

Supporting Information for

A Theoretical Study of N-Demethylation of Substituted N,N-Dimethylanilines by Cytochrome P450: The Mechanistic Significance of Kinetic Isotope Effect Profiles.

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Reference 17 in Full.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

Table S1. Relative Energies, Spin and Charge Densities at the UB3LYP/B1//B1 Level for the Species in the C–H Hydroxylation of DMA by Cpd I of Cytochrome P450

	E (a.u.)	E _{rel} (Kcal/mol)	Spin Density						Charge					
			Fe	O	SH	Por	H	rest	Fe	O	SH	Por	H	rest
⁴ RC	-1951.6515651	0.00	1.09	0.94	0.50	0.39	0.00	0.08	0.50	-0.36	-0.06	-0.14	0.22	-0.16
² RC	-1951.6514531	0.07	1.22	0.88	-0.55	-0.47	0.00	-0.08	0.51	-0.36	-0.06	-0.15	0.22	-0.16
⁴ TS1	-1951.6359965	9.8	1.43	0.69	0.24	-0.02	0.00	0.66	0.46	-0.52	-0.02	-0.39	0.37	0.10
² TS1	-1951.6384270	8.2	1.61	0.27	-0.14	-0.20	-0.01	-0.53	0.46	-0.49	-0.07	-0.36	0.33	0.13
⁴ IM	-1951.6438933	4.8	1.67	0.44	0.14	-0.10	0.01	0.84	0.47	-0.60	-0.02	-0.36	0.44	0.07
⁴ Carb.	-1951.7232220	-45.0	2.56	0.02	0.44	-0.02	0.00	0.00	0.54	-0.57	-0.17	-0.49	0.39	0.30
² Carb.	-1951.7313556	-50.1	1.08	0.00	0.00	-0.08	0.00	0.00	0.37	-0.60	0.02	-0.56	0.40	0.37

Table S2. Relative Energies, Spin and Charge Densities at the UB3LYP/B1//B1 Level for the Species in the C–H Hydroxylation of p-Cl-DMA by Cpd I of Cytochrome P450

	E (a.u.)	E _{rel} (Kcal/mol)	Spin Density						Charge					
			Fe	O	SH	Por	H	rest	Fe	O	SH	Por	H	rest
⁴ RC	-2411.230001	0.00	1.09	0.94	0.50	0.39	0.00	0.08	0.50	-0.36	-0.06	-0.14	0.22	-0.16
² RC	-2411.230044	-0.03	1.22	0.88	-0.55	-0.47	0.00	-0.08	0.51	-0.36	-0.06	-0.15	0.22	-0.16
⁴ TS1	-2411.211263	11.8	1.43	0.69	0.24	-0.02	0.00	0.66	0.46	-0.52	-0.02	-0.39	0.37	0.10
² TS1	-2411.213505	10.4	1.61	0.27	-0.14	-0.20	-0.01	-0.53	0.46	-0.49	-0.07	-0.36	0.33	0.13
⁴ IM	-2411.219953	6.3	1.87	0.31	0.02	-0.13	0.03	0.90	0.47	-0.61	0.02	-0.34	0.39	0.07
⁴ Carb.	-2411.299503	-43.6	2.51	0.01	0.46	0.02	0.00	0.00	0.52	-0.58	-0.15	-0.43	0.40	0.24
² Carb.	-2411.307028	-48.3	1.09	0.00	0.00	-0.09	0.00	0.00	0.36	-0.59	0.03	-0.57	0.41	0.36

Table S3. Relative Energies, Spin and Charge Densities at the UB3LYP/B1//B1 Level for the Species in the C–H Hydroxylation of *p*-CN-DMA by Cpd I of Cytochrome P450

	E (a.u.)	E _{rel} (Kcal/mol)	Spin Density						Charge					
			Fe	O	SH	Por	H	rest	Fe	O	SH	Por	H	rest
⁴ RC	-2043.871550	0.0	1.09	0.94	0.52	0.44	0.00	0.01	0.50	-0.35	-0.05	-0.09	0.22	-0.23
² RC	-2043.871054	0.3	1.22	0.88	-0.58	-0.51	0.00	-0.01	0.51	-0.36	-0.04	-0.10	0.21	-0.22
⁴ TS1	-2043.848861	14.2	1.41	0.68	0.27	0.00	-0.01	0.65	0.46	-0.52	-0.01	-0.37	0.37	0.07
² TS1	-2043.850786	13.0	1.64	0.23	-0.16	-0.21	0.00	-0.50	0.46	-0.50	-0.06	-0.34	0.33	0.11
⁴ IM	-2043.858425	8.2	1.85	0.30	0.03	-0.13	0.02	0.93	0.46	-0.61	0.03	-0.31	0.39	0.04
⁴ Carb.	-2043.938816	-42.2	2.50	0.00	0.47	0.03	0.00	0.00	0.52	-0.58	-0.15	-0.41	0.41	0.22
² Carb.	-2043.945636	-46.5	1.09	0.00	-0.01	-0.08	0.00	0.00	0.36	-0.59	0.03	-0.55	0.40	0.35

Table S4. Relative Energies, Spin and Charge Densities at the UB3LYP/B1//B1 Level for the Species in the C–H Hydroxylation of *p*-NO₂-DMA by Cpd I of Cytochrome P450

	E (a.u.)	E _{rel} (Kcal/mol)	Spin Density						Charge					
			Fe	O	SH	Por	H	rest	Fe	O	SH	Por	H	rest
⁴ RC	-2156.085857	0.00	1.09	0.93	0.54	0.44	0.00	0.00	0.50	-0.36	-0.04	-0.08	0.19	-0.21
² RC	-2156.085803	0.03	1.22	0.88	-0.59	-0.51	0.00	0.00	0.52	-0.36	-0.04	-0.10	0.23	-0.25
⁴ TS1	-2156.058967	16.9	1.38	0.68	0.30	0.03	-0.02	0.63	0.46	-0.52	0.01	-0.35	0.37	0.03
² TS1	-2156.060412	16.0	1.67	0.19	-0.16	-0.22	0.00	-0.48	0.46	-0.50	-0.04	-0.32	0.34	0.06
⁴ IM	-2156.069609	10.2	1.84	0.28	0.03	-0.12	0.02	0.95	0.46	-0.60	0.04	-0.30	0.38	0.02
⁴ Carb.	-2156.148378	-39.2	2.52	0.03	0.48	-0.04	0.00	0.01	0.57	-0.57	-0.16	-0.51	0.39	0.28
² Carb.	-2156.15636	-44.2	1.09	0.00	-0.01	-0.09	0.00	0.00	0.36	-0.59	0.05	-0.54	0.41	0.33

Table S5. Relative Energies at Various Levels for C–H Hydroxylation of DMA by Cpd I of Cytochrome P450

	UB3LYP/B1//B1	UB3LYP/B1//B1 +ZPE	UB3LYP/B2//B1	UB3LYP/B2//B1 +Bulk Polarity	UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond	UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond +ZPE				
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
⁴ RC	-1951.651565	0.0	-1951.186389	0.0	-1952.4062103	0.0	-1952.430017	0.0	-2065.579400	0.0
² RC	-1951.651453	0.1	-1951.186476	-0.1	-1952.4063203	-0.1	-1952.430302	-0.2	-2065.580072	-0.4
⁴ TS _H	-1951.635996	9.8	-1951.175628	6.8	-1952.3924281	8.6	-1952.418344	7.3	-2065.564903	9.1
² TS _H	-1951.638427	8.2	-1951.177214	5.8	-1952.3941055	7.6	-1952.422529	4.7	-2065.570415	5.6
⁴ IM	-1951.643893	4.8	-1951.181266	3.2	-1952.4090658	-1.8	-1952.434212	-2.6	-2065.582442	-1.9
⁴ Carb.	-1951.723222	-45.0	-1951.256320	-43.9	-1952.4914926	-53.5	-1952.517469	-54.9	-2065.669774	-56.7
² Carb.	-1951.731356	-50.1	-1951.262451	-47.7	-1952.4975512	-57.3	-1952.520173	-56.6	-2065.664191	-53.2

Table S6. Relative Energies at Various Levels for C–H Hydroxylation of *p*-Cl-DMA by Cpd I of Cytochrome P450

	UB3LYP/B1//B1	UB3LYP/B1//B1 +ZPE	UB3LYP/B2//B1	UB3LYP/B2//B1 +Bulk Polarity	UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond	UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond +ZPE				
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
⁴ RC	-2411.230001	0.00	-2410.774618	0.0	-2412.031410	0.00	-2412.054121	0.0	-2525.202785	0.0
² RC	-2411.230044	-0.03	-2410.774776	-0.1	-2412.031376	0.02	-2412.054655	-0.3	-2525.203492	-0.4
⁴ TS _H	-2411.211263	11.8	-2410.760762	8.7	-2412.015097	10.2	-2412.041681	7.8	-2525.187844	9.4
² TS _H	-2411.213505	10.4	-2410.76206	7.9	-2412.017202	8.9	-2412.046898	4.5	-2525.193548	5.8
⁴ IM	-2411.219953	6.3	-2410.766704	5.0	-2412.032546	-0.7	-2412.05936195	-3.3	-2525.19682228	3.7
⁴ Carb.	-2411.299503	-43.6	-2410.841947	-42.2	-2412.114855	-52.4	-2412.142147	-55.2	-2525.294799	-57.7
² Carb.	-2411.307028	-48.3	-2410.847644	-45.8	-2412.120802	-56.1	-2412.144057	-56.4	-2525.287998	-53.5

Table S7. Relative Energies at Various Levels for C–H Hydroxylation of *p*-CN-DMA by Cpd I of Cytochrome P450

	UB3LYP/B1//B1		UB3LYP/B1//B1 +ZPE		UB3LYP/B2//B1		UB3LYP/B2//B1 +Bulk Polarity		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond +ZPE	
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
⁴ RC	-2043.871550	0.0	-2043.407798	0.0	-2044.682871	0.0	-2044.71124875	0.0	-2157.867064	0.0	-2157.403312	0.0
² RC	-2043.871054	0.3	-2043.407290	0.3	-2044.682722	0.1	-2044.71151554	-0.2	-2157.866973	0.1	-2157.403209	0.1
⁴ TS _H	-2043.848861	14.2	-2043.390079	11.1	-2044.661809	13.2	-2044.69401743	10.8	-2157.848760	11.5	-2157.389978	8.4
² TS _H	-2043.850786	13.0	-2043.391330	10.3	-2044.663644	12.1	-2044.69707119	8.9	-2157.850731	10.2	-2157.391275	7.6
⁴ IM	-2043.858425	8.2	-2043.396838	6.9	-2044.680895	1.2	-2044.71398611	-1.7	-2157.860578	0.0	-2157.398991	2.7
⁴ Carb.	-2043.938816	-42.2	-2043.472821	-40.8	-2044.763831	-50.8	-2044.79819173	-54.6	-2157.950735	-52.5	-2157.484740	-51.1
² Carb.	-2043.945636	-46.5	-2043.477919	-44.0	-2044.768588	-53.9	-2044.79957732	-55.4	-2157.943604	-52.1	-2157.475887	-45.5

Table S8. Relative Energies at Various Levels for C–H Hydroxylation of *p*-NO₂-DMA by Cpd I of Cytochrome P450

	UB3LYP/B1//B1		UB3LYP/B1//B1 +ZPE		UB3LYP/B2//B1		UB3LYP/B2//B1 +Bulk Polarity		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond +ZPE	
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
⁴ RC	-2156.085857	0.00	-2155.617951	0.0	-2156.979788	0.0	-2157.010535	0.00	-2270.166410	0.00	-2269.698504	0.0
² RC	-2156.085803	0.03	-2155.618173	-0.1	-2156.979920	-0.1	-2157.010526	0.01	-2270.166553	-0.03	-2269.698923	-0.3
⁴ TS _H	-2156.058967	16.9	-2155.596710	13.3	-2156.956896	14.4	-2156.991626	11.9	-2270.146673	12.4	-2269.684416	8.8
² TS _H	-2156.060412	16.0	-2155.597772	12.7	-2156.95851	13.4	-2156.994212	10.8	-2270.146960	12.3	-2269.684320	8.9
⁴ IM	-2156.069609	10.2	-2155.605069	8.1	-2156.9837788	-2.5	-2157.019219	-5.4	-2270.157968	5.3	-2269.693428	3.2
⁴ Carb.	-2156.148378	-39.2	-2155.679175	-38.4	-2157.058673	-49.5	-2157.09764341	-54.7	-2270.250178	-52.5	-2269.780975	-51.8
² Carb.	-2156.156360	-44.2	-2155.685238	-42.2	-2157.064558	-53.2	-2157.09826864	-55.1	-2270.242144	-47.5	-2269.771022	-45.5

Figure S1. The Highest Occupied Molecular Orbitals (HOMOs) of the *p*-(H, Cl, CN, NO₂)-DMA Substrates.

