.482863	1.273896
1	-0.714900	-2.051356	-0.992060	1	0.878192	0.598346	2.258674	1	0.490428	1.019570	2.127668
1	-2.409983	-1.635784	-0.695203	1	0.247469	2.226294	1.960437	1	-0.664771	2.233227	1.550550
6	-2.065668	0.433008	0.844700	6	0.748993	2.391663	-0.602395	6	-0.193230	2.141360	-0.967869
1	-3.034794	-0.067371	0.837208	1	0.476154	3.288247	-0.045559	1	-0.485796	3.105886	-0.551540
1	-1.824401	0.723903	1.869168	1	1.568122	2.625782	-1.284343	1	0.478377	2.296851	-1.812352
1	-2.070458	1.330755	0.211451	1	-0.101342	2.010543	-1.180790	1	-1.074630	1.587612	-1.306146
1	0.584868	2.547216	-0.408824	1	-0.277768	-1.035452	-2.255462	1	-0.537573	-2.001951	-1.626487
1	1.151248	0.671465	-0.858756	1	1.001731	-1.324242	-0.379572	1	1.038516	-1.352219	-0.011385
				1	-1.483404	-0.446760	-0.460631	1	-1.419656	-1.250546	-0.057591
				7	-2.293127	-0.299273	0.186058	8	-2.205906	-1.113827	0.643423

	6 -3.346634 0.408350 -0.502729 1 -2.950016 1.332536 -0.935497 1 -3.818515 -0.169092 -1.322245 1 -4.149623 0.685534 0.193776 6 -2.737464 -1.579745 0.684700 1 -1.887142 -2.122333 1.109097 1 -3.484386 -1.451676 1.480030 1 -3.197411 -2.228811 -0.086433	6 -3.290238 -0.603121 -0.062113 1 -3.149958 0.442061 -0.398645 1 -3.531477 -1.191425 -0.964465 1 -4.184527 -0.610436 0.575993
<b>TS-IIc</b> Et =-463.2900721 NIMag=1 (-725.22)	<b>TS-IId</b> Et =-443.8758943 NIMag=1(-96.26)	<b>TS-IIe</b> Et =-598.4424055 NIMag=1(-129.41)
6 -1.042774 0.626850 -0.430930 6 -0.141000 1.485919 0.261046 1 -0.796559 0.358320 -1.454477 6 0.452697 2.634172 -0.544579 1 -0.253275 3.461066 -0.677095 1 1.340096 3.031878 -0.044359 1 0.758892 2.293816 -1.538881 8 0.375979 -1.328103 -1.624948 7 -2.042766 -0.062045 0.072737 6 -2.531807 0.098970 1.428956 1 -2.027382 -0.593205 2.112423 1 -2.371009 1.120799 1.771971 1 -3.602989 -0.111945 1.444854 6 -2.577531 -1.176084 -0.704035 1 -3.489421 -0.881797 -1.232452 1 -1.779127 -1.488345 -1.389098 1 -2.815633 -1.998860 -0.024910 1 1.290143 -0.905213 -0.621803 1 0.343253 -2.289892 -1.532102 7 1.861425 -0.438962 0.249113 1 0.807102 0.656895 0.371115	6 0.953913 0.841225 0.065404 6 -0.207113 1.303357 -0.667611 1 1.259448 1.341591 0.978171 1 -0.023166 1.290770 -1.748695 6 -0.772904 2.627434 -0.177750 1 -0.091661 3.468756 -0.344889 1 -1.708957 2.851144 -0.695627 1 -0.994291 2.569581 0.891813 8 -0.567537 -0.188990 2.044435 7 1.660175 -0.198909 -0.273199 6 1.258737 -1.043398 -1.399280 1 1.332569 -0.481394 -2.334229 1 1.932109 -1.898445 -1.449522 1 0.219366 -1.365191 -1.228376 6 2.741423 -0.686314 0.568033 1 3.647292 -0.809614 -0.030136 1 2.932410 0.023165 1.372645 1 2.462784 -1.652915 0.997352 1 -0.160123 -0.953933 2.469284 1 -1.039892 -0.589125 1.233889 8 -1.543873 -1.037784 -0.179475	6 -0.295953 1.317623 0.374437 6 0.179344 2.131074 -0.755380 1 -1.309693 0.927688 0.332808 1 1.153147 2.589859 -0.573846 6 -0.853720 3.162560 -1.210149 1 -1.032060 3.931793 -0.452661 1 -0.505022 3.660232 -2.118417 1 -1.808958 2.682196 -1.441076 8 -0.166859 -0.489513 -1.374243 7 0.354610 1.026569 1.456180 6 1.753065 1.376072 1.693942 1 2.371882 0.625538 1.178228 1 1.965301 2.374734 1.314269 1 1.931800 1.361593 2.769727 6 -0.231187 0.104162 2.423034 1 -0.279029 0.585284 3.403118 1 -1.226646 -0.185500 2.084531 1 0.403547 -0.783187 2.491247 1 -1.733562 -0.777730 -0.599454 1 0.287859 1.333936 -1.524938 1 1.467637 -0.769491 -0.724439

1 -0.432131 1.769053 1.274976	6 -2.898588 -1.228774 -0.311883	7 2.435432 -0.974830 -0.384711			
6 3.194796 -0.012788 -0.110343	1 -3.501776 -0.709293 0.462151	6 2.499673 -2.354602 0.045033			
1 3.654321 0.592108 0.683916	1 -3.296798 -0.878096 -1.287178	1 1.711255 -2.550338 0.778842			
1 3.870947 -0.862106 -0.306761	1 -3.189606 -2.298604 -0.243357	1 2.379389 -3.086323 -0.776892			
1 3.150889 0.595390 -1.018505	1 -0.962470 0.416978 -0.512060	1 3.463730 -2.567269 0.525091			
6 1.837236 -1.314771 1.398276		6 3.370943 -0.703715 -1.454328			
1 2.466494 -2.210283 1.261611		1 3.240627 0.324072 -1.806691			
1 2.186833 -0.805080 2.306783		1 4.404619 -0.807833 -1.099642			
1 0.810405 -1.654337 1.569079		1 3.258281 -1.374333 -2.327372			
		1 -0.179520 -1.390772 -1.728745			
		7 -2.586636 -0.909634 -0.009875			
		6 -3.772316 -0.566869 -0.763691			
		1 -3.663687 0.435220 -1.190717			
		1 -3.990311 -1.263562 -1.594910			
		1 -4.655693 -0.557065 -0.111975			
		6 -2.624831 -2.274612 0.468213			
		1 -1.662005 -2.530218 0.921339			
		1 -3.402289 -2.398619 1.233404			
		1 -2.829681 -3.018688 -0.324713			
<b>TS-III<sup>f</sup></b> Et = -559.5863922 NIImag=1(-71.84)		<b>TS-II<sup>g</sup></b> Et = -559.5858266 NIImag=2(-31.59, -4.39)		<b>TS-III<sup>g</sup></b> Et = -559.5834682 NIImag=1(-142.83)	
6 1.489449 -0.098440 0.385102	6 1.687700 -0.405024 0.098850	6 1.502476 -0.395630 0.217090			
6 2.342434 -0.356256 -0.791378	6 1.969281 1.029313 -0.131874	6 1.752936 1.022805 0.219421			
1 1.390146 0.929843 0.726676	1 1.892261 -0.838348 1.069601	1 1.382936 -0.925055 1.161486			
1 2.675426 -1.394768 -0.855601	1 2.539085 1.151485 -1.062909	1 2.311076 1.360333 -0.660208			
6 3.517067 0.612715 -0.889088	6 2.675385 1.680164 1.050490	6 2.301689 1.585202 1.521610			
1 4.226015 0.479443 -0.066739	1 3.666277 1.247655 1.219908	1 3.346345 1.305619 1.693848			
1 4.056201 0.451523 -1.825352	1 2.803520 2.750422 0.873069	1 2.247939 2.676802 1.514511			
1 3.169417 1.649683 -0.878003	1 2.075641 1.547168 1.954029	1 1.714982 1.234954 2.376767			
8 -0.388339 0.549874 -1.450709	8 0.011830 -0.208703 2.262896	8 -0.420123 -1.579446 2.278724			

7	0.749153	-0.946521	1.007499	7	1.131967	-1.176684	-0.768525	7	1.192826	-1.086975	-0.842050
6	0.584331	-2.346508	0.627411	6	0.737033	-0.694215	-2.094836	6	1.110073	-0.455808	-2.157676
1	-0.382617	-2.411817	0.115512	1	1.611483	-0.288377	-2.608173	1	0.814000	-1.208122	-2.887537
1	1.390484	-2.673395	-0.023880	1	0.347747	-1.536099	-2.664071	1	0.366853	0.350501	-2.107805
1	0.575996	-2.953549	1.534572	1	-0.031313	0.079272	-1.986283	1	2.084379	-0.050279	-2.442551
6	-0.179307	-0.501768	2.048743	6	0.646634	-2.501056	-0.386411	6	0.704766	-2.455531	-0.735555
1	0.043848	-1.034283	2.975976	1	0.853537	-3.210510	-1.188537	1	1.280707	-3.103029	-1.400812
1	-0.082178	0.574424	2.175659	1	1.143262	-2.820227	0.529419	1	0.796296	-2.795020	0.294841
1	-1.186536	-0.736023	1.694181	1	-0.430068	-2.364169	-0.206991	1	-0.351385	-2.465460	-1.013933
1	-0.782871	0.949636	-2.235472	1	-0.036617	-0.980340	2.841129	1	-0.561730	-0.972235	3.015626
1	-1.374073	-0.376095	-0.862950	1	-0.700233	-0.397164	1.551282	1	-0.976590	-1.207901	1.547727
8	-2.019641	-1.042433	-0.376837	8	-1.632160	-0.748013	0.360998	8	-1.747065	-0.571177	0.148669
6	-3.184684	-1.158795	-1.133596	6	-2.945895	-0.941219	0.734921	6	-3.145032	-0.589932	0.067302
1	-3.003154	-1.562288	-2.144734	1	-3.340185	-0.153690	1.409960	1	-3.622995	0.132108	0.748004
1	-3.877034	-1.845017	-0.630808	1	-3.638513	-0.970866	-0.130053	1	-3.499361	-0.370238	-0.950498
1	-3.711368	-0.197607	-1.258306	1	-3.098775	-1.898916	1.272163	1	-3.505144	-1.588694	0.337189
1	1.609336	-0.171649	-1.600392	1	0.982928	1.493313	-0.315492	1	0.646468	1.419627	-0.029655
1	-0.333092	1.651430	-0.434239	1	-1.400704	0.553622	-0.340737	1	-1.389138	0.357883	-0.179343
8	-0.282105	2.310920	0.366063	8	-1.113021	1.411189	-0.852475	8	-0.742549	1.571654	-0.681078
6	-1.601502	2.617378	0.713730	6	-2.119109	2.373976	-0.744845	6	-1.431263	2.746812	-0.453116
1	-2.070622	3.330304	0.013136	1	-2.320473	2.663227	0.298921	1	-1.800761	2.854361	0.586577
1	-2.243604	1.723947	0.748293	1	-1.807335	3.277817	-1.281589	1	-0.809523	3.640397	-0.650727
1	-1.619832	3.085064	1.706308	1	-3.074668	2.044102	-1.184092	1	-2.321119	2.846515	-1.104141
<b>TS-IIh</b>				<b>TS-IIIi</b>							
Et = -598.4325752 NImag=1(-608.96)				Et = -559.5852625 NImag=2(-74.02,-51.7)							

6	2.623864	-0.342625	0.293459					
6	2.765748	0.438514	-0.913490					
1	3.132853	0.025689	1.178242					
1	2.386468	-0.035953	-1.818792					
6	4.107589	1.127364	-1.105240	6	1.628795	0.720880	0.040419	
1	4.906324	0.429375	-1.378094	6	0.390179	1.534137	0.138837	
1	4.036793	1.876231	-1.898553	1	2.483581	0.981700	0.653755	
1	4.414816	1.648478	-0.192208	6	0.527999	2.667331	1.148417	
8	1.013957	1.454777	0.759508	1	1.320086	3.369788	0.871170	
7	1.872081	-1.390196	0.496395	1	-0.406734	3.228154	1.218319	
6	1.076519	-2.037880	-0.537784	1	0.755855	2.272348	2.142858	
1	0.031295	-1.691566	-0.506846	8	1.117171	-0.716147	1.821906	
1	1.506745	-1.840157	-1.517842	7	1.844108	-0.183871	-0.862551	
1	1.099814	-3.115835	-0.358099	6	0.778526	-0.715408	-1.709909	
6	1.471244	-1.680012	1.866183	1	0.186556	-1.421868	-1.114214	
1	1.132404	-2.713404	1.942709	1	0.101614	0.076526	-2.026007	
1	2.314767	-1.526258	2.541290	1	1.232499	-1.192219	-2.578656	
1	0.667332	-0.984977	2.132397	6	3.085551	-0.946263	-0.859565	
1	1.223843	2.264308	1.246344	1	3.496600	-0.974100	-1.870885	
1	1.946360	1.197656	-0.482908	1	3.803990	-0.486275	-0.182772	
1	-0.671125	1.548726	0.457382	1	2.878112	-1.965347	-0.523508	
7	-1.693343	1.648405	0.240458	1	0.839525	-0.290811	2.643394	
6	-2.389530	2.092896	1.427330	1	0.221585	-0.958386	1.347210	
1	-2.175040	1.410200	2.255306	8	-1.070420	-1.139472	0.623545	
1	-2.110275	3.113843	1.752054	6	-1.950820	-1.855723	1.411376	
1	-3.475493	2.093274	1.265770	1	-2.050210	-2.917567	1.105326	
6	-1.841707	2.582514	-0.853632	1	-1.649601	-1.880444	2.477775	
1	-1.222607	2.259287	-1.695667	1	-2.977223	-1.442058	1.396562	
1	-2.884287	2.620848	-1.195692	1	0.138387	1.922148	-0.855106	
1	-1.545551	3.617697	-0.597079	1	-0.424464	0.847117	0.417919	
1	-2.059896	-0.255557	-0.262056	8	-2.263655	0.019685	-1.397996	
7	-2.201445	-1.247684	-0.508687	1	-1.845465	-0.443768	-0.605810	
6	-2.968250	-1.896385	0.532437	6	-3.242011	0.893445	-0.916151	
1	-3.015852	-2.977665	0.351260	1	-2.851240	1.625777	-0.189718	
1	-2.481136	-1.742112	1.499984	1	-3.652410	1.460196	-1.759806	
1	-4.010290	-1.534495	0.616520	1	-4.083882	0.373255	-0.430122	
6	-2.852079	-1.334616	-1.797858					
1	-2.278178	-0.770932	-2.539359					

**Table S60.** The B3LYP/6-311+G\*\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Transition States for Carbinolamine Formation (**Step-I**)

TS-I			TS-Ia				TS-Ib				
Et = -328.3659407 NImag=1(-1573.11)			Et = -463.5849549 NImag=1 (-1584.56)				Et = -444.1483177 NImag=1(-1594.02)				
6	-0.311719	0.766445	-0.353631	6	1.141954	0.255276	0.871288	6	-0.636074	0.276605	-0.829699
6	-1.607498	0.237930	0.257686	6	0.982725	1.584638	0.139113	6	-0.423563	1.567813	-0.048916
1	-0.352373	0.625893	-1.452882	1	2.059202	0.294252	1.488366	1	-1.431002	0.433084	-1.579296
1	-1.514928	0.188309	1.346172	1	0.183743	1.508496	-0.602853	1	0.256775	1.394314	0.787869
6	-2.103306	-1.089649	-0.324762	6	2.272382	2.128574	-0.484725	6	-1.717218	2.250745	0.407338
1	-1.417010	-1.917557	-0.121385	1	2.656089	1.479966	-1.278133	1	-2.280143	1.641653	1.121023
1	-3.073744	-1.363763	0.096692	1	2.106406	3.114571	-0.925903	1	-1.500717	3.203305	0.896961
1	-2.224499	-1.022160	-1.410366	1	3.061620	2.233460	0.266319	1	-2.376910	2.459683	-0.440697
8	0.111926	1.983690	0.059580	8	0.041876	-0.222185	1.531672	8	0.489475	-0.328692	-1.348252
7	1.036835	-0.003386	0.063455	7	1.340170	-1.031777	-0.027543	7	-1.108701	-0.985466	-0.019897
6	1.034005	-0.760348	1.324508	6	0.801219	-0.980706	-1.400616	6	-0.747307	-1.035098	1.411188
1	0.570514	-0.155296	2.102792	1	-0.218102	-0.591586	-1.370899	1	0.304426	-0.773782	1.527650
1	0.496407	-1.707642	1.226724	1	1.424144	-0.360822	-2.051550	1	-1.369907	-0.359929	2.004555
1	2.065283	-0.970419	1.617007	1	0.777067	-1.995943	-1.802715	1	-0.894171	-2.055741	1.769741
6	1.755987	-0.684577	-1.023089	6	2.648387	-1.697325	0.065216	6	-2.469899	-1.469903	-0.295986
1	1.268251	-1.626580	-1.291724	1	3.415406	-1.143359	-0.484747	1	-3.222335	-0.829834	0.174897
1	1.780099	-0.033218	-1.897563	1	2.942246	-1.768660	1.113269	1	-2.636056	-1.483103	-1.373857
1	2.781426	-0.894953	-0.710853	1	2.575116	-2.704200	-0.350888	1	-2.579066	-2.484971	0.090701
1	1.204863	1.187742	0.229420	1	0.463978	-1.272463	0.795770	1	-0.159524	-1.326229	-0.731982
1	-2.342362	1.025014	0.060869	1	0.620961	2.282249	0.901364	1	1.894763	-0.214632	-0.290041
				1	-1.746098	0.016620	0.537329	8	2.505456	-0.206301	0.482149
				7	-2.455485	-0.019182	-0.197928	6	3.836732	-0.036951	0.033527
				6	-3.297726	-1.193054	-0.010895	1	3.972754	0.906196	-0.513443
				1	-3.949071	-1.331382	-0.881152	1	4.486851	-0.017497	0.911426
				1	-2.672918	-2.084992	0.083578	1	4.163726	-0.860712	-0.615578

	1 -3.944595 -1.136652 0.882732 6 -3.218547 1.221138 -0.223434 1 -2.537784 2.073428 -0.292853 1 -3.870394 1.242724 -1.103881 1 -3.857194 1.367249 0.666079	1 0.115975 2.227134 -0.736538
<b>TS-Id</b> Et =-463.6019163 NImag=1 (-1163.19)	<b>TS-Id</b> Et =-444.1711245 NImag=1(-813.40)	<b>TS-Ie</b> Et =-598.8032174 NImag=1(-1597.45)
6 -0.833756 -0.778991 0.189938 6 -2.286971 -0.992838 -0.279621 1 -0.821749 -0.804319 1.305999 1 -2.328577 -0.845763 -1.363320 6 -3.397049 -0.202689 0.422503 1 -3.405576 0.855015 0.145706 1 -4.379089 -0.606986 0.160264 1 -3.303590 -0.260383 1.512126 8 0.015743 -1.611895 -0.400247 7 -0.314001 0.737591 -0.048928 6 -0.546233 1.204915 -1.420544 1 -0.303048 0.392885 -2.107637 1 -1.587608 1.507056 -1.580255 1 0.094876 2.064929 -1.641980 6 -0.701840 1.734872 0.954348 1 -1.737275 2.069677 0.840371 1 -0.587542 1.309377 1.953906 1 -0.051680 2.613791 0.876884 1 1.006735 0.462390 0.060881 1 1.416767 -1.070451 -0.122696 7 2.072031 -0.214844 0.088866 6 2.702088 -0.308744 1.408488 1 3.467284 -1.092757 1.428964 1 3.172679 0.640502 1.684377	6 0.462426 -0.734085 -0.184744 6 1.913645 -1.087470 0.146256 1 0.308132 -0.756741 -1.280687 1 2.068111 -0.969883 1.222742 6 3.020431 -0.388579 -0.650243 1 3.158218 0.656088 -0.359499 1 3.977186 -0.890306 -0.485273 1 2.821175 -0.414352 -1.726135 8 -0.398641 -1.494396 0.512251 7 0.075508 0.798625 0.122541 6 0.406574 1.213970 1.504157 1 0.112109 0.409893 2.176587 1 1.475228 1.414344 1.598557 1 -0.156261 2.114916 1.753102 6 0.469362 1.794311 -0.896297 1 1.536191 2.007325 -0.848536 1 0.221915 1.408697 -1.885745 1 -0.088710 2.717671 -0.728059 1 -1.014554 0.677518 0.075981 1 -1.456308 -0.993340 0.384390 8 -2.303009 -0.085707 0.243104 6 -3.391304 -0.308281 -0.616483 1 -4.132105 -0.976347 -0.154310 1 -3.903167 0.635826 -0.847967	6 -0.199184 0.868474 -0.386458 6 0.820009 1.641532 -1.216110 1 -1.212789 1.225274 -0.632093 1 1.831032 1.432870 -0.858569 6 0.556563 3.148907 -1.298645 1 0.626808 3.637468 -0.322389 1 1.280844 3.635140 -1.956895 1 -0.441438 3.354084 -1.698126 8 -0.083771 -0.511272 -0.406697 7 -0.097665 0.996087 1.171611 6 1.184210 1.446279 1.745853 1 2.000676 0.877476 1.297956 1 1.341025 2.517505 1.590165 1 1.168657 1.248904 2.819704 6 -1.283351 1.574024 1.830040 1 -1.327225 2.657737 1.681451 1 -2.177542 1.105990 1.413743 1 -1.234535 1.368276 2.901339 1 -0.110821 -0.209298 0.887847 1 0.758245 1.203319 -2.217411 1 1.896443 -1.161127 -0.333961 7 2.872155 -1.254681 -0.046533 6 3.013605 -2.392288 0.852813 1 4.019402 -2.404353 1.286941