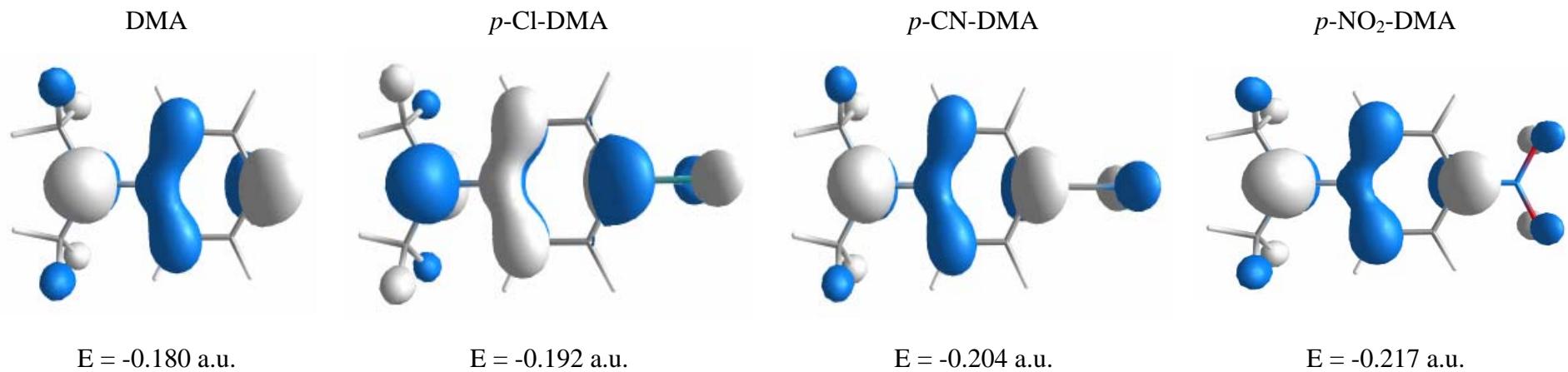


Figure S2. Some Occupied Orbitals of $^{2,4}\text{TS}_\text{H}$ Showing Conjugation of the O---H---C Bonding into the Aromatic Ring

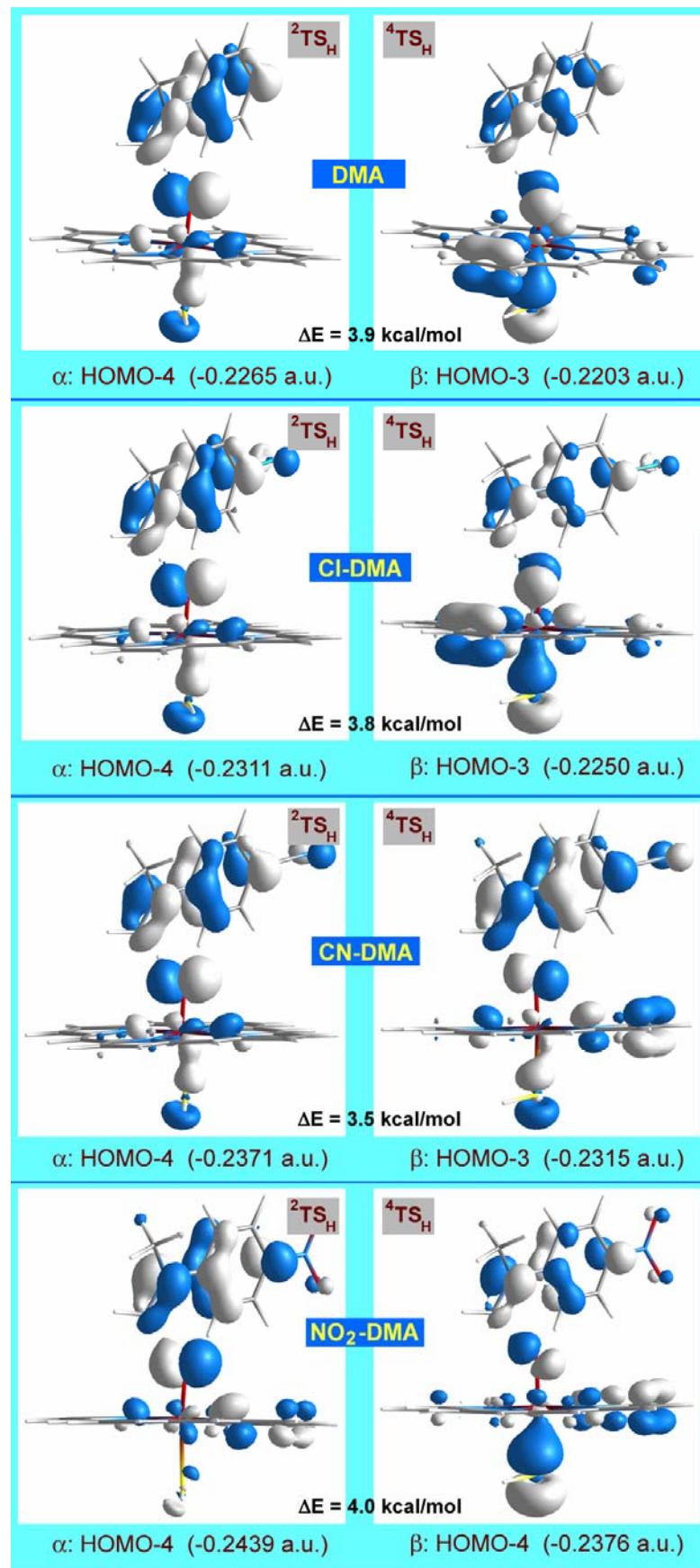


Figure S3. Some Occupied Orbitals of $^{2,4}\text{TS}_\text{H}$ Showing Conjugation of the O---H---C Bonding into the Aromatic Ring

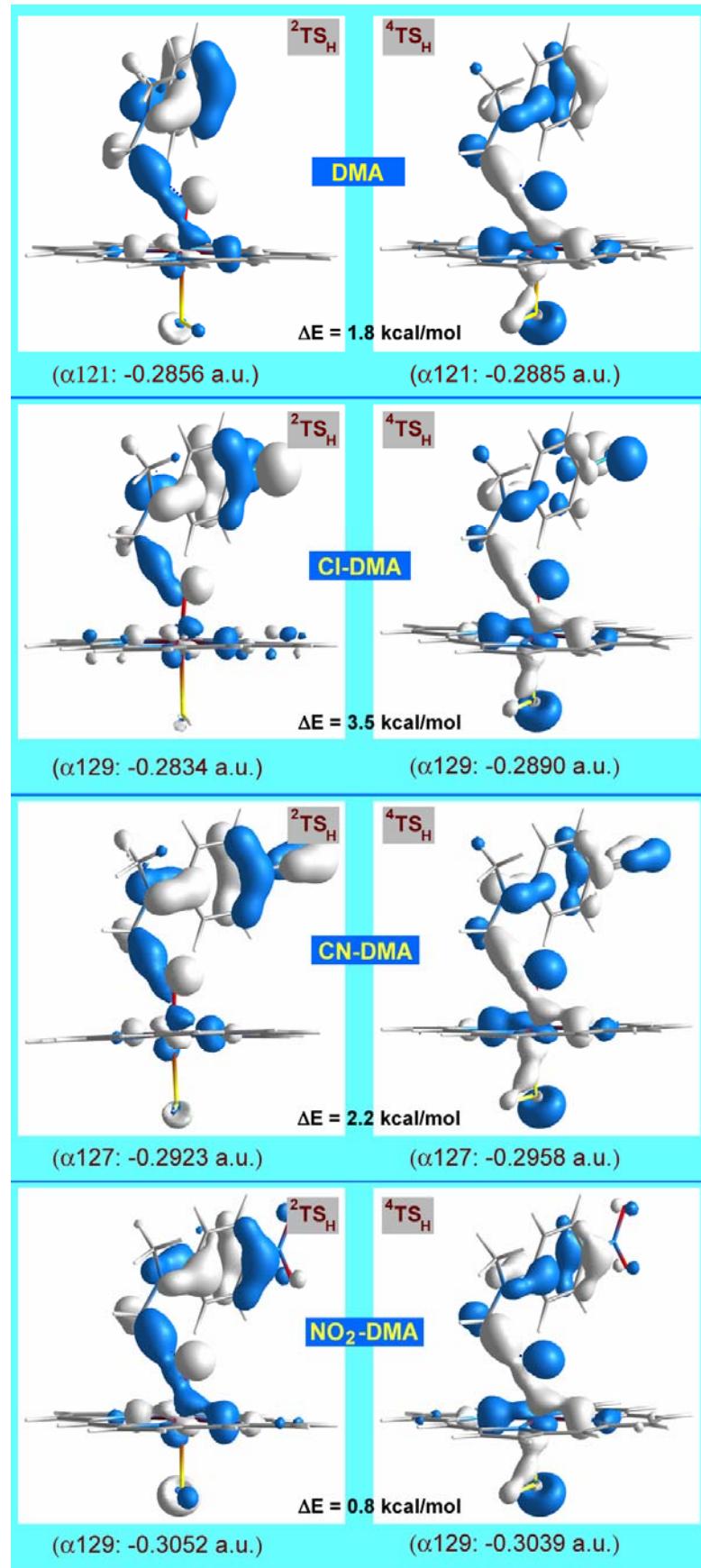
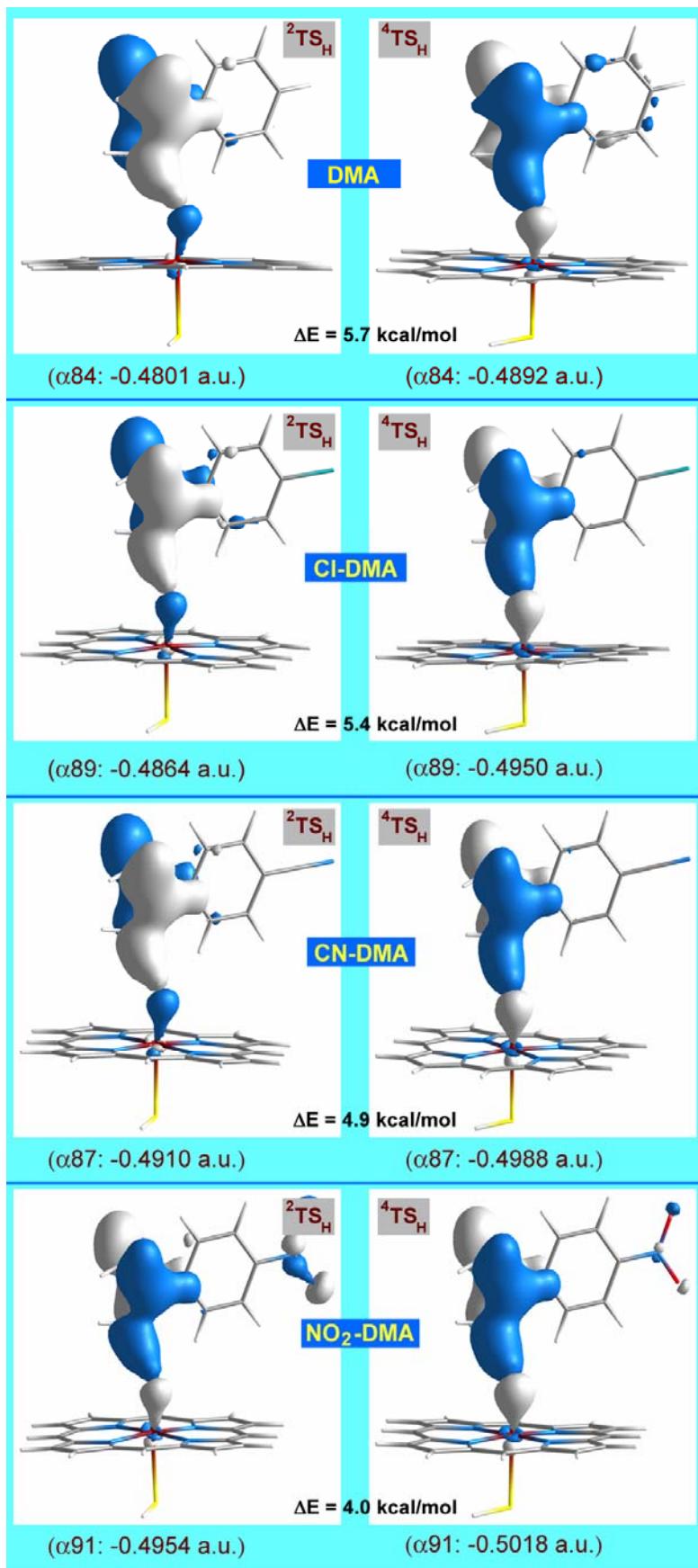
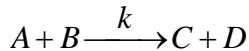