1 1.943137 -0.553560 2.153979	1 -3.091436 -0.765326 -1.574684	1 2.297411 -2.306011 1.674140			
1 -2.452053 -2.063142 -0.124473	1 1.962124 -2.164736 -0.036971	1 2.851829 -3.368605 0.362222			
6 3.009598 0.052628 -1.004857		6 3.732029 -1.355737 -1.218443			
1 2.468625 0.038582 -1.952159		1 3.535209 -0.520707 -1.895427			
1 3.483164 1.032224 -0.882099		1 4.783897 -1.300141 -0.917351			
1 3.797340 -0.708049 -1.047970		1 3.598178 -2.293562 -1.786521			
		1 -2.098304 -1.028043 -0.416739			
		7 -3.092138 -0.952322 -0.193003			
		6 -3.864967 -0.759165 -1.413210			
		1 -3.867821 -1.638995 -2.081058			
		1 -4.907233 -0.531550 -1.163997			
		1 -3.464686 0.088449 -1.975338			
		6 -3.516771 -2.124940 0.560774			
		1 -3.511345 -3.057988 -0.030418			
		1 -2.859901 -2.268263 1.422525			
		1 -4.535174 -1.979778 0.937628			
<b>TS-If</b> Et =-559.9406447 NIImg=1(-111.99)		<b>TS-Ig</b> Et =-598.8245672 NIImg=1(-682.1)		<b>TS-Ih</b> Et =-559.9574335 NIImg=1 (-507.45)	
6 0.179717 0.909631 0.782323	6 -1.113203 -0.713985 0.344277	6 0.967927 -0.377572 -0.607435			
6 -0.603963 0.250201 1.861836	6 -2.414693 -1.560687 0.486953	6 2.446251 -0.577323 -0.964147			
1 1.241239 0.689955 0.680754	1 -0.607313 -0.768735 1.344808	1 0.410540 -0.138961 -1.526726			
1 -0.846681 1.013521 2.616735	1 -2.101344 -2.476098 1.002226	1 2.425236 -1.316686 -1.771138			
6 0.158989 -0.919408 2.492257	6 -3.081010 -1.961459 -0.832902	6 3.352370 -1.105245 0.153017			
1 1.099649 -0.591871 2.943305	1 -2.317952 -2.314944 -1.528922	1 2.885079 -1.957581 0.648341			
1 -0.446916 -1.384752 3.272353	1 -3.809345 -2.762093 -0.670389	1 4.307760 -1.433004 -0.264636			
1 0.380960 -1.666051 1.728125	1 -3.609782 -1.131962 -1.309167	1 3.575038 -0.350196 0.910799			
8 0.342475 -1.165754 -0.900895	8 -0.348792 -1.031804 -0.681963	8 0.453469 -1.429480 0.059175			
7 -0.304181 1.772806 -0.045825	7 -1.405827 0.854263 0.313114	7 0.690104 0.949689 0.234785			
6 -1.736463 2.114379 -0.087464	6 -2.192455 1.267158 -0.853849	6 1.055757 0.854559 1.670875			
1 -2.281183 1.268767 -0.520617	1 -1.831152 0.712471 -1.720225	1 0.796984 -0.143752 2.016993			
1 -2.103539 2.309207 0.919649	1 -3.262857 1.066854 -0.720535	1 2.121649 1.035210 1.805603			

1 -1.860068 3.010112 -0.693359	1 -2.074024 2.342320 -1.034359	1 0.481557 1.597368 2.225905
6 0.520947 2.272048 -1.155644	6 -1.956571 1.398070 1.554626	6 1.199399 2.185438 -0.399667
1 0.527643 3.363874 -1.139615	1 -3.002185 1.103036 1.715021	1 2.283826 2.247250 -0.306778
1 1.528393 1.868999 -1.068325	1 -1.369322 1.040098 2.404716	1 0.921271 2.188298 -1.454316
1 0.079296 1.920259 -2.090302	1 -1.918237 2.493432 1.542320	1 0.746128 3.050340 0.087478
1 0.387729 -1.412094 -1.830908	1 -0.033287 1.266381 0.094805	1 -0.394867 1.029101 0.206815
1 -1.208204 -1.092575 -0.712232	1 1.329556 -1.299040 -0.154502	1 -0.631201 -1.471593 -0.094266
8 -2.211272 -0.944658 -0.575571	7 2.301138 -1.099608 0.167675	8 -1.956478 -1.314414 -0.322562
6 -2.915960 -2.109763 -0.948449	6 3.249740 -1.534392 -0.854834	6 -2.825865 -2.230922 0.297204
1 -2.569521 -2.994743 -0.396662	1 2.965493 -1.116296 -1.823362	1 -2.798238 -2.161191 1.396713
1 -3.977501 -1.964505 -0.726101	1 4.260789 -1.185682 -0.614489	1 -3.864304 -2.062808 -0.020101
1 -2.823724 -2.325233 -2.023156	1 3.291068 -2.630441 -0.961828	1 -2.561711 -3.260756 0.022905
1 -1.550561 -0.098551 1.436048	1 -3.132826 -1.073123 1.159274	1 2.860840 0.333553 -1.408394
1 1.797852 -0.678459 -0.666945	1 1.632752 0.627282 0.075651	1 -2.077326 -0.076520 -0.008143
8 2.668473 -0.180209 -0.457984	7 1.110792 1.513655 -0.148542	8 -1.927194 1.023252 0.237668
6 3.756125 -1.078341 -0.405670	6 1.630816 2.627964 0.663143	6 -2.812218 1.865630 -0.469997
1 3.599616 -1.876495 0.333853	1 1.064781 3.538425 0.454073	1 -2.499884 2.911794 -0.366728
1 3.945550 -1.552974 -1.379068	1 1.527008 2.383353 1.721164	1 -2.845563 1.623429 -1.542021
1 4.655485 -0.523551 -0.122291	1 2.686634 2.811924 0.445286	1 -3.833644 1.786621 -0.075156
<b>TS-Ii</b>		
Et = -598.8039785 NImag=1(-1582.00)		
6 1.842393 -0.957819 0.193353	6 1.338724 -0.720222 0.549051	6 1.481590 0.686322 -0.166438
6 1.461790 -0.324594 1.528448	6 0.886563 0.392149 1.487356	6 2.840268 0.265721 -0.726623
<b>TS-Ij</b>		
Et = -559.9307369 NImag=1(-1589.25)		
<b>TS-Ik</b>		
Et = -559.9541741 NImag=1(-654.23)		

1	2.763425	-1.553916	0.327129	1	2.220344	-1.223450	0.978409	1	1.609867	1.206431	0.801588
1	0.671765	0.415066	1.376839	1	0.122796	1.006098	1.004320	1	2.679929	-0.338800	-1.623744
6	2.638502	0.262646	2.314947	6	2.031163	1.248807	2.039517	6	3.829256	-0.412058	0.227384
1	3.114855	1.096577	1.791311	1	2.553156	1.801804	1.253097	1	3.553936	-1.443153	0.462995
1	2.308922	0.637997	3.287044	1	1.654319	1.983565	2.755079	1	4.823161	-0.447140	-0.225440
1	3.407764	-0.494091	2.498664	1	2.772645	0.633566	2.559235	1	3.921257	0.135570	1.170574
8	0.844425	-1.619032	-0.479232	8	0.362506	-1.611338	0.128949	8	0.757322	1.358569	-1.071087
7	2.175984	0.034506	-0.988635	7	1.767668	-0.304572	-0.898711	7	0.563020	-0.561867	0.309534
6	1.705747	1.430099	-0.885973	6	1.315831	1.006455	-1.408840	6	0.377726	-1.587402	-0.750043
1	0.666243	1.456654	-0.551237	1	0.256689	1.150874	-1.194300	1	0.254684	-1.067713	-1.698821
1	2.330448	2.009646	-0.199980	1	1.897159	1.822569	-0.970579	1	1.250522	-2.240278	-0.783855
1	1.765657	1.885961	-1.876991	1	1.458193	1.018714	-2.491352	1	-0.527250	-2.153093	-0.532106
6	3.536229	-0.078471	-1.538077	6	3.162309	-0.612587	-1.253950	6	0.856799	-1.149957	1.638514
1	4.271662	0.384608	-0.872802	1	3.855772	0.092257	-0.784633	1	1.745337	-1.775747	1.592062
1	3.785090	-1.132339	-1.669252	1	3.403453	-1.624613	-0.926477	1	1.013973	-0.345536	2.357431
1	3.578363	0.418664	-2.509282	1	3.280632	-0.554200	-2.337505	1	0.001131	-1.749715	1.951743
1	1.321717	-0.753897	-1.386571	1	0.915005	-1.199919	-1.002303	1	-0.341948	-0.037310	0.405914
1	1.009463	-1.138492	2.104419	1	-1.268208	-1.341734	0.383819	1	-0.327817	1.485545	-0.626024
1	-1.093909	-1.541106	-0.169542	8	-2.229761	-1.098716	0.451274	8	-1.382140	1.295614	0.003788
7	-2.107562	-1.415953	-0.085297	6	-3.024552	-2.204152	0.051728	6	-1.847121	2.405274	0.738028
6	-2.755785	-1.925257	-1.288978	1	-2.832773	-3.081576	0.680590	1	-2.407523	3.103571	0.100184
1	-3.823557	-1.679842	-1.275235	1	-4.074431	-1.924276	0.162820	1	-2.516855	2.082570	1.546313
1	-2.314683	-1.455677	-2.171667	1	-2.847644	-2.480248	-0.995926	1	-1.021713	2.970804	1.197681
1	-2.665638	-3.019100	-1.405464	1	0.382142	-0.119560	2.313375	1	3.269388	1.206480	-1.083560
6	-2.581308	-2.079074	1.124106	1	-2.170620	0.512313	-0.289039	1	-2.385248	-0.115751	-0.053074
1	-2.019189	-1.716735	1.988646	8	-1.943740	1.394335	-0.654661	8	-2.695716	-1.048309	0.035156
1	-3.638883	-1.847138	1.291975	6	-2.988486	2.304247	-0.357554	6	-4.013315	-1.165521	-0.470251
1	-2.482225	-3.177985	1.089487	1	-3.932064	2.021718	-0.843385	1	-4.315100	-2.212081	-0.384304
1	-1.927298	0.722981	-0.002078	1	-3.167510	2.389530	0.722448	1	-4.729557	-0.557623	0.098873
7	-1.718834	1.726929	0.005300	1	-2.694093	3.286140	-0.735056	1	-4.078266	-0.875234	-1.527461
6	-2.326754	2.357456	-1.159694								

1 -3.431085 2.363430 -1.134578		
1 -1.995455 3.398981 -1.241099		
1 -2.013831 1.835708 -2.067826		
6 -2.175762 2.313124 1.258955		
1 -1.753835 1.759934 2.101908		
1 -1.833861 3.351367 1.336642		
1 -3.274752 2.317963 1.371295		
<b>TS-II</b>		<b>TS-Im</b>
Et = -598.8205906 NImag=1 (-1101.14)		Et = -559.9508999 NImag=1(-730.99)

6	-0.315405	0.793310	-0.393408					
6	0.306521	2.160465	-0.044359					
1	-0.543895	0.787779	-1.484117					
1	0.425535	2.225061	1.041949					
6	-0.373117	3.420248	-0.593085	6	0.628859	-0.369128	-0.756318	
1	-1.305626	3.662489	-0.075906	6	0.502967	-1.890924	-0.828249	
1	0.285215	4.286421	-0.481762	1	1.424855	-0.026472	-1.438498	
1	-0.600053	3.321277	-1.659875	1	-0.246313	-2.223710	-0.105439	
8	0.448256	-0.227661	0.016750	6	1.793537	-2.707216	-0.701131	
7	-1.784934	0.590576	0.204234	1	2.190861	-2.715910	0.317212	
6	-1.858401	0.881761	1.641894	1	1.605059	-3.748166	-0.974522	
1	-0.976491	0.459008	2.125142	1	2.578489	-2.332768	-1.365908	
1	-1.894131	1.958592	1.840735	8	-0.572465	0.232349	-1.016800	
1	-2.756304	0.426400	2.072407	7	1.132606	0.190003	0.628074	
6	-2.887773	1.204694	-0.545367	6	0.427964	-0.380650	1.804106	
1	-2.956827	2.284605	-0.386434	1	-0.642254	-0.412613	1.602955	
1	-2.747800	1.023260	-1.613248	1	0.794724	-1.386521	2.016321	
1	-3.838669	0.754852	-0.239322	1	0.614498	0.261914	2.665894	
1	-1.834205	-0.765169	0.068085	6	2.601944	0.218451	0.801202	
1	-0.438413	-1.523815	-0.090910	1	3.005286	-0.783761	0.938743	
7	-1.436926	-1.946255	-0.085961	1	3.058018	0.675500	-0.077257	
6	-1.789660	-2.539560	-1.380536	1	2.840439	0.824104	1.677294	
1	-1.225562	-3.460664	-1.561871	1	0.787893	1.250700	0.506951	
1	-2.857806	-2.773249	-1.419586	1	-0.454897	1.331446	-0.693292	
1	-1.554657	-1.831482	-2.177072	8	-0.041907	2.322900	0.000500	
1	1.322945	2.095935	-0.443034	6	0.330150	3.522012	-0.632211	
6	-1.657197	-2.833258	1.061369	1	-0.555177	4.088334	-0.952531	
1	-1.313618	-2.336378	1.969550	1	0.898151	4.164629	0.054114	
1	-2.720017	-3.071210	1.167159	1	0.955015	3.357501	-1.526207	
1	-1.101719	-3.770657	0.949336	1	0.059163	-2.071234	-1.811740	
1	2.406318	-0.097146	-0.037871	1	-2.022978	-0.521545	-0.223130	
7	3.424605	-0.007115	-0.094316	8	-2.629078	-0.986134	0.388409	
6	4.014168	-0.165225	1.223701	6	-3.943648	-0.482610	0.220940	
1	3.932745	-1.191892	1.630945	1	-4.591085	-1.004961	0.928487	
1	5.080293	0.090091	1.196237	1	-4.003426	0.593748	0.429085	
1	3.527846	0.514585	1.927960	1	-4.327611	-0.662781	-0.791958	
6	3.954977	-0.944599	-1.068415					
1	3.871731	-2.005609	-0.761326					

**Table S61.** The B3LYP/6-311+G\*\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Transition States for Dehydration step (**Step-II**)

TS-II				TS-IIa				TS-IIb			
Et = -328.3547369 NImag=1(-572.60)				Et = -463.5791845 NImag=1(-409.35)				Et = -444.1498509 NImag=1(-258.08)			
6 0.209019	-0.210006	0.536602		6 1.752677	0.368763	-0.231914		6 1.289869	0.396770	-0.385720	
6 1.365828	-0.366834	-0.311785		6 1.987797	-0.916991	0.393881		6 1.924492	-0.554731	0.511072	
1 0.352107	0.263564	1.501346		1 2.154564	0.509847	-1.228918		1 1.470478	0.262183	-1.447524	
1 1.237557	-1.076223	-1.129240		1 1.742151	-0.954676	1.454739		1 1.908109	-0.260384	1.560368	
6 2.711819	-0.495422	0.397942		6 3.329892	-1.572639	0.063471		6 3.298006	-1.052662	0.054949	
1 2.846235	-1.471827	0.874350		1 4.176740	-1.064025	0.534647		1 4.069947	-0.279785	0.120101	
1 3.526419	-0.359351	-0.316702		1 3.330044	-2.609178	0.406969		1 3.612481	-1.892193	0.678036	
1 2.821674	0.277148	1.164107		1 3.497971	-1.589697	-1.017013		1 3.257780	-1.412401	-0.976914	
8 0.247021	1.929315	-0.572325		8 0.036648	-1.156814	-1.373113		8 -0.232069	-1.823671	-0.498645	
7 -1.039614	-0.508732	0.247230		7 1.031138	1.360993	0.216917		7 0.427768	1.324756	-0.092530	
6 -1.417053	-0.974160	-1.088745		6 0.304261	1.324142	1.492797		6 -0.047337	1.599155	1.269700	
1 -1.395149	-0.128523	-1.782696		1 -0.694989	0.899759	1.315193		1 -0.982836	1.048340	1.408886	
1 -0.728613	-1.745118	-1.430074		1 0.848186	0.721941	2.216727		1 0.693778	1.289897	2.001360	

1 -2.420947 -1.395543 -1.042969	1 0.221524 2.344463 1.870098	1 -0.223241 2.671675 1.363580			
6 -2.090212 0.208503 0.970775	6 0.607228 2.421945 -0.699319	6 -0.367358 1.966732 -1.149690			
1 -3.024539 -0.351058 0.922149	1 0.670790 3.389067 -0.197750	1 -0.382387 3.045879 -0.986321			
1 -1.799583 0.335111 2.013106	1 1.243475 2.423756 -1.582295	1 0.071354 1.746725 -2.121199			
1 -2.198736 1.198065 0.509764	1 -0.425033 2.232540 -1.005532	1 -1.377912 1.551893 -1.096486			
1 0.177921 2.880400 -0.710136	1 -0.214380 -1.652057 -2.160201	1 -0.482260 -2.660032 -0.902660			
1 1.230373 0.727469 -0.753748	1 1.140105 -1.442808 -0.219134	1 1.137194 -1.389673 0.347484			
	1 -1.484031 -0.647233 -0.452279	1 -1.441207 -0.965009 -0.179978			
	7 -2.258896 -0.306083 0.148157	8 -2.183434 -0.283668 0.059288			
	6 -3.292837 0.293534 -0.682796	6 -3.394321 -0.972839 0.267726			
	1 -2.852740 1.057341 -1.330318	1 -3.738972 -1.492168 -0.639389			
	1 -3.812876 -0.433771 -1.332705	1 -3.313598 -1.720307 1.071032			
	1 -4.055007 0.778471 -0.060630	1 -4.169167 -0.253778 0.553965			
	6 -2.768580 -1.412280 0.946937				
	1 -1.944726 -1.888108 1.485423				
	1 -3.493223 -1.051435 1.687196				
	1 -3.270058 -2.192905 0.346823				
<b>TS-IIc</b> Et =-463.5736391 NIImg=1(-597.10)		<b>TS-IIId</b> Et =-444.1515521 NIImg=1(-120.37)		<b>TS-IIe</b> Et =-598.8027708 NIImg=1 (-88.80)	
6 -1.143932 0.798510 -0.351039	6 1.181479 .553242 .123271	6 -0.403909 1.278776 0.448256			
6 -0.084582 1.435907 0.360679	6 .367604 1.525201 -.635786	6 0.025721 2.160473 -0.652654			
1 -1.154450 0.885460 -1.431502	1 1.628022 .845694 1.065182	1 -1.396105 0.839185 0.394632			
6 0.477123 2.713688 -0.267445	1 .704630 1.548805 -1.680022	1 0.937251 2.714092 -0.423371			
1 -0.184289 3.575491 -0.132462	6 .366867 2.924268 -.018058	6 -1.090480 3.091480 -1.147153			
1 1.442202 2.964554 0.179718	1 1.365189 3.372546 .000061	1 -1.383132 3.825067 -0.390433			
1 0.640661 2.582356 -1.341044	1 -.284526 3.587195 -.590753	1 -0.752252 3.637496 -2.030100			
8 -0.000185 -1.484932 -1.290211	1 -.014406 2.889443 1.005222	1 -1.976592 2.519430 -1.431632			
7 -2.098328 0.030166 0.134440	8 -.506945 -.259683 1.809371	8 -0.062805 -0.550379 -1.259903			
6 -2.149985 -0.346412 1.543969	7 1.432703 -.655704 -.270575	7 0.282606 0.961736 1.501908			
1 -1.470565 -1.182290 1.738630	6 .787277 -1.233253 -1.463707	6 1.678508 1.364847 1.733229			
1 -1.873433 0.497086 2.174807	1 .976446 -.598452 -2.330416	1 2.332126 0.668133 1.187513			