Figure S4. Some Occupied Orbitals of $^{2,4}\text{TS}_\text{H}$ Showing Conjugation of the O---H---C Bonding into the Aromatic Ring



KIE Formulation based on the Theory of Absolute Reaction Rates

According to the theory of absolute reaction rate, the rate of the reaction



can be written as the following,

$$k = \frac{Q^{\#}}{Q_A Q_B} \exp\left(-\frac{\Delta E}{RT}\right)$$

with Q being the partition function, R the gas constant, T the absolute temperature, and ΔE the activation free energy of the reaction.

Then, we can get the function of reaction rates for the non-deuterated and deuterated cases

$$k_H = \frac{Q_H^{\#}}{Q_{AH} Q_B} \exp\left(-\frac{\Delta E_H}{RT}\right)$$

$$k_D = \frac{Q_D^{\#}}{Q_{AD} Q_B} \exp\left(-\frac{\Delta E_D}{RT}\right) \quad (\text{assuming that A is deuterated})$$

So, the semi-classical Ering KIE value is determined as

$$\left(\frac{k_H}{k_D}\right)_S = \frac{Q_H^{\#} Q_{AD}}{Q_{AH} Q_D^{\#}} \exp\left[-\frac{(\Delta E_H - \Delta E_D)}{RT}\right]$$

with $\Delta E = E^{\#} - E^R$, s denotes for semi-classical, # for transition state, R for reagent.

Taking the Teller-Redlich role in the statistic mechanism into account, we can get

$$\frac{Q_H^{\#} Q_{AD}}{Q_{AH} Q_D^{\#}} \approx 1$$

Then, the function for the semi-classical Ering KIE calculation will be

$$\left(\frac{k_H}{k_D}\right)_S = \exp\left[-\frac{(E_H^{\#} - E_H^R) - (E_D^{\#} - E_D^R)}{RT}\right] \quad (1)$$

The “quantum correction” on the KIE is done by multiplying $(k_H/k_D)_S$ with a Q^{corr} factor.

For the Winger quantum corrected KIE, the function of KIE is

$$\left(\frac{k_H}{k_D}\right)_W = Q_w^{\text{corr}} \left(\frac{k_H}{k_D}\right)_S \quad (2)$$

$$Q_w^{\text{corr}} = (1 + u_t^2 / 24) / (1 + u'_t^2 / 24) \quad (3)$$

with $u_t = h\nu_H / k_B T$, $u'_t = h\nu_D / k_B T$, where ν is the imaginary frequency of the transition state.

Basic information on the theory of absolute reaction rate and KIE can be found in the following books:

1. Glasstone, S.; Laidler, K. J.; Eyring, H. *The Theory of Rate Processes*, McGraw-Hill, New York, 1941.
2. Melander, L.; Saunders, Jr. W. H. *Reaction Rates of Isotopic Molecules*, John Wiley & Sons, Inc, 1987.

A book in Chinese edited by Wei (ISBN: 7-03-011477) is also recommended.

Fortran Codes for Intramolecular KIE calculation

```
Program IntraKIE
IMPLICIT REAL*8 (A-H,O-Z)
C
C PROGRAM for KIE calculation with ethanol oxidation by CYP450.
C
C Formulation can be found in the following book, (fun2.5&2.15 at page 11&16)
C Melander,L.; Saunders, W. H. Jr.
C <<Reaction rates of isotopic molecules>>
C Robert E. Krieger Publishing Company; Malabar, FL, 1987.
C

OPEN(4,FILE='inp.txt',STATUS='OLD')
OPEN(6,FILE='out.txt',STATUS='UNKNOWN')
read(4,*) T
C Temperature for incubation (normally to be 310.15 K.)
write(6,*) 'Temperature---', T, 'K'
write(6,*)

C
C G value is got from .out file with "Sum of electronic and thermal Free Energies"
C

read(4,*)
read(4,*) vhh
read(4,*) Ghreag,Ghts
read(4,*)
read(4,*) vdh
read(4,*) Gdreas,Gdts
C 1 a.u.=627.509 Kcal/mol
C 1 K=1.98722×10_-3 kcal/mol
Ghreag=Ghreag*627.509
Ghts=Ghts*627.509
Gdreas=Gdreas*627.509
Gdts=Gdts*627.509
deltaGD=Gdts-Gdreas
deltaGH=Ghts-Ghreag
C semiclassical Eyring KIE
v1KIE=exp((deltaGD-deltaGH)/((1.98722e-3)*T))

C 1 cm_-1=2.85914×10_-3 Kcal/mol
C frequency is scaled by 0.9704, for the using of 6-31G basis set.
vkbt=T*1.98722e-3
vhhv=vhh*0.9704*2.85914e-3
uth=(vhhv)/(vkbt)
qth=1.0+(uth*uth)/24.0
```

```
vdhv=vdh*0.9704*2.85914e-3  
utd=(vdhv)/(vkbT)  
qtd=1.0+(utd*utd)/24.0
```

```
qt=qth/qtd  
C KIE with quantum Wigner correction  
v1KIE1=v1KIE*qt
```

```
Write(*,*) 'Successful! Find the results in the out.txt file'
```

```
write(6,*) '*****'  
write(6,*)  
write(6,*) 'the semiclassical Eyring KIE: ', v1KIE  
write(6,*)  
write(6,*) 'the KIE value with Wigner correction: ', v1KIE1  
write(6,*) '*****'  
write(6,*)
```

```
close (4)  
close (6)
```

```
END
```

Table S9. Calculated KIE Values for the *p*-(H, Cl, CN, NO₂)-DMA *N*-Demethylation by Cpd I at the B3LYP/LACVP Level.

	$k_{\text{CH}_3\text{CH}_2\text{H}-\text{O}}/k_{\text{CH}_3\text{CH}_2\text{D}-\text{O}}$	$k_{\text{CD}_2\text{HCD}_2\text{H}-\text{O}}/k_{\text{CD}_2\text{HCHDD}-\text{O}}$	$k_{\text{CH}_3\text{CH}_2\text{H}-\text{O}}/k_{\text{CD}_3\text{CD}_2\text{D}-\text{O}}$	$k_{\text{CD}_3\text{CH}_2\text{H}-\text{O}}/k_{\text{CH}_3\text{CD}_2\text{D}-\text{O}}$
H-DMA^b (KIE _{exp} =2.6)	For the doublet reaction route			
	<i>KIE</i> =3.8 (4.1) ^a	<i>KIE</i> =3.6 (3.7)	<i>KIE</i> =4.1 (4.4)	<i>KIE</i> =4.4 (4.7)
	For the quartet reaction route			
	<i>KIE</i> =5.8 (7.7)	<i>KIE</i> =5.5 (7.3)	<i>KIE</i> =6.3 (8.6)	<i>KIE</i> =6.7 (9.1)
Cl-DMA (KIE _{exp} =2.8)	For the doublet reaction route			
	<i>KIE</i> =4.1 (4.4)	<i>KIE</i> =3.8 (4.1)	<i>KIE</i> =4.4 (4.9)	<i>KIE</i> =4.6 (5.1)
	For the quartet reaction route			
	<i>KIE</i> =5.8 (7.9)	<i>KIE</i> =5.4 (7.3)	<i>KIE</i> =6.5 (8.9)	<i>KIE</i> =6.8 (9.3)
CN-DMA (KIE _{exp} =3.6)	For the doublet reaction route			
	<i>KIE</i> =4.5 (5.1)	<i>KIE</i> =4.2 (4.7)	<i>KIE</i> =4.9 (5.7)	<i>KIE</i> =5.0 (5.8)
	For the quartet reaction route			
	<i>KIE</i> =5.9 (8.2)	<i>KIE</i> =5.5 (7.6)	<i>KIE</i> =6.7 (9.3)	<i>KIE</i> =7.0 (9.7)
NO₂-DMA (KIE _{exp} =4.0)	For the doublet reaction route			
	<i>KIE</i> =5.3 (6.2)	<i>KIE</i> =4.4 (5.1)	<i>KIE</i> =4.4 (4.9)	<i>KIE</i> =4.5 (5.4)
	For the quartet reaction route			
	<i>KIE</i> =6.0 (8.4)	<i>KIE</i> =5.6 (7.8)	<i>KIE</i> =6.9 (9.7)	<i>KIE</i> =7.1 (10.0)

a Figures outside of the parenthesis are values of the semiclassical Eyring KIEs and those inside of the parenthesis are values of the Wigner-corrected ones.

b Experimental KIE values are got from references 4b and 4d. R denotes separated substrate and Cpd I reagents.

Table S10. Data for KIE calculations for hydrogen abstraction of the DMA at UB3LYP/LACVP level.

	Doublet State		Quartet State	
	642.428 ^a		1282.15	
(k _{CH₃CH₂H-O}	-1951.268954	-1951.245486	-1951.269591	-1951.244010
/k _{CH₃CH₂D-O})	552.728		964.899	
	-1951.272399	-1951.247611	-1951.273036	-1951.245732
	611.313		1265.86	
(k _{CD₂HCD₂H-O}	-1951.282825	-1951.259297	-1951.283462	-1951.257841
/k _{CD₂HCHDD-O})	543.542		958.931	
	-1951.282765	-1951.257990	-1951.283402	-1951.256099
	642.428		1282.15	
(k _{CH₃CH₂H-O}	-1951.268954	-1951.245486	-1951.269591	-1951.244010
/k _{CD₃CD₂D-O})	532.126		953.848	
	-1951.289838	-1951.264991	-1951.290475	-1951.263079
	641.508		1282.00	
(k _{CD₃CH₂H-O}	-1591.279396	-1951.255961	-1951.280033	-1951.254479
/k _{CH₃CD₂D-O})	532.808		953.975	
	-1591.279396	-1951.254516	-1951.280033	-1951.252610

a. Figures in vertical sequence are the imaginary frequency (unit in cm⁻¹) of H-abstraction transition state and free energies of reagents and transition states (unit in a.u.) for the non-deuterated and the deuterated cases.

Table S11. Data for KIE calculations for hydrogen abstraction of the *p*-Cl-DMA at UB3LYP/LACVP level.