1 -3.166888 -0.649664 1.792503	1 1.212123 -2.219143 -1.642034	1 1.840469 2.383307 1.386861
6 -2.844904 -0.830110 -0.794246	1 -.298298 -1.277132 -1.264683	1 1.873336 1.319579 2.804624
1 -3.770576 -1.155520 -0.318670	6 2.115889 -1.599784 .619758	6 -0.229975 -0.070249 2.412176
1 -3.086254 -0.265052 -1.694887	1 2.897944 -2.121660 .065336	1 -0.198650 0.300835 3.438529
1 -2.186420 -1.664558 -1.062683	1 2.547799 -1.063697 1.461651	1 -1.248448 -0.327087 2.127379
1 1.185581 -1.044065 -0.542194	1 1.382035 -2.312523 .999342	1 0.403670 -0.956067 2.326006
1 0.175180 -2.008397 -2.078072	1 -1.023094 .108107 2.532015	1 -1.839165 -0.899540 -0.593250
7 1.898564 -0.494793 0.107642	1 -1.179700 -.363105 .946190	1 0.254637 1.401006 -1.429699
1 0.845032 0.583357 0.284802	8 -1.801965 -.414177 -.265216	1 1.721195 -0.776425 -0.747346
1 -0.246242 1.525915 1.436223	6 -3.165073 -.696393 -.237149	7 2.704098 -0.865890 -0.424101
6 3.088092 -0.093018 -0.630791	1 -3.710369 -.111712 .529446	6 2.957918 -2.243275 -0.025032
1 3.708651 0.596102 -0.044314	1 -3.649289 -.468818 -1.202529	1 2.206868 -2.562679 0.703010
1 3.716945 -0.953639 -0.907612	1 -3.378371 -1.761085 -.022902	1 2.930596 -2.957954 -0.867490
1 2.789395 0.410695 -1.553395	1 -.658043 1.086663 -.660299	1 3.943846 -2.332406 0.446996
6 2.196192 -1.226646 1.329309		6 3.602370 -0.425686 -1.483274
1 2.759034 -2.152210 1.134966		1 3.323897 0.579810 -1.809893
1 2.786046 -0.617005 2.026125		1 4.636450 -0.388100 -1.119704
1 1.262190 -1.508289 1.823565		1 3.587669 -1.081227 -2.372288
<b>TS-IIIIf</b>		
Et =-559.9417843 NImag=1 (-193.92)	Et =-559.9398519 NImag=1 (-187.01)	Et =-559.9377426 NImag=1 (-63.33)
6 0.975055 -1.126030 0.386943	6 1.789698 0.031594 0.056873	6 1.563511 -0.438975 0.120883

6	1.426423	-1.228775	-0.973914	6	1.558355	1.486984	-0.173375	6	1.859367	0.978911	0.232125
1	1.505287	-0.424464	1.026514	1	2.413724	-0.277804	0.883245	1	1.553701	-1.057112	1.015044
1	0.995519	-2.053558	-1.542320	1	2.021086	1.754117	-1.133422	1	2.365820	1.366981	-0.657442
6	2.928568	-1.051077	-1.198437	6	2.130832	2.359477	0.945716	6	2.553482	1.394548	1.528953
1	3.504536	-1.927291	-0.884990	1	3.213099	2.234431	1.047060	1	3.582718	1.027627	1.590902
1	3.128971	-0.882638	-2.258683	1	1.936044	3.413367	0.737884	1	2.585033	2.483379	1.603869
1	3.300109	-0.180679	-0.651890	1	1.667650	2.110837	1.901971	1	2.007871	1.022991	2.400276
8	0.035054	1.069400	-1.479886	8	0.354965	-0.431934	1.892580	8	-0.342675	-1.815802	2.092026
7	-0.123275	-1.611913	0.899656	7	1.427698	-0.909337	-0.756961	7	1.131606	-1.023927	-0.957505
6	-1.038924	-2.498253	0.171333	6	0.568103	-0.703132	-1.932159	6	0.920531	-0.275467	-2.208673
1	-1.797268	-1.882477	-0.321584	1	1.035919	-1.190338	-2.790646	1	0.582899	-0.970724	-2.974239
1	-0.490748	-3.088863	-0.559196	1	-0.403424	-1.146635	-1.707074	1	0.168564	0.502870	-2.021645
1	-1.512121	-3.168539	0.890384	1	0.422597	0.353853	-2.127163	1	1.857185	0.183947	-2.530767
6	-0.653428	-1.083108	2.162614	6	1.638747	-2.317953	-0.404007	6	0.635969	-2.406157	-0.926470
1	-0.867022	-1.907490	2.846517	1	2.066016	-2.846224	-1.258730	1	1.159829	-2.996198	-1.681537
1	0.070541	-0.402158	2.604660	1	2.304258	-2.388530	0.453374	1	0.785933	-2.826434	0.065126
1	-1.570281	-0.532670	1.937909	1	0.667930	-2.744300	-0.144344	1	-0.435124	-2.387977	-1.135531
1	0.075136	1.563085	-2.304567	1	0.037047	0.188675	2.554848	1	-0.688313	-1.742749	2.985220
1	-1.441965	0.629726	-0.944552	1	-0.528500	-0.721516	1.258327	1	-0.977596	-1.323093	1.508550
8	-2.282599	0.269456	-0.526780	8	-1.447722	-1.034210	0.377864	8	-1.816812	-0.501016	0.279961
6	-3.355459	1.137329	-0.828220	6	-2.506856	-1.797670	0.883034	6	-3.221941	-0.528112	0.134419
1	-3.529158	1.222282	-1.910515	1	-3.229900	-1.197388	1.463954	1	-3.723288	0.174903	0.814647
1	-4.264874	0.735113	-0.372452	1	-3.075418	-2.281716	0.072874	1	-3.526131	-0.280023	-0.891557
1	-3.194021	2.148672	-0.429306	1	-2.154352	-2.601319	1.551952	1	-3.587107	-1.535232	0.360639
1	0.863308	-0.238761	-1.367736	1	0.480560	1.654149	-0.296527	1	0.789983	1.435804	0.128008
1	0.788449	1.679382	-0.131124	1	-1.686626	0.390727	-0.351444	1	-1.430988	0.444633	-0.002083
8	1.252815	1.815330	0.744959	8	-1.644360	1.282858	-0.817128	8	-0.754118	1.637738	-0.434806
6	1.279439	3.191976	1.060534	6	-2.821327	2.014127	-0.544369	6	-1.437846	2.847758	-0.306741
1	1.820719	3.779732	0.305649	1	-2.955678	2.202745	0.530735	1	-1.843975	3.008814	0.709274
1	0.269519	3.613623	1.161928	1	-2.752903	2.981082	-1.050923	1	-0.785468	3.711363	-0.525411
1	1.796076	3.315503	2.016308	1	-3.721384	1.502876	-0.914039	1	-2.292395	2.921325	-1.003222

TS-IIh				TS-IIIi				
Et = -598.7958519 NIImg=1 (-413.60 )				Et = -559.9364032 NIImg=1 (-43.93)				
6	-2.521113	-0.514165	-0.315836	6	-1.706916	0.691111	-0.021195	
6	-2.903198	0.393914	0.748242	6	-0.599834	1.613899	-0.365319	
1	-2.936554	-0.306461	-1.295215	1	-2.591991	0.686068	-0.646065	
1	-2.599822	0.082247	1.746743	6	-1.007162	2.667024	-1.398513	
6	-4.353944	0.880605	0.690878	1	-1.800798	3.322170	-1.027133	
1	-5.074990	0.095880	0.940143	1	-0.149861	3.294244	-1.648883	
1	-4.495804	1.701856	1.396454	1	-1.353883	2.195075	-2.321414	
1	-4.593650	1.263827	-0.304994	8	-1.224875	-1.224501	-1.640755	
8	-1.254724	1.689117	-0.875717	7	-1.731633	-0.120060	0.983860	
7	-1.664110	-1.498045	-0.281712	6	-0.574018	-0.355715	1.862762	
6	-0.929965	-1.931842	0.912591	1	0.066901	-1.096551	1.369165	
1	0.137197	-1.709842	0.778571	1	0.015856	0.548654	1.986235	
1	-1.310726	-1.429966	1.796329	1	-0.939533	-0.709042	2.826078	
1	-1.060989	-3.011262	1.026744	6	-2.829047	-1.085313	1.126544	
6	-1.202751	-2.119582	-1.526040	1	-3.194868	-1.065728	2.154337	
1	-1.256401	-3.206581	-1.434666	1	-3.632230	-0.837816	0.436618	
1	-1.822403	-1.787868	-2.356512	1	-2.448012	-2.078117	0.882827	
1	-0.167065	-1.824256	-1.707189	1	-1.155600	-1.391632	-2.584453	
1	-1.346700	2.461006	-1.445212	1	-0.240133	-1.207347	-1.266745	
1	-2.213247	1.254783	0.353958	8	1.068417	-1.095204	-0.622422	
1	0.524097	1.707777	-0.396571	6	1.926559	-2.100823	-1.081864	
7	1.525493	1.767506	-0.125641	1	2.595088	-2.473211	-0.285879	
6	2.267553	2.380108	-1.221533	1	1.373780	-2.979738	-1.459354	
1	2.086384	1.823759	-2.144760	1	2.579242	-1.761312	-1.907268	
1	1.987771	3.433364	-1.402298	1	-0.190872	2.073171	0.539432	
1	3.345041	2.357322	-1.018502	1	0.215093	0.979110	-0.745995	
6	1.631754	2.542889	1.104830	8	2.238167	0.599759	1.016846	
1	0.995011	2.100559	1.875507	1	1.861968	-0.063370	0.360332	
1	2.663981	2.537991	1.475451	6	3.565199	0.920482	0.660902	

1	1.327286	3.597386	0.983431	1	3.637669	1.331710	-0.356995
1	2.094143	-0.197224	0.161540	1	3.935522	1.678521	1.357380
7	2.331148	-1.189396	0.306374	1	4.235732	0.051142	0.721515
6	3.062115	-1.689610	-0.850891				
1	3.185128	-2.776970	-0.783629				
1	2.503695	-1.470528	-1.765013				
1	4.069576	-1.250566	-0.960349				
6	3.084255	-1.336975	1.545803				
1	2.532810	-0.878101	2.370621				
1	3.221270	-2.398426	1.783049				
1	4.086809	-0.875149	1.510697				

**Table S62.** The PCM-B3LYP/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Transition States for Carbinolamine Formation (**Step-I**)

TS-I				TS-Ia				TS-Ib			
Et = -328.2646744 NImag=1 (-1592.18)				Et = -463.4175539 NImag=1 (-480.75)				Et = -444.0003013 NImag=1(-1605.69)			
6	-0.306445	0.743664	-0.416740	6	1.850130	0.335283	-0.180640	6	-0.269602	-0.040859	-0.353908
6	-1.598540	0.256421	0.240661	6	1.919232	-1.021910	0.326139	6	-0.061587	1.346741	0.247616
1	-0.364438	0.530464	-1.507553	1	2.327479	0.531314	-1.136795	1	-0.319392	0.048056	-1.456154
1	-1.502670	0.307803	1.331277	1	1.618628	-1.133379	1.370198	1	-0.201949	1.308193	1.333751
6	-2.069421	-1.129965	-0.211665	6	3.191273	-1.797421	-0.017393	6	-0.922736	2.446946	-0.381508
1	-1.364778	-1.920163	0.074452	1	4.062213	-1.452703	0.553049	1	-1.994201	2.281323	-0.215552
1	-3.038091	-1.380824	0.233846	1	3.053040	-2.861861	0.198575	1	-0.674854	3.425958	0.041882
1	-2.185359	-1.171731	-1.301546	1	3.429727	-1.707953	-1.084060	1	-0.762285	2.504101	-1.464982
8	0.117276	1.990668	-0.081839	8	-0.043066	-0.737827	-1.400273	8	0.585734	-1.030309	0.093983
7	1.032476	0.004299	0.023818	7	1.172819	1.344263	0.309844	7	-1.574862	-0.807982	0.041965
6	1.058413	-0.558388	1.385073	6	0.374220	1.247704	1.538684	6	-2.223788	-0.425828	1.309851
1	0.648226	0.182853	2.073857	1	-0.618470	0.833152	1.301092	1	-1.466030	-0.371041	2.093514
1	0.482083	-1.487415	1.451874	1	0.883660	0.610921	2.262896	1	-2.742483	0.535115	1.226744

1 2.095809 -0.764271 1.664861	1 0.275202 2.250680 1.961619	1 -2.949476 -1.198977 1.576747
6 1.685926 -0.856132 -0.975808	6 0.775231 2.408062 -0.616523	6 -2.535885 -1.063339 -1.045382
1 1.158091 -1.811169 -1.080311	1 0.520229 3.311771 -0.060048	1 -3.089662 -0.153778 -1.305273
1 1.691575 -0.342809 -1.940794	1 1.595158 2.625378 -1.305216	1 -1.994706 -1.419475 -1.925342
1 2.717533 -1.053748 -0.669749	1 -0.086850 2.040433 -1.188548	1 -3.245219 -1.832298 -0.727027
1 1.230244 1.214970 0.055898	1 -0.329875 -1.130511 -2.242310	1 -0.615507 -1.580992 0.234856
1 -2.353363 1.007003 -0.027255	1 1.015356 -1.351668 -0.368037	1 2.156072 -0.465571 0.556807
	1 -1.506122 -0.474419 -0.449715	8 3.048145 -0.049070 0.669856
	7 -2.316860 -0.290642 0.187586	6 3.804803 -0.406973 -0.465441
	6 -3.353900 0.421568 -0.538141	1 3.325143 -0.108881 -1.412493
	1 -2.925976 1.314004 -1.010008	1 4.772204 0.105741 -0.405406
	1 -3.841834 -0.177404 -1.335032	1 4.004996 -1.490747 -0.523292
	1 -4.151067 0.753539 0.143496	1 1.003118 1.564058 0.099387
	6 -2.791726 -1.552392 0.728365	
	1 -1.951178 -2.099684 1.170014	
	1 -3.536874 -1.383506 1.519884	
	1 -3.266379 -2.216207 -0.023828	
TS-Id	TS-Id	TS-Id
Et =-463.4601171 NImag=1(-1121.86)	Et =-444.0273752 NImag=1(-766.37)	Et =-598.615733 NImag=1 (-1601.36)
6 -0.828986 -0.771837 0.151475	6 0.413536 -0.727169 -0.122490	6 -0.177439 0.866122 -0.396821
6 -2.309328 -0.964939 -0.256995	6 1.880216 -1.075560 0.143193	6 0.878320 1.644790 -1.177382
1 -0.776783 -0.808125 1.272032	1 0.199811 -0.796191 -1.207640	1 -1.176914 1.255445 -0.656101
1 -2.401674 -0.780257 -1.334666	1 2.097736 -0.910501 1.205069	1 1.878598 1.400603 -0.804880
6 -3.387379 -0.198356 0.518241	6 2.943651 -0.417929 -0.743330	6 0.650324 3.160627 -1.210211
1 -3.425999 0.862924 0.250574	1 3.104253 0.637906 -0.500249	1 0.713724 3.612351 -0.213343
1 -4.381055 -0.614945 0.314332	1 3.906808 -0.922795 -0.613126	1 1.398443 3.653488 -1.840228
1 -3.223138 -0.261415 1.601575	1 2.680572 -0.482711 -1.806063	1 -0.338461 3.402077 -1.618826
8 -0.022877 -1.606291 -0.494135	8 -0.408244 -1.460662 0.660419	8 -0.092961 -0.520612 -0.475994
7 -0.308238 0.734677 -0.084380	7 0.047037 0.807885 0.145948	7 -0.107890 0.930044 1.159869
6 -0.490234 1.164830 -1.474880	6 0.430345 1.259490 1.504356	6 1.166179 1.342698 1.781479
1 -0.237901 0.315264 -2.115381	1 0.156981 0.467383 2.202683	1 1.984697 0.767265 1.339821

1 -1.523516 1.479039 -1.677954	1 1.504231 1.456543 1.554156	1 1.345545 2.416367 1.657082			
1 0.174127 2.006672 -1.705319	1 -0.118534 2.172928 1.747812	1 1.112310 1.119293 2.850971			
6 -0.723604 1.755454 0.883221	6 0.408450 1.775193 -0.915772	6 -1.302282 1.500261 1.813263			
1 -1.743505 2.117865 0.706977	1 1.476353 1.996352 -0.896258	1 -1.334599 2.589830 1.692976			
1 -0.674271 1.337426 1.894070	1 0.141179 1.354087 -1.887947	1 -2.190849 1.045045 1.365288			
1 -0.045494 2.617015 0.830051	1 -0.153101 2.700660 -0.759451	1 -1.270383 1.264644 2.881063			
1 1.028972 0.449428 0.073022	1 -1.044796 0.687668 0.152608	1 -0.136789 -0.278122 0.826133			
1 1.453784 -1.092370 -0.089085	1 -1.464165 -0.981779 0.528885	1 0.829009 1.245642 -2.198467			
7 2.071902 -0.232985 0.131228	8 -2.362366 -0.093730 0.352664	1 1.854604 -1.100430 -0.333720			
6 2.680349 -0.290951 1.466845	6 -3.145149 -0.345205 -0.782852	7 2.828577 -1.226390 -0.039823			
1 3.450794 -1.070378 1.517502	1 -3.893484 -1.136001 -0.596838	6 2.920849 -2.392087 0.829364			
1 3.140521 0.671267 1.717344	1 -3.703703 0.555892 -1.086461	1 3.924961 -2.453311 1.269749			
1 1.905520 -0.515417 2.205370	1 -2.557928 -0.669883 -1.664859	1 2.200877 -2.297746 1.649795			
1 -2.474292 -2.042145 -0.128787	1 1.917114 -2.162535 0.002751	1 2.728480 -3.353913 0.315518			
6 3.025156 0.033046 -0.954047		6 3.683482 -1.342566 -1.213740			
1 2.495194 -0.015866 -1.908729		1 3.520263 -0.484994 -1.875507			
1 3.467491 1.028778 -0.839563		1 4.739106 -1.336130 -0.911035			
1 3.832751 -0.709760 -0.961375		1 3.516775 -2.265510 -1.802468			
		1 -2.078662 -0.936766 -0.442323			
		7 -3.074345 -0.873570 -0.206712			
		6 -3.855971 -0.697382 -1.423319			
		1 -3.847141 -1.576110 -2.097278			
		1 -4.904586 -0.494148 -1.168154			
		1 -3.476219 0.163088 -1.985194			
		6 -3.468699 -2.061338 0.538947			
		1 -3.450659 -2.994795 -0.056701			
		1 -2.801329 -2.195292 1.397378			
		1 -4.490081 -1.940318 0.923585			
<b>TS-If</b>		<b>TS-Ig</b>		<b>TS-Ih</b>	
Et =-559.735774 NImag= 1(-1603.67)		Et =-598.6407093 NImag=1( -727.93)		Et =-559.7671932 NImag=1(-441.61)	
6 -0.123254 -0.745637 -0.536563		6 -1.092856 -0.704904 0.277267		6 0.947764 -0.328773 -0.644634	