	Doublet State		Quartet State	
	727.334		1339.66	
(k _{CH₃CH₂H-O}	-2410.857650	-2410.831881	-2410.851858	-2410.831241
/k _{CH₃CH₂D-O})	641.782		1007.50	
	-2410.861098	-2410.833946	-2410.855373	-2410.832958
	695.928		1323.56	
(k _{CD₂HCD₂H-O}	-2410.871533	-2410.845699	-2410.865523	-2410.845046
/k _{CD₂HCHDD-O})	605.431		1001.24	
	-2410.871473	-2410.844328	-2410.865567	-2410.843322
	727.334		1339.66	
(k _{CH₃CH₂H-O}	-2410.857650	-2410.831881	-2410.851858	-2410.831241
/k _{CD₃CD₂D-O})	595.077		996.399	
	-2410.878552	-2410.851326	-2410.872563	-2410.850305
	726.481		1339.49	
(k _{CD₃CH₂H-O}	-2410.868101	-2410.842353	-2410.862119	-2410.841713
/k _{CH₃CD₂D-O})	595.077		996.538	
	-2410.868101	-2410.840854	-2410.862285	-2410.839832

Table S12. Data for KIE calculations for hydrogen abstraction of the *p*-CN-DMA at UB3LYP/LACVP level.

	Doublet State		Quartet State	
	848.272		1418.06	
(k _{CH₃CH₂H-O}	-2043.489417	-2043.461679	-2043.480965	-2043.460830
/k _{CH₃CH₂D-O})	701.353		1066.21	
	-2043.492870	-2043.463651	-2043.484435	-2043.462534
	817.445		1402.65	
(k _{CD₂HCD₂H-O}	-2043.503321	-2043.475514	-2043.494828	-2043.474648
/k _{CD₂HCHDD-O})	691.813		1059.74	
	-2043.503263	-2043.474047	-2043.494801	-2043.472907
	848.272		1418.06	
(k _{CH₃CH₂H-O}	-2043.489417	-2043.461679	-2043.480965	-2043.460830
/k _{CD₃CD₂D-O})	681.678		1054.88	
	-2043.510350	-2043.481046	-2043.501870	-2043.479899
	847.660		1417.87	
(k _{CD₃CH₂H-O}	-2043.499883	-2043.472154	-2043.491403	-2043.471317
/k _{CH₃CD₂D-O})	682.211		1055.04	
	-2043.499883	-2043.470564	-2043.491432	-2043.469412

Table S13. Data for KIE calculations for hydrogen abstraction of the *p*-NO₂-DMA at UB3LYP/LACVP level.

	Doublet State		Quartet State	
	969.244		1482.06	
(k _{CH₃CH₂H-O}	-2155.698637	-2155.597772	-2155.692734	-2155.668550
/k _{CH₃CH₂D-O})	788.415		1115.58	
	-2155.702095	-2155.599591	-2155.696250	-2155.670241
	939.537		1465.73	
(k _{CD₂HCD₂H-O}	-2155.712560	-2155.611040	-2155.706615	-2155.682377
/k _{CD₂HCHDD-O})	778.968		1101.81	
	-2155.712503	-2155.609524	-2155.706624	-2155.680622
	969.244		1482.06	
(k _{CH₃CH₂H-O}	-2155.698637	-2155.597772	-2155.692734	-2155.668550
/k _{CD₃CD₂D-O})	769.343		1103.74	
	-2155.719597	-2155.616273	-2155.713710	-2155.687618
	968.630		1481.86	
(k _{CD₃CH₂H-O}	-2155.709117	-2155.607764	-2155.703199	-2155.679048
/k _{CH₃CD₂D-O})	769.806		1103.91	
	-2155.709117	-2155.606281	-2155.703245	-2155.677120

Table S14. Relative Energies, and Spin and Charge Densities at the UB3LYP/B1//B1 Level for Species During Carbinolaniline Decomposition in the **Enzymatic** Environment, with and without One Water Assistance

Without One Water Assisted (in heme pocket)														
E (a.u.)	E _{rel} (Kcal/mol)	Spin Density						Charge						
		Fe	SH	Por	O	H	N _{sub}	Fe	SH	Por	O	H	N _{sub}	
⁴ Carb	-1951.7232220	-45.0	2.56	0.44	-0.02	0.02	0.00	0.00	0.54	-0.17	-0.49	-0.57	0.39	-0.64
² Carb	-1951.7313556	-50.1	1.08	0.00	-0.08	0.00	0.00	0.00	0.37	0.02	-0.56	-0.60	0.40	-0.64
⁴ TS _p	-1951.6641755	-7.9	2.60	0.40	-0.07	0.05	0.00	0.00	0.59	-0.23	-0.57	-0.63	0.43	-0.74
² TS _p	-1951.6789481	-17.2	1.05	0.02	-0.08	0.02	0.00	0.00	0.40	-0.04	-0.62	-0.64	0.45	-0.75
⁴ Form	-1951.7068390	-34.7	2.56	0.45	-0.02	0.02	0.00	0.00	0.56	-0.17	-0.49	-0.35	0.33	-0.71
² Form	-1951.7139691	-39.2	1.49	-0.32	-0.17	0.00	0.00	0.00	0.48	-0.06	-0.51	-0.34	0.33	-0.72
The Decomplexation Step (in heme pocket)														
⁴ Carb _{free}	-1951.7140009	-39.2	2.49	0.47	0.04	0.00	0.00	0.00	0.62	-0.20	-0.42	-0.59	0.35	-0.62
² Carb _{free}	-1951.7117812	-37.8	1.31	-0.15	-0.16	0.00	0.00	0.00	0.45	-0.03	-0.42	-0.59	0.35	-0.62
With One Water Assisted (in heme pocket)														
			Fe	O	H	OH ^{H2O}	H ^{H2O}	N	Fe	O	H	OH ^{H2O}	H ^{H2O}	N
⁴ Carb ^{H2O}	-2028.1327194	0.0	2.59	0.03	0.00	0.00	0.00	0.00	0.56	-0.63	0.47	-0.36	0.39	-0.63
² Carb ^{H2O}	-2028.1442303	-7.2	1.07	0.01	0.00	0.00	0.00	0.00	0.37	-0.68	0.49	-0.34	0.40	-0.64
⁴ TS _p ^{H2O}	-2028.0977163	22.0	3.10	0.02	0.00	0.00	0.00	0.00	0.53	-0.66	0.49	-0.47	0.45	-0.74
² TS _p ^{H2O}	-2028.1195107	8.3	1.06	0.01	0.00	0.00	0.00	0.00	0.36	-0.67	0.50	-0.48	0.45	-0.74
⁴ Form ^{H2O}	-2028.1196113	8.2	2.56	0.01	0.00	0.00	0.00	0.00	0.56	-0.43	0.43	-0.40	0.38	-0.72
² Form ^{H2O}	-2028.1260032	4.2	1.05	0.02	0.00	0.00	0.00	0.00	0.33	-0.63	0.49	-0.43	0.43	-0.72

Table S15. Relative Energies, and Spin and Charge Densities at the UB3LYP/B1//B1 Level for Species During Carbinolaniline Decomposition in the Non-enzymatic Environment, with and without One Water Assistance

Without One Water Assisted (in non-enzymatic environment)													
E (a.u.)	E _{rel} (Kcal/mol)	Spin Density				Charge							
		O	H	N	rest	O	H	N	rest				
RC	-441.3137896	0.0	0.00	0.00	0.00	0.00	-0.60	0.35	-0.63	0.88			
TS	-441.2453035	43.0	0.00	0.00	0.00	0.00	-0.65	0.39	-0.72	0.99			
PC	-441.2986806	9.5	0.00	0.00	0.00	0.00	-0.39	0.31	-0.71	0.78			
With One Water Assisted (in non-enzymatic environment)													
		O _{cab}	H _{cab}	OH _w	H _w	N _{cab}	O _{cab}	O _{cab}	H _{cab}				
		0.00	0.00	0.00	0.00	0.00	0.00	-0.62	0.39	-0.39	0.41	-0.64	-0.62
RC	-517.71936641	0.0	0.00	0.00	0.00	0.00	0.00	-0.63	0.43	-0.51	0.43	-0.72	-0.63
TS	-517.69523062	15.1	0.00	0.00	0.00	0.00	0.00	-0.44	0.41	-0.39	0.38	-0.73	-0.44
PC	-517.71002961	5.9	0.00	0.00	0.00	0.00	0.00						

Table S16. Relative Energies for Carbinolaniine Decomposition in the Enzymatic Environment, with and without One Water Assistance, at Various Levels.

	UB3LYP/B1//B1		UB3LYP/B1//B1 +ZPE		UB3LYP/B2//B1		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond		UB3LYP/B2//B1 +Bulk Polarity +NH---S H-bond +ZPE	
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
Without One Water Assisted (in heme pocket)										
⁴ Carb	-1951.723222	-45.0	-1951.256320	-43.9	-1952.491493	-53.5	-1952.517469	-54.9	-2065.669774	-56.7
² Carb	-1951.731356	-50.1	-1951.262451	-47.7	-1952.497551	-57.3	-1952.520173	-56.6	-2065.664191	-53.2
⁴ TS _p	-1951.664176	-7.9	-1951.201927	-9.8	-1952.429960	-14.9	-1952.463065	-20.7	-2065.614874	-22.2
² TS _p	-1951.678948	-17.2	-1951.214495	-17.6	-1952.443104	-23.2	-1952.470391	-25.3	-2065.614423	-22.0
⁴ Form	-1951.706839	-34.7	-1951.243909	-36.1	-1952.479439	-46.0	-1952.507908	-48.9	-2065.659245	-50.1
² Form	-1951.713969	-39.2	-1951.247593	-38.4	-1952.485319	-50.0	-1952.508806	-49.4	-2065.653787	-46.7
The Decomplexation Step (in heme pocket)										
⁴ Carb _{free}	-1951.7140009	-39.2	-	-	-1952.487295	-50.9	-	-	-	-
² Carb _{free}	-1951.7117812	-37.8	-	-	-1952.484013	-48.8	-	-	-	-
With One Water Assisted (in heme pocket)										
⁴ Carb ^{H2O}	-2028.132719	0.0	-2027.640511	0.0	-2028.950025	0.0	-2028.9802087	0.0	-2142.132283	0.0
² Carb ^{H2O}	-2028.144230	-7.2	-2027.650110	-6.0	-2028.957839	-4.9	-2028.9829814	-1.7	-2142.126383	3.7
⁴ TS _p ^{H2O}	-2028.097716	22.0	-2027.611019	18.5	-2028.903554	29.2	-2028.9360776	27.7	-2142.085191	29.6
² TS _p ^{H2O}	-2028.119511	8.3	-2027.630555	6.2	-2028.922929	17.0	-2028.9522523	17.5	-2142.096607	22.4
⁴ Form ^{H2O}	-2028.119611	8.2	-2027.630217	6.4	-2028.938768	7.1	-2028.9685416	7.3	-2142.121080	7.0
² Form ^{H2O}	-2028.126003	4.2	-2027.631683	5.5	-2028.937847	7.6	-2028.9697927	6.5	-2142.114186	11.4
										-2141.619866
										12.7

Table S17. Relative Energies for Carbinolaniine Decomposition in the **Non-enzymatic** Environment, with and without One Water Assistance, at Various Levels.