6	-1.451156	-1.043013	-1.221290	6	-2.396539	-1.531847	0.507707	6	2.427909	-0.521232	-0.997269
1	0.626886	-1.482541	-0.857757	1	-0.524557	-0.771569	1.246355	1	0.408209	-0.010379	-1.552475
1	-2.241242	-0.402494	-0.817470	1	-2.053016	-2.487772	0.928122	1	2.411515	-1.217853	-1.844711
6	-1.855837	-2.521846	-1.185491	6	-3.203548	-1.832765	-0.758522	6	3.320214	-1.112203	0.100354
1	-2.041186	-2.879655	-0.166171	1	-2.512099	-2.130647	-1.552558	1	2.842306	-1.987195	0.549409
1	-2.774000	-2.683032	-1.759716	1	-3.920956	-2.644911	-0.588336	1	4.279072	-1.425715	-0.326101
1	-1.075099	-3.155970	-1.622424	1	-3.770394	-0.965338	-1.113722	1	3.541363	-0.395433	0.897845
8	0.346301	0.577844	-0.676563	8	-0.409706	-1.032760	-0.802197	8	0.415574	-1.438990	-0.073869
7	-0.079661	-0.740627	1.007824	7	-1.360886	0.866878	0.285087	7	0.671003	0.913018	0.298569
6	-1.356669	-0.586085	1.732886	6	-2.111166	1.328320	-0.887555	6	0.995128	0.686839	1.731823
1	-1.901655	0.260404	1.308812	1	-1.766675	0.746019	-1.745162	1	0.730199	-0.342399	1.972088
1	-1.964866	-1.495380	1.682322	1	-3.194749	1.191291	-0.764882	1	2.056454	0.859280	1.917739
1	-1.128914	-0.373234	2.780927	1	-1.925619	2.395810	-1.066333	1	0.398760	1.378002	2.332414
6	0.841286	-1.725823	1.606185	6	-1.910433	1.397831	1.533647	6	1.213116	2.195657	-0.210787
1	0.437957	-2.742831	1.534353	1	-2.973175	1.146522	1.664644	1	2.297901	2.228292	-0.089380
1	1.797406	-1.664276	1.079939	1	-1.352032	0.983891	2.380926	1	0.958244	2.298329	-1.268694
1	0.991332	-1.477749	2.660481	1	-1.818422	2.491395	1.557019	1	0.761396	3.018921	0.348728
1	0.401628	0.368310	0.603058	1	-0.008051	1.269817	0.116364	1	-0.417347	1.002741	0.262814
1	-1.058468	1.696521	-0.573558	1	1.265582	-1.331060	-0.211313	1	-0.644013	-1.453936	-0.246073
8	-1.883398	2.166797	-0.303461	7	2.228258	-1.164024	0.156023	8	-2.043888	-1.294753	-0.442107
6	-1.509939	3.409562	0.261489	6	3.206619	-1.558010	-0.853999	6	-2.763060	-2.136196	0.420592
1	-1.020439	4.074151	-0.468314	1	2.962348	-1.080174	-1.808486	1	-2.382453	-2.128095	1.460018
1	-2.421794	3.906255	0.609695	1	4.213299	-1.234792	-0.557450	1	-3.827738	-1.850501	0.467067
1	-0.834092	3.300273	1.125116	1	3.245070	-2.649860	-1.020627	1	-2.725022	-3.181976	0.073355
1	-1.311674	-0.729049	-2.263399	1	-3.029393	-1.076307	1.283110	1	2.852013	0.411743	-1.387827
1	2.097687	0.272117	-0.885871	1	1.662496	0.608697	0.134580	1	-2.103367	-0.076219	-0.037789
8	2.996547	-0.117215	-0.764688	7	1.165651	1.509646	-0.092586	8	-1.959648	1.013395	0.291808
6	3.811775	0.873254	-0.167871	6	1.682764	2.608853	0.743848	6	-2.632464	1.865605	-0.608824
1	3.411048	1.235289	0.793080	1	1.131283	3.529177	0.528776	1	-2.389501	2.914505	-0.387701
1	4.793357	0.427374	0.025067	1	1.549537	2.352187	1.798152	1	-2.367900	1.674856	-1.663333
1	3.960930	1.748034	-0.821313	1	2.747517	2.781152	0.550422	1	-3.725056	1.756514	-0.521565

	6 2.431495 -1.866357 1.419748 1 1.652305 -1.578096 2.132540 1 2.410892 -2.966378 1.316139 1 3.404942 -1.595710 1.850264 6 1.324736 1.733158 -1.545693 1 0.889146 0.866882 -2.046986 1 0.792059 2.641969 -1.841348 1 2.382718 1.836705 -1.810991	
<b>TS-Ii</b> Et = -598.6148138 NImag=1(-1591.67)	<b>TS-Ij</b> Et = -559.7374909 NImag=1(-1605.91)	<b>TS-Ik</b> Et = -559.7635751 NImag=1 (-734.05)
6 1.848396 -0.924484 0.219423 6 1.372817 -0.280033 1.520782 1 2.800312 -1.457700 0.413556 1 0.544411 0.406526 1.315760 6 2.477484 0.403234 2.335394 1 2.916336 1.256897 1.806102 1 2.086121 0.777001 3.287738 1 3.290775 -0.296730 2.563304 8 0.920496 -1.670275 -0.472216 7 2.170781 0.053243 -0.971387 6 1.632390 1.428064 -0.924689 1 0.581125 1.417259 -0.619330 1 2.210268 2.055841 -0.236767 1 1.706568 1.856274 -1.929239 6 3.556576 -0.002086 -1.468222 1 4.241677 0.514990 -0.786151 1 3.863117 -1.047029 -1.563438 1 3.608342 0.475918 -2.450680 1 1.369714 -0.800186 -1.384552 1 0.947805 -1.105677 2.106201 1 -0.977163 -1.502938 -0.174173	6 1.343400 -0.869871 -0.163710 6 0.770459 -0.852992 1.250680 1 2.261526 -1.483673 -0.171594 1 -0.051198 -0.133299 1.324144 6 1.815795 -0.612366 2.346751 1 2.274214 0.380370 2.270875 1 1.359218 -0.684973 3.339387 1 2.621712 -1.354581 2.296435 8 0.463880 -1.210297 -1.187538 7 1.758077 0.497710 -0.786312 6 1.174222 1.727826 -0.211079 1 0.102784 1.594147 -0.040016 1 1.665153 1.995086 0.731224 1 1.325502 2.541315 -0.926707 6 3.188712 0.640923 -1.109809 1 3.784871 0.805182 -0.204513 1 3.537737 -0.264608 -1.612562 1 3.321458 1.494469 -1.780283 1 1.001416 -0.080883 -1.607153 1 -1.165238 -1.078827 -0.965652 8 -2.154798 -0.963168 -0.838554	6 1.382583 0.622781 -0.368909 6 2.671069 0.068024 -0.981729 1 1.618124 1.372327 0.413541 1 2.421347 -0.781730 -1.628062 6 3.825528 -0.280191 -0.035355 1 3.654569 -1.206933 0.521967 1 4.749653 -0.420202 -0.606141 1 4.007587 0.520876 0.691358 8 0.516557 1.025005 -1.307214 7 0.584506 -0.470124 0.543016 6 0.226493 -1.694590 -0.220155 1 -0.010037 -1.380235 -1.237762 1 1.068155 -2.390575 -0.218378 1 -0.657856 -2.146143 0.232742 6 1.121211 -0.756536 1.895933 1 1.984664 -1.418001 1.829653 1 1.413659 0.183209 2.370643 1 0.342561 -1.237731 2.494114 1 -0.303086 0.081812 0.662742 1 -0.520462 1.283080 -0.729164 8 -1.439202 1.263010 0.062943

7	-1.999244	-1.420213	-0.080824	6	-2.663984	-2.147377	-0.248440	6	-1.710186	2.515228	0.646413
6	-2.628585	-1.971627	-1.275086	1	-2.220315	-2.353919	0.737652	1	-2.356298	3.136198	0.003785
1	-3.710175	-1.783853	-1.253380	1	-3.743710	-2.023492	-0.116777	1	-2.228348	2.388950	1.608214
1	-2.218940	-1.481376	-2.164811	1	-2.494526	-3.023749	-0.890751	1	-0.789836	3.092383	0.838776
1	-2.484838	-3.062907	-1.389759	1	0.322784	-1.845617	1.390149	1	2.993172	0.866864	-1.660509
6	-2.423510	-2.107535	1.132839	1	-2.191954	0.473561	0.145026	1	-2.504626	-0.085116	0.236851
1	-1.868788	-1.713423	1.991271	8	-2.079160	1.301462	0.675674	8	-2.924550	-0.972877	0.371565
1	-3.492177	-1.931180	1.312734	6	-2.987354	2.264082	0.175393	6	-3.631312	-1.291095	-0.810006
1	-2.270394	-3.203134	1.100499	1	-2.824279	2.490564	-0.890403	1	-4.088168	-2.278124	-0.675790
1	-1.939359	0.666640	-0.013343	1	-4.037580	1.953704	0.297593	1	-4.439830	-0.573491	-1.025863
7	-1.757398	1.679553	-0.025157	1	-2.842994	3.189935	0.742736	1	-2.981225	-1.339388	-1.699342
6	-2.385814	2.265319	-1.201557								
1	-3.492970	2.239716	-1.180266								
1	-2.087405	3.317352	-1.304557								
1	-2.053294	1.733581	-2.099927								
6	-2.241845	2.274793	1.212616								
1	-1.803869	1.751429	2.069622								
1	-1.933907	3.327485	1.270196								
1	-3.343682	2.249469	1.323703								
<b>TS-Im</b> Et = -559.7620837 NImag=1(-628.11)											

6	0.863918	0.002667	-0.762219
6	1.768400	-1.228391	-0.832989
1	1.306884	0.826964	-1.347895
1	1.347154	-2.018286	-0.200157
6	3.256700	-1.022571	-0.529735
1	3.450861	-0.845792	0.533672
1	3.823207	-1.915977	-0.812264
1	3.671209	-0.178414	-1.093674
8	-0.404816	-0.313097	-1.192465
7	0.733499	0.644470	0.662087
6	0.486193	-0.334525	1.752709
1	-0.289384	-1.034497	1.433057
1	1.405693	-0.872623	1.998522
1	0.144054	0.212777	2.635013
6	1.791882	1.624045	1.008452
1	2.745167	1.125853	1.192898
1	1.905755	2.336210	0.187923
1	1.487686	2.162716	1.909860
1	-0.234459	1.209734	0.508057
1	-1.064048	0.548976	-0.867718
8	-1.527088	1.507434	-0.086113
6	-1.707015	2.754331	-0.705200
1	-2.580941	2.746146	-1.377597
1	-1.883339	3.545306	0.042042
1	-0.839172	3.074079	-1.314198
1	1.656251	-1.582779	-1.864484
1	-1.288528	-1.689742	-0.413863
8	-1.802946	-2.260116	0.201972
6	-3.080440	-1.651762	0.343968
1	-3.566660	-2.092676	1.221291
1	-3.004073	-0.565343	0.487013
1	-3.726823	-1.840444	-0.529172

**Table S63.** The PCM-B3LYP/6-31G\* Optimized Geometries (in Cartesian coordinates), Total Electronic Energies (in hartree/particle), and Number of Imaginary Frequencies ( $\text{cm}^{-1}$ ) of Transition States for Dehydration Step (**Step-II**)