	UB3LYP/B1//B1		UB3LYP/B1//B1 +ZPE		UB3LYP/B2//B1		UB3LYP/B2//B1 +Bulk Polarity (chlorobenzene)		UB3LYP/B2//B1 +Bulk Polarity (water)		UB3LYP/B2//B1 +Bulk Polarity (water)+ZPE	
	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}	E (a.u.)	E _{rel}
Without One Water Assisted (in non-enzymatic environment)												
RC	-441.3137896	0.0	-441.1336276	0.0	-441.537562	0.0	-441.549888828	0.0	-441.554835182	0.0	-441.3746732	0.0
TS	-441.2453035	43.0	-441.0706545	39.5	-441.4693838	42.8	-441.492978215	35.7	-441.502177706	33.0	-441.3275287	29.6
PC	-441.2986806	9.5	-441.1231436	6.6	-441.5263383	7.0	-441.539467825	6.5	-441.545309230	6.0	-441.3697722	3.0
With One Water Assisted (in non-enzymatic environment)												
RC	-517.71936641	0.0	-517.5139964	0.0	-517.993004172	0.0	-518.009636321	0.0	-518.016334973	0.0	-517.8109650	0.0
TS	-517.69523062	15.1	-517.4946946	12.1	-517.957468178	22.3	-517.978467304	19.6	-517.987888594	17.9	-517.7873526	14.8
PC	-517.71002961	5.9	-517.5083846	3.5	-517.984455519	5.4	-518.000538524	5.7	-518.006939440	5.9	-517.8052944	3.6

Table S18. Data Computed at the UB3LYP/B1 Level for KIE Calculations During Proton Shift in the *para*-Substituted Carbinolaniine Decomposition Processes

DMA	<i>p</i> -Cl-DMA	<i>p</i> -CN-DMA	<i>p</i> -NO ₂ -DMA
755.1041 ^a	782.4103	827.4180	866.7431
-517.801231 -517.770397	-977.098854 -977.092867	-609.729238 -609.720519	-721.936298 -721.925523
622.2072	644.6737	683.6340	717.9936
-517.801192 -517.769263	-977.098506 -977.091739	-609.728887 -609.719408	-721.935945 -721.924426

a. Figures in vertical sequence are the imaginary frequency (unit in cm⁻¹) of H-abstraction transition state and free energies of reagents and transition states (unit in a.u.) for the non-deuterated and the deuterated cases.

Table S19 Cartesian Coordinates for Various Reaction Species in C–H Hydroxylation of DMA by Cpd I

I. For 4RC

26	-2.375368000	-0.071265000	0.067303000	6	-2.564478000	1.387590000	-2.351926000
7	-2.643161000	-2.035744000	0.452692000	6	-2.616481000	-2.472488000	-0.410612000
7	-1.848910000	0.220949000	1.992178000	6	-0.764684000	-3.084316000	2.853107000
7	-2.377001000	1.922783000	-0.228268000	6	-0.023661000	-2.147263000	3.514459000
7	-3.155183000	-0.344813000	-1.775004000	6	1.111201000	2.679212000	2.732017000
6	-3.056325000	-3.017721000	-0.443896000	6	0.819799000	3.592444000	1.759826000
6	-2.312424000	-2.707014000	1.624777000	6	-1.894742000	3.546320000	-2.459161000
6	-1.623557000	-0.752662000	2.950811000	6	-2.638072000	2.611786000	-3.119695000
6	-1.534049000	1.430681000	2.594970000	6	-3.745268000	-2.225216000	-2.354656000
6	-1.987204000	2.897745000	0.669407000	6	-3.452452000	-3.140826000	-1.384365000
6	-2.682731000	2.585746000	-1.403197000	6	-2.101047000	-3.070103000	0.729162000
6	-3.348288000	0.628052000	-2.743269000	6	0.525591000	0.264592000	3.086089000
6	-3.482731000	-1.548608000	-2.373951000	6	-0.529732000	3.524047000	-0.354511000
6	-3.005649000	-4.316254000	0.191563000	1	-3.163897000	0.192463000	-2.708094000
6	-2.545702000	-4.125415000	1.462258000	1	-2.352671000	-4.111001000	0.903517000
6	-1.160090000	-0.141119500	4.178423000	1	1.105839000	0.275216000	4.002555000
6	-1.109581000	1.205789000	3.960342000	1	-0.267757000	4.561393000	-0.532896000
6	-2.047694000	4.202318000	0.044152000	1	-3.736885000	0.176494000	-3.629189000
6	-2.476610000	4.009363000	-1.237354000	1	-0.952353000	-4.110900000	3.131879000
6	-3.813182000	0.018487000	-3.970436000	1	0.517989000	-2.252180000	4.443048000
6	-3.895516000	-1.325707000	-3.742772000	1	1.707920000	2.813742000	3.622241000
6	-3.438025000	-2.791634000	-1.754543000	1	1.129591000	4.625123000	1.694887000
6	-1.824008000	-2.1141154000	2.775793000	1	-1.714136000	4.575168000	-2.733959000
6	-1.601064000	2.671356000	1.983902000	1	-3.186710000	2.722571000	-4.043576000
6	-3.133360000	1.986668000	-2.570196000	1	-4.345778000	-2.357333000	-3.242796000
1	-3.726944000	-3.653939000	-2.346150000	8	0.124803000	-0.244931000	-0.752470000
1	-1.596819000	-2.763642000	3.614285000	16	-3.251311000	1.170821000	1.352597000
1	-1.323683000	3.535737000	2.577810000	1	-4.217200000	0.878940000	0.407265000
1	-3.333417000	2.634401000	-3.417276000	1	6.023012000	2.252591000	0.729362000
1	-3.285479000	-5.243092000	-0.287501000	6	5.596496000	1.360587000	0.282231000
1	-2.374615000	-4.864764000	2.230872000	6	6.415656000	0.420730000	-0.353995000
1	-0.917978000	-0.684541000	5.079933000	6	4.215970000	1.126709000	0.329944000
1	-0.816754000	1.986142000	4.647352000	6	5.876001000	-0.729450000	-0.931106000
1	-1.793712000	5.130337000	0.534916000	1	7.489348000	0.579693000	-0.401942000
1	-2.645392000	4.747800000	-2.007364000	6	3.654840000	-0.016814000	-0.238700000
1	-4.042512000	0.560734000	-4.876094000	1	3.560281000	1.843898000	0.815383000
1	-4.205834000	-2.104011000	-4.424545000	6	4.478468000	-0.972842000	-0.890266000
8	-0.818011000	-0.242178000	-0.467640000	1	6.541076000	-1.436964000	-1.410096000
16	-4.743604000	-0.013741000	1.047207000	1	2.581339000	-0.154532000	-0.195053000
1	-5.381295000	-0.760433000	0.073743000	7	3.930511000	-2.114814000	-1.468583000
1	4.231289000	0.388414000	3.774873000	6	2.507929000	-2.419802000	-1.295274000
6	4.023283000	-0.031084000	2.795966000	6	4.798976000	-3.100737000	-2.103515000
6	5.067427000	-0.447545000	1.962284000	1	2.257891000	-3.296124000	-1.896524000
6	2.705029000	-0.167520000	2.341496000	1	2.258594000	-2.635532000	-0.245477000
6	4.809188000	-0.990457000	0.702853000	1	1.868424000	-1.589846000	-1.613196000
1	6.097877000	-0.353361000	2.293547000	1	5.493711000	-3.570652000	-1.389519000
6	2.423892000	-0.708372000	1.086835000	1	4.183685000	-3.886258000	-2.544975000
1	1.878067000	0.150380000	2.970040000	1	5.397068000	-2.649116000	-2.906016000
6	3.477426000	-1.129722000	0.233171000				
1	5.642262000	-1.307131000	0.088016000				
1	1.392655000	-0.783395000	0.764673000				
7	3.210608000	-1.667131000	-1.023440000	26	-2.216985000	-0.090426000	-0.037756000
6	1.829710000	-1.938394000	-1.431540000	7	-2.282589000	-2.118708000	0.252649000
6	4.307154000	-2.128586000	-1.868331000	7	-1.701724000	0.157674000	1.900997000
1	1.826868000	-2.270488000	-2.471527000	7	-2.193553000	1.884886000	-0.305925000
1	1.365955000	-2.723668000	-0.815429000	7	-2.906575000	-0.356217000	-1.911514000
1	1.196019000	-1.048673000	-1.352940000	7	-2.611002000	-3.081014000	-0.685425000
1	4.855461000	-2.973445000	-1.422153000	6	-2.015077000	-2.793799000	1.430917000
1	3.904649000	-2.454913000	-2.828633000	6	-1.512815000	-0.840151000	2.846973000
1	5.029372000	-1.324280000	-2.061209000	6	-1.410484000	1.353761000	2.528912000

III. For 4TS_H

26	-2.216985000	-0.090426000	-0.037756000
7	-2.282589000	-2.118708000	0.252649000
6	-1.701724000	0.157674000	1.900997000
1	-2.193553000	1.884886000	-0.305925000
1	-2.906575000	-0.356217000	-1.911514000
6	-2.611002000	-3.081014000	-0.685425000
6	-2.015077000	-2.793799000	1.430917000
6	-1.512815000	-0.840151000	2.846973000
6	-1.410484000	1.353761000	2.528912000
6	-1.823454000	2.846791000	0.621308000
6	-2.531872000	2.569183000	-1.461987000
6	-3.145367000	0.634270000	-2.846832000
6	-3.135163000	-1.565539000	-2.554976000
6	-2.532439000	-4.396654000	-0.083421000
6	-2.167617000	-4.219418000	1.221293000
6	-1.103051000	-0.245433000	4.102195000
6	-1.038708000	1.105747000	3.905750000
6	-1.915492000	4.163254000	0.022475000

6	-2.353856000	3.992851000	-1.257778000	6	-2.402463000	2.449156000	0.111314000
6	-3.558032000	0.036400000	-4.099049000	6	-2.414901000	-2.407659000	0.162668000
6	-3.548493000	-1.317508000	-3.920259000	1	3.215013000	-3.167791000	0.206066000
6	-2.995767000	-2.825995000	-1.994779000	1	3.224842000	3.220233000	-0.121576000
6	-1.655560000	-2.203310000	2.634095000	1	-3.167333000	3.218061000	0.130039000
6	-1.457933000	2.607265000	1.934280000	1	-3.181029000	-3.175316000	0.180303000
6	-2.981616000	1.996188000	-2.639055000	1	5.092485000	-1.332035000	0.113306000
1	-3.223671000	-3.679442000	-2.624658000	1	5.100104000	1.370520000	-0.042281000
1	-1.474562000	-2.860274000	3.478260000	1	1.371246000	5.105012000	-0.078018000
1	-1.202062000	3.463789000	2.548466000	1	-1.334550000	5.094924000	0.051141000
1	-3.210182000	2.660509000	-3.465375000	1	-5.054279000	1.383504000	0.166433000
1	-2.745074000	-5.321390000	-0.600227000	1	-5.064495000	-1.323979000	0.172932000
1	-2.020571000	-4.970292000	1.984153000	1	-1.335296000	-5.052443000	0.257242000
1	-0.899801000	-0.802318000	5.005498000	1	1.372475000	-5.049853000	0.279620000
1	-0.773474000	1.875013000	4.616505000	8	-0.147359000	-0.061244000	-1.703630000
1	-1.679893000	5.085022000	0.534265000	16	0.037859000	0.169371000	2.417766000
1	-2.548293000	4.746684000	-2.006799000	1	-0.627946000	-1.009926000	2.690328000
1	-3.810632000	0.593760000	-4.989392000	1	-0.539297000	5.394332000	-5.765576000
1	-3.794330000	-2.089968000	-4.634614000	6	-0.184072000	4.391990000	-5.551551000
8	-0.558364000	-0.232795000	-0.555193000	6	0.000700000	3.470839000	-6.590154000
16	-4.450837000	-0.082667000	0.791695000	6	0.082429000	4.000672000	-4.233063000
1	-5.073215000	-0.651085000	-0.303227000	6	0.453377000	2.178497000	-6.323089000
1	4.888058000	0.578888000	3.535877000	1	-0.205102000	3.759259000	-7.616061000
6	4.378402000	0.109671000	2.701104000	6	0.536524000	2.713523000	-3.947600000
6	5.102144000	-0.321900000	1.582982000	1	-0.079746000	4.691637000	-3.412443000
6	2.987977000	-0.059846000	2.723567000	6	0.738288000	1.785773000	-4.995332000
6	4.453405000	-0.923739000	0.503508000	1	0.604227000	1.488660000	-7.144371000
1	6.179589000	-0.194568000	1.549973000	1	0.678981000	2.412936000	-2.918182000
6	2.323853000	-0.658767000	1.653412000	7	1.214940000	0.492247000	-4.718699000
1	2.406610000	0.291187000	3.569884000	6	1.759547000	0.165337000	-3.449474000
6	3.053432000	-1.109095000	0.530536000	6	1.004579000	-0.583915000	-5.695863000
1	5.036470000	-1.266015000	-0.342904000	1	2.297038000	-0.782603000	-3.476397000
1	1.244087000	-0.727322000	1.663191000	1	2.377100000	0.965412000	-3.036629000
7	2.392026000	-1.735893000	-0.544396000	1	0.877330000	0.013686000	-2.617303000
6	1.068802000	-2.210474000	-0.416845000	1	1.709768000	-0.504614000	-6.533273000
6	3.032293000	-1.772642000	-1.865953000	1	1.158144000	-1.543581000	-5.202099000
1	0.783090000	-2.867864000	-1.236696000	1	-0.015681000	-0.553106000	-6.089832000
1	0.851646000	-2.638362000	0.562516000				
1	0.205243000	-1.217282000	-0.493945000				
1	3.804415000	-2.551401000	-1.914146000	26	-2.295072000	-0.000841000	0.030299000
1	2.273592000	-1.988113000	-2.618823000	7	-2.159910000	-2.009247000	0.318840000
1	3.489838000	-0.806666000	-2.098257000	7	-1.813848000	0.301931000	1.964258000