TS-II			TS-IIa			TS-IIb					
	Et = -328.2348707	NImag = 1(-1104.19)		Et = -463.4175539	NImag = 1(		Et = -443.9854632	NImag = 1(-281.89)			
6	0.209574	-0.101244	0.519864	6	1.850130	0.335283	-0.180640	6	1.393777	0.486965	-0.317948
6	1.369601	-0.393376	-0.292605	6	1.919232	-1.021910	0.326139	6	1.871096	-0.655685	0.447547
1	0.359927	0.499808	1.412258	1	2.327479	0.531314	-1.136795	1	1.742022	0.580315	-1.344066
1	1.230075	-1.187903	-1.028286	1	1.618628	-1.133379	1.370198	1	1.709839	-0.566885	1.524691
6	2.711761	-0.460153	0.431323	6	3.191273	-1.797421	-0.017393	6	3.279803	-1.137712	0.095702
1	2.833317	-1.376867	1.022850	1	4.062213	-1.452703	0.553049	1	4.057292	-0.447702	0.443881
1	3.534310	-0.422748	-0.290926	1	3.053040	-2.861861	0.198575	1	3.467693	-2.111985	0.557608
1	2.836506	0.392688	1.110303	1	3.429727	-1.707953	-1.084060	1	3.395961	-1.259956	-0.987756
8	0.194597	1.853662	-0.816868	8	-0.043066	-0.737827	-1.400273	8	-0.327668	-1.378365	-0.933700
7	-1.045140	-0.474789	0.317426	6	0.374220	1.247704	1.538684	6	-0.193424	1.306661	1.340304
6	-1.427711	-1.186435	-0.901766	1	-0.618470	0.833152	1.301092	1	-0.997267	0.554662	1.295231
1	-1.437937	-0.494132	-1.752825	1	0.883660	0.610921	2.262896	1	0.522204	1.049518	2.122429
1	-0.726215	-1.997887	-1.101127	1	0.275202	2.250680	1.961619	1	-0.603044	2.297403	1.548054
1	-2.424735	-1.610624	-0.764537	6	0.775231	2.408062	-0.616523	6	-0.196413	2.134022	-1.001284
6	-2.077248	0.398957	0.879084	1	0.520229	3.311771	-0.060048	1	-0.491520	3.105437	-0.599482
1	-3.048708	-0.098509	0.846359	1	1.595158	2.625378	-1.305216	1	0.469067	2.276980	-1.854698
1	-1.832663	0.638072	1.917431	1	-0.086850	2.040433	-1.188548	1	-1.079123	1.568481	-1.321805
1	-2.078383	1.327137	0.288796	1	-0.329875	-1.130511	-2.242310	1	-0.554377	-2.101073	-1.540872
1	0.619947	2.584559	-0.333658	1	1.015356	-1.351668	-0.368037	1	1.053556	-1.367517	0.021451
1	1.177895	0.694143	-0.829082	1	-1.506122	-0.474419	-0.449715	1	-1.458338	-1.254089	0.005131
				7	-2.316860	-0.290642	0.187586	8	-2.250233	-1.063917	0.677452
				6	-3.353900	0.421568	-0.538141	6	-3.328988	-0.606691	-0.089887

	1 -2.925976 1.314004 -1.010008 1 -3.841834 -0.177404 -1.335032 1 -4.151067 0.753539 0.143496 6 -2.791726 -1.552392 0.728365 1 -1.951178 -2.099684 1.170014 1 -3.536874 -1.383506 1.519884 1 -3.266379 -2.216207 -0.023828	1 -3.154215 0.382351 -0.558002 1 -3.597368 -1.298633 -0.909491 1 -4.216714 -0.503452 0.551029
<b>TS-IIc</b> Et =-463.4104 NImag=1(-920.97)	<b>TS-IId</b> Et =-443.9941529 NImag=1(-61.73)	<b>TS-IIe</b> HF = -598.6014211 NImag = 1 (-119.3)
6 -1.053673 0.642241 -0.435531 6 -0.130419 1.481479 0.256184 1 -0.831793 0.398917 -1.469663 6 0.473270 2.639731 -0.542446 1 -0.222586 3.480795 -0.652990 1 1.373822 3.017364 -0.046208 1 0.762459 2.311826 -1.547895 8 0.384186 -1.358937 -1.624000 7 -2.060830 -0.047917 0.072548 6 -2.527086 0.095305 1.448289 1 -2.010478 -0.607479 2.114738 1 -2.357500 1.113403 1.802175 1 -3.599468 -0.114914 1.481339 6 -2.621321 -1.154342 -0.714895 1 -3.535447 -0.842509 -1.232971 1 -1.838540 -1.475438 -1.412367 1 -2.866095 -1.980749 -0.040190 1 1.293485 -0.929977 -0.637603 1 0.308699 -2.316325 -1.475113 7 1.870127 -0.447837 0.240679 1 0.829072 0.636908 0.356569 1 -0.406654 1.756986 1.277621	6 0.983717 0.847552 0.130598 6 -0.176524 1.455234 -0.502478 1 1.318537 1.206738 1.099497 1 -0.045947 1.533147 -1.589728 6 -0.626518 2.774593 0.126683 1 0.098904 3.583637 -0.022514 1 -1.576466 3.095126 -0.312470 1 -0.787103 2.654081 1.203979 8 -0.423493 -0.647486 2.033720 7 1.630247 -0.183835 -0.340793 6 1.168837 -0.880419 -1.555115 1 1.200494 -0.198155 -2.409986 1 1.837532 -1.720128 -1.748114 1 0.133252 -1.216104 -1.377733 6 2.642392 -0.867266 0.466220 1 3.522686 -1.076351 -0.147418 1 2.927069 -0.240420 1.312246 1 2.226262 -1.808575 0.840902 1 -0.130534 -1.537641 2.282968 1 -0.976131 -0.807877 1.192637 8 -1.601756 -0.899266 -0.278975 6 -2.959114 -1.128952 -0.384832	6 -0.335766 1.362016 0.371845 6 0.075974 2.174872 -0.790624 1 -1.333814 0.932692 0.362121 1 1.019086 2.704165 -0.631679 6 -1.031365 3.130626 -1.263593 1 -1.250971 3.909274 -0.524305 1 -0.723928 3.624143 -2.190907 1 -1.957257 2.582125 -1.469100 8 -0.153379 -0.478295 -1.390180 7 0.357700 1.107422 1.442242 6 1.760397 1.505589 1.637012 1 2.390214 0.748974 1.144804 1 1.939736 2.491355 1.206908 1 1.959438 1.544506 2.710157 6 -0.168305 0.168594 2.442649 1 -0.201834 0.659061 3.420302 1 -1.163469 -0.160120 2.138915 1 0.501048 -0.695841 2.498334 1 -1.733233 -0.821892 -0.579776 1 0.228075 1.370858 -1.546684 1 1.508267 -0.762400 -0.728381 7 2.477150 -0.962112 -0.388161

6 3.210672 -0.014395 -0.119917	1 -3.558974 -0.675212 0.435407	6 2.531760 -2.332853 0.097072
1 3.667655 0.597289 0.672952	1 -3.397417 -0.735583 -1.328871	1 1.743982 -2.490952 0.843206
1 3.890131 -0.864044 -0.310833	1 -3.216348 -2.212239 -0.371577	1 2.399121 -3.096308 -0.696070
1 3.164437 0.589052 -1.033018	1 -0.982279 0.611970 -0.398097	1 3.498002 -2.536006 0.580349
6 1.842596 -1.316965 1.406175		6 3.407338 -0.736871 -1.484537
1 2.474496 -2.213515 1.278907		1 3.271900 0.276712 -1.878332
1 2.188053 -0.797807 2.312864		1 4.446071 -0.827308 -1.136225
1 0.813451 -1.656330 1.573935		1 3.284507 -1.445008 -2.328458
<b>TS-IIf</b>		
Et =-559.7376971 NIImag=1(-80.00)	Et =-559.741987 NIImag=1 (-90.32)	

6	1.518941	-0.098784	0.392084	6	-1.720075	-0.286447	-0.222558
6	2.386610	-0.363149	-0.783599	6	-2.015323	1.086198	0.312787
1	1.429854	0.927996	0.740624	1	-2.179451	-0.580623	-1.159114
1	2.759430	-1.391797	-0.804614	1	-2.703309	0.970039	1.163350
6	3.536211	0.644989	-0.903080	6	-2.644145	2.000672	-0.743261
1	4.238263	0.566127	-0.065577	1	-3.601379	1.601812	-1.098475
1	4.094414	0.466573	-1.826914	1	-2.831124	2.992898	-0.321572
1	3.152671	1.670503	-0.934898	1	-1.980325	2.109718	-1.605356
8	-0.374523	0.532874	-1.456288	8	-0.075638	0.314388	-1.575440
7	0.769696	-0.948197	1.010068	7	-1.268410	-1.268912	0.511470
6	0.586960	-2.350952	0.607881	6	-0.619842	-1.080223	1.816518
1	-0.388921	-2.400055	0.110162	1	-0.975556	-1.860061	2.496425
1	1.380985	-2.671620	-0.062879	1	0.459612	-1.165375	1.655974
1	0.588878	-2.973079	1.506602	1	-0.860499	-0.101953	2.227044
6	-0.157470	-0.504790	2.068408	6	-1.027888	-2.588490	-0.085139
1	0.070051	-1.049700	2.989126	1	-1.346870	-3.365467	0.615631
1	-0.051656	0.570130	2.205441	1	-1.592272	-2.681127	-1.014964
1	-1.169163	-0.729836	1.719012	1	0.047493	-2.658463	-0.281411
1	-0.755635	0.942263	-2.248542	1	0.249700	1.132449	-1.147223
1	-1.406072	-0.365460	-0.854129	1	0.641591	-0.342481	-1.176245
8	-2.069189	-1.005811	-0.354073	8	1.652381	-0.964736	-0.244591
6	-3.214423	-1.169191	-1.149060	6	2.868510	-1.292453	-0.831925
1	-2.994393	-1.620872	-2.133631	1	3.223890	-0.541746	-1.570778
1	-3.919335	-1.836231	-0.634651	1	3.685600	-1.396105	-0.088874
1	-3.742384	-0.217462	-1.338772	1	2.833618	-2.257894	-1.378062
1	1.665039	-0.233532	-1.611051	1	-1.090808	1.522899	0.706308
1	-0.334750	1.658940	-0.425869	1	1.589330	0.525852	0.336954
8	-0.305848	2.315748	0.376670	8	1.313387	1.489273	0.544418
6	-1.646047	2.596767	0.707194	6	2.466142	2.280203	0.734847
1	-2.110487	3.323642	0.014848	1	3.135495	2.275763	-0.140945
1	-2.273591	1.691140	0.702947	1	2.151993	3.316082	0.910003
1	-1.689287	3.037888	1.712851	1	3.056832	1.957999	1.608332