V. For 4IM

26	0.020550000	0.021559000	-0.000294000	6	-2.461030000	-3.002671000	-0.600294000
7	2.034028000	0.025837000	-0.000248000	6	-1.817178000	-2.655112000	1.496685000
7	0.030504000	2.040434000	0.027326000	6	-1.504480000	-0.666210000	2.907845000
7	-2.000219000	0.018866000	0.120796000	6	-1.654552000	1.526651000	2.590005000
7	0.016847000	-1.992714000	0.168207000	6	-2.171012000	2.971467000	0.673109000
6	2.863459000	-1.084008000	0.077733000	6	-2.770745000	2.626347000	-1.434075000
6	2.869461000	1.131987000	-0.046309000	6	-3.230061000	0.640375000	-2.803657000
6	1.134438000	2.873399000	-0.037910000	6	-3.125048000	-1.553917000	-2.472622000
6	-1.081327000	2.865636000	0.064886000	6	-2.271224000	-4.301115000	0.009035000
6	-2.823652000	1.129658000	0.128584000	6	-1.873956000	-4.087288000	1.298862000
6	-2.831816000	-1.086348000	0.137177000	6	-1.158034000	-0.028608000	4.159403000
6	-1.092029000	-2.822968000	0.181975000	6	-1.252026000	1.320734000	3.964254000
6	1.125130000	-2.820717000	0.195875000	6	-2.344939000	4.272073000	0.060553000
6	4.247344000	-0.661069000	0.060062000	6	-2.712818000	4.059822000	-1.236460000
6	4.251288000	0.702440000	-0.019281000	6	-3.602232000	0.002164000	-4.046884000
6	0.703978000	4.255967000	-0.042367000	1	-3.538974000	-1.347374000	-3.842984000
6	-0.661000000	4.250600000	0.024202000	1	-2.903146000	-2.795675000	-1.897865000
6	-4.210703000	0.708795000	0.152542000	1	-1.501674000	-2.036255000	2.696505000
6	-4.215853000	-0.655649000	0.155202000	1	-1.819013000	2.768285000	1.996404000
6	-0.664808000	-4.205618000	0.232409000	1	-3.144230000	2.011324000	-2.617196000
6	0.700783000	-4.204400000	0.243797000	1	-3.091698000	-3.671329000	-2.509350000
6	2.447101000	-2.402884000	0.161576000	1	-1.246440000	-2.672040000	3.537088000
6	2.456763000	2.455329000	-0.083816000	1	-1.655331000	3.644852000	2.613350000
6				1	-3.389278000	2.648603000	-3.459634000
6				1	-2.437158000	-5.242876000	-0.493646000
6				1	-1.650463000	-4.819004000	2.061575000
6				1	-0.881636000	-0.558691000	5.059162000
6				1	-1.068517000	2.115264000	4.672817000
6				1	-2.203255000	5.212492000	0.572798000
6				1	-2.933412000	4.791348000	-2.000110000

1	-3.867115000	0.532094000	-4.950229000
1	-3.742335000	-2.141975000	-4.546121000
8	-0.576959000	0.043671000	-0.509365000
16	-4.532358000	-0.081153000	0.820681000
1	-5.167406000	-0.177501000	-0.402270000
1	4.718421000	1.064828000	3.532783000
6	4.306575000	0.504984000	2.699657000
6	5.155665000	-0.122399000	1.780373000
6	2.919902000	0.412192000	2.523341000
6	4.632605000	-0.846867000	0.706612000
1	6.232595000	-0.056678000	1.901449000
6	2.381290000	-0.301995000	1.452267000
1	2.246225000	0.912889000	3.211667000
6	3.236436000	-0.950716000	0.536591000
1	5.307716000	-1.346181000	0.021273000
1	1.311467000	-0.303148000	1.284194000
7	2.692877000	-1.699375000	-0.536011000
6	1.417897000	-2.234588000	-0.475120000
6	3.492682000	-1.901122000	-1.752219000
1	1.096083000	-2.826132000	-1.321622000
1	1.005758000	-2.448936000	0.502858000
1	-0.047094000	-0.796832000	-0.601803000
1	4.187490000	-2.744846000	-1.646439000
1	2.820150000	-2.108555000	-2.586956000
1	4.063749000	-0.998198000	-1.981614000

VI. For ⁴ Carbinolaniline Complex.

26	-2.559880000	0.011284000	0.213802000
7	-2.107530000	-1.952957000	0.229126000
7	-2.377617000	0.058989000	2.223874000
7	-2.769605000	2.008190000	0.188253000
7	-2.349464000	0.020128000	-1.810849000
6	-1.974714000	-2.790291000	-0.873959000
6	-2.005330000	-2.772347000	1.348802000
6	-2.220017000	-1.029818000	3.070568000
6	-2.537266000	1.164840000	3.046507000
6	-2.872426000	2.849638000	1.288313000
6	-2.897624000	2.820612000	-0.931437000
6	-2.560836000	1.102070000	-2.658520000
6	-2.189723000	-1.088011000	-2.637230000
6	-1.784359000	-4.151870000	-0.432510000
6	-1.805129000	-4.140876000	0.935814000
6	-2.264748000	-0.590877000	4.448769000
6	-2.458361000	0.760947000	4.433933000
6	-3.089948000	4.208015000	0.846703000
6	-3.107275000	4.189905000	-0.520260000
6	-2.500138000	0.665396000	-4.035221000
6	-2.270494000	-0.681926000	-4.022225000
6	-2.007260000	-2.391355000	-2.203195000
6	-2.055044000	-2.345422000	2.668196000
6	-2.766398000	2.461621000	2.615584000
6	-2.811512000	2.402642000	-2.251547000
1	-1.897993000	-3.161447000	-2.959082000
1	-1.956608000	-3.098775000	3.442156000
1	-2.873458000	3.230952000	3.372481000
1	-2.947815000	3.152249000	-3.023377000
1	-1.659579000	-4.998243000	-1.092271000
1	-1.698060000	-4.976001000	1.612699000
1	-2.165522000	-1.244180000	5.303380000
1	-2.548917000	1.434029000	5.274030000
1	-3.206098000	5.055608000	1.506311000
1	-3.239517000	5.019809000	-1.199037000
1	-2.626791000	1.313980000	-4.889796000
1	-2.174125000	-1.352186000	-4.863976000
8	-0.047834000	0.447868000	0.006912000
16	-4.988184000	-0.480941000	0.193102000
1	-5.445860000	0.820348000	0.279567000
1	5.834712000	3.315898000	-0.102561000
6	5.090356000	2.526757000	-0.093434000
6	5.426708000	1.227505000	-0.484819000
6	3.772866000	2.794573000	0.298681000
6	4.473029000	0.205144000	-0.473966000

VII. For ² Carbinolaniline Complex.

1	6.441424000	0.998895000	-0.797071000
6	2.805820000	1.788355000	0.305989000
1	3.486707000	3.801442000	0.587825000
6	3.147043000	0.468503000	-0.068845000
1	4.769196000	-0.794439000	-0.767301000
1	1.778840000	2.027949000	0.552825000
7	2.180156000	-0.559835000	-0.035746000
6	0.959333000	-0.388562000	0.698181000
6	2.481245000	-1.864826000	-0.630515000
1	0.521542000	-1.368260000	0.898931000
1	1.121317000	0.143160000	1.637268000
1	-0.078523000	0.227384000	-0.948395000
1	3.246666000	-2.416278000	-0.065136000
1	1.571095000	-2.468078000	-0.649686000
1	2.836778000	-1.751731000	-1.661272000
26	-2.234446000	-0.511582000	0.193499000
7	-2.472781000	-2.517163000	0.056064000
7	-2.064891000	-0.635765000	2.200434000
7	-1.863739000	1.462607000	0.323189000
7	-2.274157000	-0.420783000	-1.822963000
6	-2.683367000	-3.276091000	-1.087492000
6	-2.577310000	-3.395985000	1.124838000
6	-2.229813000	-1.784061000	2.962720000
6	-1.858229000	0.399553000	3.104304000
6	-1.664305000	2.231980000	1.466365000
6	-1.808479000	2.345689000	-0.743409000
6	-2.177746000	0.737594000	-2.579218000
6	-2.513336000	-1.449700000	-2.723615000
6	-2.903979000	-4.660278000	-0.726242000
6	-2.839070000	-4.734330000	0.636149000
6	-2.115463000	-1.459539000	4.369409000
6	-1.886029000	-0.115257000	4.456288000
6	-1.473277000	3.612406000	1.105667000
6	-1.563027000	3.688110000	-0.255525000
6	-2.344652000	0.422264000	-3.983555000
6	-2.550838000	-0.924684000	-4.072436000
6	-2.695741000	-2.782933000	-2.384442000
6	-2.458514000	-3.060250000	2.466024000
6	-1.659526000	1.730463000	2.764053000
6	-1.955528000	2.013235000	-2.082620000
1	-2.877783000	-3.486927000	-3.189331000
1	-2.566701000	-3.861814000	3.189391000
1	-1.501481000	2.438123000	3.570911000
1	-1.895304000	2.822227000	-2.803150000
1	-3.091523000	-5.456172000	-1.432494000
1	-2.963578000	-5.603366000	1.266116000
1	-2.206194000	-2.176214000	5.172975000
1	-1.751465000	0.485141000	5.344460000
1	-1.298736000	4.411539000	1.811544000
1	-1.477791000	4.562425000	-0.884650000
1	-2.310059000	1.148563000	-4.782683000
1	-2.718912000	-1.520117000	-4.958147000
8	-0.172613000	-0.818868000	-0.048903000
1	-4.503081000	-0.189182000	0.292310000
1	-4.532997000	0.673141000	1.372085000
1	4.818833000	3.355759000	-0.886181000
6	4.282307000	2.454402000	-0.609567000
6	4.959214000	1.239355000	-0.469778000
6	2.898598000	2.485719000	-0.398248000
6	4.274265000	0.074050000	-0.111826000
1	6.031522000	1.191448000	-0.634059000
6	2.197709000	1.329733000	-0.050541000
6	2.348803000	3.414128000	-0.518308000
6	2.882277000	0.104997000	0.113257000
1	4.830166000	-0.848273000	0.002148000

1	1.120899000	1.371068000	0.052062000	1	-0.026352000	-1.433620000	-0.794903000
7	2.186256000	-1.066790000	0.497307000	1	3.668083000	-2.448074000	1.179873000
6	0.864129000	-0.987525000	1.018510000	1	2.134784000	-3.157748000	0.641486000
6	2.860980000	-2.367678000	0.438696000	1	3.291149000	-2.544720000	-0.553965000
1	0.623953000	-1.890527000	1.581308000				
1	0.712228000	-0.107152000	1.640244000				

I-1. For $^4\text{RC} + 2\text{NH}_3$ Complex.

26	-1.014796000	-0.194321000	-0.101012000	1	-3.518571000	0.197903000	-4.712866000
7	-0.359361000	-0.803302000	1.705587000	1	-3.283244000	-4.440824000	-2.217609000
7	-0.472672000	1.695676000	0.346003000	1	-2.279467000	-5.290132000	0.149543000
7	-1.910999000	0.475149000	-1.782851000	8	0.415692000	-0.560307000	-0.850436000
7	-1.792507000	-2.027706000	-0.436564000	16	-3.251328000	0.570948000	0.878271000
6	-0.413560000	-2.087536000	2.217846000	1	-4.088102000	-0.259425000	0.156039000
6	0.310646000	-0.045251000	2.646531000	1	5.558920000	3.338445000	0.158611000
6	0.209137000	2.120377000	1.477753000	6	5.357290000	2.301806000	-0.090978000
6	-0.605098000	2.813717000	-0.461063000	6	6.406059000	1.422562000	-0.384955000
6	-1.850318000	1.762409000	-2.303757000	6	4.043390000	1.817125000	-0.125696000
6	-2.586354000	-0.287313000	-2.731450000	6	6.155988000	0.088537000	-0.708803000
6	-2.469253000	-2.453631000	-1.565668000	1	7.433427000	1.775303000	-0.362593000
6	-1.646642000	-3.147879000	0.366341000	6	3.769470000	0.486580000	-0.443814000
6	0.241586000	-2.134272000	3.508243000	1	3.213572000	2.482008000	0.096244000
6	0.689587000	-0.872041000	3.772965000	6	4.827827000	-0.409597000	-0.750340000
6	0.499875000	3.535010000	1.376839000	1	6.992052000	-0.563467000	-0.928650000
6	0.001108000	3.961410000	0.179618000	1	2.739399000	0.151030000	-0.465461000
6	-2.519902000	1.807191000	-3.585510000	7	4.568201000	-1.736484000	-1.081021000
6	-2.974314000	0.547411000	-3.847724000	6	3.198576000	-2.253791000	-1.032616000
6	-2.758974000	-3.867953000	-1.466711000	6	5.671037000	-2.649772000	-1.362051000
6	-2.252703000	-4.296150000	-0.272573000	1	3.194324000	-3.280477000	-1.403566000
6	-1.012488000	-3.175000000	1.599096000	1	2.791541000	-2.249895000	-0.011448000
6	0.573152000	1.314545000	2.543477000	1	2.515074000	-1.659945000	-1.648351000
6	-1.232914000	2.842420000	-1.697381000	1	6.331610000	-2.787082000	-0.491953000
6	-2.837888000	-1.644440000	-2.633428000	1	5.265840000	-3.624754000	-1.636936000
1	-0.979738000	-4.125416000	2.121462000	1	6.287932000	-2.291509000	-2.197605000
1	1.109262000	1.782069000	3.362380000	1	-3.172963000	3.193573000	0.440895000
1	-1.254065000	3.790309000	-2.224298000	1	-2.855403000	0.225193000	3.485816000
1	-3.368849000	-2.114229000	-3.454612000	7	-2.738888000	0.165752000	4.489657000
1	0.334134000	-3.021113000	4.117940000	7	-3.170667000	4.201769000	0.349569000
1	1.223848000	-0.517351000	4.642080000	1	-2.821317000	-0.808975000	4.745069000
1	1.015686000	4.109713000	2.132090000	1	-3.267963000	0.789865000	5.083530000
1	0.027306000	4.955366000	-0.242198000	1	-3.380403000	4.417057000	-0.615720000
1	-2.618781000	2.694985000	-4.192718000	1	-3.692324000	4.756562000	1.014549000

II-1. For $^2\text{RC} + 2\text{NH}_3$ Complex.

26	-1.014302000	-0.164476000	-0.138713000	6	0.441696000	0.880261000	2.789865000
7	-0.586365000	-1.030701000	1.626152000	6	-0.833832000	3.044673000	-1.365111000
7	-0.364403000	1.606599000	0.579727000	6	-2.710990000	-1.135671000	-2.970922000
7	-1.699755000	0.778027000	-1.793272000	1	-1.524771000	-4.304315000	1.586951000
7	-1.911735000	-1.863204000	-0.756829000	1	0.937214000	1.197798000	3.701097000
6	-0.800792000	-2.352707000	1.975396000	1	-0.725282000	4.043927000	-1.772846000
6	0.052749000	-0.450350000	2.705609000	1	-3.198146000	-1.458129000	-3.885080000
6	0.247832000	1.833116000	1.804198000	1	-0.326245000	-3.558718000	3.808236000
6	-0.328223000	2.816135000	-0.094154000	1	0.721900000	-1.226776000	4.702302000
6	-1.477823000	2.103232000	-2.148747000	1	1.159928000	3.649113000	2.756266000
6	-2.338316000	0.193946000	-2.883067000	1	0.460329000	4.849884000	0.432698000
6	-2.513812000	-2.091278000	-1.981632000	1	-1.973530000	3.309879000	-3.972830000
6	-1.936984000	-3.076319000	-0.087373000	1	-3.024962000	0.983774000	-4.866931000
6	-0.281036000	-2.605298000	3.302513000	1	-3.428796000	-3.904737000	-2.935743000
6	0.247117000	-1.429639000	3.753567000	1	-2.726031000	-5.109893000	-0.615017000
6	0.665632000	3.215890000	1.899143000	8	0.437053000	-0.546010000	-0.832359000
6	0.313127000	3.821193000	0.727216000	16	-3.278699000	0.706270000	0.735693000
6	-2.011110000	2.354606000	-3.470134000	1	-4.107057000	0.046143000	-0.153038000
6	-2.541997000	1.181150000	-3.921087000	1	5.728479000	3.199553000	0.260290000
6	-2.930220000	-3.473646000	-2.079914000	6	5.485482000	2.169731000	0.019597000
6	-2.575795000	-4.081415000	-0.909211000	6	6.491248000	1.265768000	-0.341544000
6	-1.427294000	-3.302526000	1.181858000	6	4.159848000	1.718554000	0.063863000

6	6.188112000	-0.060471000	-0.652021000	1	2.434658000	-1.729903000	-1.277144000
1	7.526741000	1.592228000	-0.381066000	1	6.297073000	-2.953937000	-0.440593000
6	3.833844000	0.396914000	-0.240864000	1	5.150703000	-3.743634000	-1.541986000
1	3.362252000	2.403070000	0.338118000	1	6.178812000	-2.430321000	-2.134751000
6	4.847795000	-0.525255000	-0.612883000	1	-2.931928000	3.341342000	0.627318000
1	6.992900000	-0.732637000	-0.921916000	1	-3.169671000	0.032505000	3.306636000
1	2.795534000	0.089882000	-0.210535000	7	-3.156937000	-0.150540000	4.302195000
7	4.535290000	-1.845328000	-0.926819000	7	-2.833686000	4.348386000	0.659206000
6	3.169360000	-2.343496000	-0.745557000	1	-3.347702000	-1.135160000	4.429687000
6	5.596745000	-2.784671000	-1.273753000	1	-3.685382000	0.451237000	4.919229000
1	3.109999000	-3.362771000	-1.132229000	1	-2.929140000	4.690269000	-0.287433000
1	2.873383000	-2.355663000	0.314174000	1	-3.367683000	4.872893000	1.338809000

III-1. For $^4 TS_H + 2NH_3$ Complex.

26	0.995795000	0.109167000	-0.033255000	1	2.963497000	-2.140527000	-4.328782000
7	0.517509000	1.406483000	1.480278000	1	4.079923000	2.889795000	-3.239932000
7	0.004862000	-1.363788000	0.933320000	1	3.359859000	4.629813000	-1.295100000
7	1.494910000	-1.165561000	-1.482487000	8	-0.426480000	0.620929000	-0.901742000
7	2.125795000	1.545253000	-0.880547000	16	2.831323000	-0.533851000	1.343519000
6	0.881873000	2.737452000	1.578415000	1	3.603085000	0.602279000	1.192200000
6	-0.227268000	1.118655000	2.610803000	1	-6.505220000	-2.548035000	-0.645247000
6	-0.671131000	-1.259676000	2.140965000	6	-5.892177000	-1.656632000	-0.724865000
6	-0.181796000	-2.659181000	0.489655000	6	-6.334327000	-0.558916000	-1.473047000
6	1.094880000	-2.487470000	-1.603011000	6	-4.644180000	-1.595172000	-0.091423000
6	2.301072000	-0.901965000	-2.577851000	6	-5.550067000	0.590518000	-1.582925000
6	2.843396000	1.437626000	-2.057990000	1	-7.297739000	-0.593046000	-1.971909000
6	2.255800000	2.863073000	-0.461971000	6	-3.847692000	-0.454711000	-0.191201000
6	0.337965000	3.304115000	2.796014000	1	-4.272857000	-2.445182000	0.471664000
6	-0.343394000	2.305921000	3.433308000	6	-4.298078000	0.660245000	-0.932792000
6	-1.286280000	-2.530740000	2.462160000	1	-5.920980000	1.434194000	-2.152280000
6	-0.985973000	-3.392240000	1.444293000	1	-2.862159000	-0.448329000	0.255311000
6	1.650569000	-3.057348000	-2.814041000	7	-3.508962000	1.824577000	-1.019038000
6	2.394664000	-2.083253000	-3.412130000	6	-2.422520000	2.042412000	-0.144619000
6	3.459657000	2.708886000	-2.374075000	6	-3.725538000	2.765518000	-2.126075000
6	3.095226000	3.586879000	-1.393543000	1	-2.064167000	3.070285000	-0.176369000
6	1.679939000	3.419368000	0.669807000	1	-2.603162000	1.689640000	0.871410000
6	-0.781421000	-0.115928000	2.917864000	1	-1.374747000	1.332069000	-0.512987000
6	0.317113000	-3.183920000	-0.694764000	1	-4.603609000	3.399098000	-1.945721000
6	2.935374000	0.298965000	-2.845262000	1	-2.848128000	3.405907000	-2.220530000
1	1.885035000	4.465650000	0.870529000	1	-3.866527000	2.225913000	-3.067016000
1	-1.343917000	-0.194734000	3.842182000	1	3.539743000	-2.858764000	0.262539000
1	0.091302000	-4.220910000	-0.918343000	1	1.619668000	-1.104404000	3.641769000
1	3.538514000	0.358653000	-3.744723000	7	1.204725000	-1.387519000	4.520674000
1	0.479802000	4.327209000	3.113189000	7	3.815396000	-3.772870000	-0.073964000
1	-0.871562000	2.350028000	4.374841000	1	0.963605000	-0.545071000	5.024921000
1	-1.864358000	-2.722460000	3.354604000	1	1.675796000	-2.081118000	5.085594000
1	-1.268298000	-4.429716000	1.338329000	1	4.344028000	-3.633740000	-0.924441000
1	1.488189000	-4.074071000	-3.141150000	1	4.241627000	-4.425499000	0.569870000

IV-1. For $^2 TS_H + 2NH_3$ Complex.

26	-0.951112000	0.050163000	-0.165470000	6	1.219588000	3.237581000	1.699557000
7	-0.843568000	-1.312814000	1.312651000	6	-0.940221000	3.416181000	-2.824221000
7	0.089173000	1.350023000	0.976847000	6	-1.661304000	2.544219000	-3.586758000
7	-1.160985000	1.462330000	-1.600710000	6	-3.410567000	-2.117104000	-2.930778000
7	-2.155052000	-1.180996000	-1.223996000	6	-3.348150000	-3.038537000	-1.924779000
6	-1.450821000	-2.560460000	1.333008000	6	-2.238301000	-3.095261000	0.326190000
6	-0.178251000	-1.185426000	2.522925000	6	0.528895000	-0.068873000	2.942705000
6	0.640938000	1.112973000	2.224292000	6	0.105880000	3.292803000	-0.545902000
6	0.433716000	2.647621000	0.636162000	6	-2.496086000	0.199954000	-3.239506000
6	-0.625693000	2.737123000	-1.582624000	1	-2.638701000	-4.091571000	0.480452000
6	-1.800426000	1.322350000	-2.819251000	1	1.003935000	-0.112025000	3.916833000
6	-2.661979000	-0.957219000	-2.493668000	1	0.454908000	4.312176000	-0.671002000
6	-2.556602000	-2.454710000	-0.861979000	1	-2.955398000	0.232833000	-4.221602000
6	-1.140701000	-3.233794000	2.575898000	1	-1.495016000	-4.219025000	2.842495000
6	-0.355109000	-2.388978000	3.307061000	1	0.060641000	-2.543819000	4.292214000
6	1.350302000	2.291409000	2.676951000	1	1.862591000	2.371435000	3.624871000

1	1.606141000	4.246385000	1.686595000	1	2.818482000	0.098329000	0.508415000
1	-0.640815000	4.426711000	-3.061350000	7	3.362737000	-2.141410000	-0.871988000
1	-2.072704000	2.696900000	-4.573982000	6	2.142150000	-2.267877000	-0.158846000
1	-3.912675000	-2.197380000	-3.884050000	6	3.614102000	-3.038657000	-2.007325000
1	-3.788648000	-4.024410000	-1.889279000	1	1.693898000	-3.250941000	-0.303297000
8	0.441750000	-0.496961000	-1.000331000	1	2.245507000	-2.025539000	0.900646000
16	-2.924049000	0.996242000	0.874538000	1	1.310051000	-1.469920000	-0.564665000
1	-3.811197000	0.787639000	-0.163625000	1	4.403283000	-3.764878000	-1.773589000
1	6.740810000	1.823601000	0.162928000	1	2.697796000	-3.583031000	-2.236202000
6	6.049933000	1.015206000	-0.051239000	1	3.911230000	-2.467413000	-2.891907000
6	6.455731000	-0.072418000	-0.834667000	1	-2.083450000	3.433351000	1.529895000
6	4.739079000	1.053587000	0.441460000	1	-3.068383000	-0.390454000	3.139893000
6	5.572226000	-1.114259000	-1.118169000	7	-3.138567000	-0.848630000	4.039867000
1	7.467321000	-0.113658000	-1.225833000	7	-1.799385000	4.350483000	1.850802000
6	3.842772000	0.020685000	0.169079000	1	-3.516912000	-1.772221000	3.878759000
1	4.398195000	1.900244000	1.028078000	1	-3.573807000	-0.357247000	4.808783000
6	4.253730000	-1.085961000	-0.609137000	1	-1.782872000	4.959844000	1.044249000
1	5.913673000	-1.952746000	-1.712717000	1	-2.257625000	4.752570000	2.657228169

V-1. For $^4\text{IM} + 2\text{NH}_3$ Complex.

26	-1.050118000	-0.105045000	-0.097882000	1	-3.099575000	2.161936000	-4.358826000
7	-0.443667000	-1.426227000	1.324058000	1	-3.776389000	-2.992997000	-3.531274000
7	-0.219343000	1.399173000	0.955961000	1	-3.017015000	-4.739347000	-1.606922000
7	-1.648385000	1.195526000	-1.504414000	8	0.455922000	-0.414355000	-1.036659000
7	-2.038048000	-1.590539000	-1.041867000	16	-2.986955000	0.338587000	1.201523000
6	-0.732839000	-2.781221000	1.376427000	1	-3.846880000	-0.543386000	0.576360000
6	0.280269000	-1.134826000	2.469889000	1	6.198252000	3.052799000	-0.383001000
6	0.486414000	1.293531000	2.145124000	6	5.733815000	2.080040000	-0.506210000
6	-0.178742000	2.734192000	0.591340000	6	6.464923000	1.008795000	-1.033052000
6	-1.398489000	2.556645000	-1.532196000	6	4.392476000	1.884171000	-0.152650000
6	-2.372369000	0.905686000	-2.647950000	6	5.874315000	-0.247074000	-1.192379000
6	-2.709423000	-1.494154000	-2.250497000	1	7.504386000	1.145701000	-1.315064000
6	-2.083926000	-2.927533000	-0.672616000	6	3.785546000	0.637699000	-0.311739000
6	-0.148188000	-3.356384000	2.568331000	1	3.802582000	2.709297000	0.234030000
6	0.476136000	-2.343661000	3.240499000	6	4.527619000	-0.447193000	-0.824490000
6	0.966615000	2.599747000	2.540302000	1	6.465963000	-1.069183000	-1.578214000
6	0.555850000	3.486505000	1.585015000	1	2.729017000	0.518524000	-0.106033000
6	-1.969185000	3.131425000	-2.732607000	7	3.922720000	-1.720658000	-0.961617000
6	-2.567455000	2.115371000	-3.419872000	6	2.832026000	-2.092692000	-0.194992000
6	-3.212130000	-2.795531000	-2.631474000	6	4.452655000	-2.667229000	-1.952941000
6	-2.828631000	-3.676898000	-1.660418000	1	2.456854000	-3.097472000	-0.335407000
6	-1.488127000	-3.482541000	0.449230000	1	2.703332000	-1.613384000	0.767269000
6	0.723224000	0.123004000	2.849031000	1	1.112616000	-1.104166000	-0.738898000
6	-0.724038000	3.277118000	-0.561460000	1	5.311665000	-3.227825000	-1.560958000
6	-2.867585000	-0.338684000	-2.999836000	1	3.667112000	-3.377605000	-2.218276000
1	-1.625146000	-4.545586000	0.614754000	1	4.759421000	-2.134320000	-2.856221000
1	1.285947000	0.199401000	3.772856000	1	-3.239411000	2.972433000	0.928173000
1	-0.609669000	4.344265000	-0.716057000	1	-2.098523000	-0.085302000	3.672676000
1	-3.421330000	-0.415103000	-3.929029000	7	-1.798698000	-0.179106000	4.635023000
1	-0.225620000	-4.397427000	2.846485000	7	-3.349931000	3.978404000	0.903404000
1	1.010845000	-2.390965000	4.178015000	1	-1.740405000	-1.167984000	4.837121000
1	1.541068000	2.794820000	3.434114000	1	-2.269872000	0.357128000	5.350963000
1	0.726559000	4.552329000	1.541508000	1	-3.749016000	4.215363000	0.005238000
1	-1.912425000	4.177578000	-2.995664000	1	-3.794461000	4.443232000	1.683435000

VI-1. For $^4\text{Carbinolaniline} + 2\text{NH}_3$ Complex.

26	1.053491000	0.297828000	0.212824000	6	0.545410000	-0.578115000	3.113621000
7	1.177945000	-1.304888000	-1.003280000	6	0.811924000	-2.337740000	1.784215000
7	1.005736000	1.507714000	-1.402657000	6	1.445221000	-3.472446000	-1.782817000
7	0.686992000	1.874579000	1.401020000	6	1.557343000	-2.638538000	-2.862118000
7	0.708602000	-0.950038000	1.783635000	6	1.236816000	2.317008000	-3.565264000
6	1.211071000	-2.643089000	-0.624219000	6	1.038278000	3.395507000	-2.751288000
6	1.390195000	-1.288972000	-2.378131000	6	0.416531000	4.040405000	2.182973000
6	1.222239000	1.139891000	-2.723665000	6	0.342960000	3.208883000	3.265736000
6	0.902713000	2.891371000	-1.401557000	6	0.515022000	-1.755546000	3.951719000
6	0.623799000	3.208570000	1.019954000	6	0.677693000	-2.838365000	3.133659000
6	0.501412000	1.858048000	2.777759000	6	1.036620000	-3.124788000	0.665979000

6	1.408842000	-0.155575000	-3.178507000	1	-7.906789000	-1.219070000	-0.445286000
6	0.724733000	3.683883000	-0.279022000	6	-4.575759000	0.734894000	-0.065991000
6	0.445363000	0.724400000	3.575572000	1	-5.777333000	2.342736000	0.686752000
1	1.097433000	-4.197861000	0.811452000	6	-4.554627000	-0.580200000	-0.584665000
1	1.581901000	-0.295154000	-4.240021000	1	-5.797440000	-2.284124000	-1.100713000
1	0.662094000	4.756559000	-0.426222000	1	-3.644024000	1.260872000	0.102052000
1	0.309734000	0.869404000	4.641775000	7	-3.336315000	-1.179813000	-0.971479000
1	1.519490000	-4.4550024000	-1.760219000	6	-2.165868000	-0.378402000	-1.186390000
1	1.738529000	-2.901600000	-3.894126000	6	-3.296328000	-2.607908000	-1.297596000
1	1.386417000	2.303511000	-4.635053000	1	-1.455750000	-0.938174000	-1.798075000
1	0.992899000	4.440204000	-3.022495000	1	-2.405896000	0.568708000	-1.672415000
1	0.333651000	5.117232000	2.159247000	1	-1.462240000	-0.694435000	0.703789000
1	0.187200000	3.471442000	4.301964000	1	-3.832972000	-2.840035000	-2.229129000
1	0.392995000	-1.740583000	5.024978000	1	-2.256274000	-2.918890000	-1.416893000
1	0.716596000	-3.882943000	3.406464000	1	-3.740272000	-3.205059000	-0.492625000
8	-1.487434000	0.044841000	0.059582000	1	4.359634000	0.287883000	-2.023788000
16	3.514202000	0.355297000	0.497382000	1	4.003753000	-2.048618000	1.525547000
1	3.589620000	1.504540000	1.261482000	7	4.252309000	-2.969057000	1.865867000
1	-7.933984000	1.112921000	0.437903000	7	4.736191000	0.207815000	-2.960057000
6	-6.997923000	0.643454000	0.154561000	1	4.016831000	-3.000375000	2.848562000
6	-6.979117000	-0.664648000	-0.338274000	1	5.168097000	-3.340815000	1.653145000
6	-5.786163000	1.332758000	0.287824000	1	4.643383000	1.113194000	-3.400279000
6	-5.776681000	-1.275430000	-0.706970000	1	5.643667000	-0.218507000	-3.089893000

VII. For ² Carbinolaniline + 2NH₃ Complex.

26	-0.833332000	0.065471000	0.316798000	1	2.065420000	3.668696000	2.785499000
7	-1.944417000	-0.942631000	-1.042344000	1	-0.335307000	4.873284000	-1.723077000
7	-0.666929000	-1.590230000	1.458255000	1	-1.895549000	3.550218000	-3.493654000
7	0.381939000	1.026435000	1.601839000	8	0.866128000	-0.468887000	-0.792542000
7	-0.898760000	1.674894000	-0.900336000	16	-2.716098000	0.772929000	1.419117000
6	-2.510653000	-0.455807000	-2.212993000	1	-2.321226000	0.458610000	2.705853000
6	-2.391988000	-2.249815000	-0.913962000	1	7.161714000	1.313242000	-0.310166000
6	-1.299216000	-2.804641000	1.229606000	6	6.289968000	0.713247000	-0.548670000
6	0.010508000	-1.730238000	2.663680000	6	6.359439000	-0.283589000	-1.526205000
6	0.938924000	0.543799000	2.777404000	6	5.073264000	0.932023000	0.108640000
6	0.787402000	2.347353000	1.495560000	6	5.240202000	-1.061817000	-1.837479000
6	-0.323071000	2.908537000	-0.636210000	1	7.291782000	-0.466591000	-2.051918000
6	-1.602328000	1.824705000	-2.087602000	6	3.943558000	0.171288000	-0.197129000
6	-3.311792000	-1.486509000	-2.838272000	1	4.990574000	1.712386000	0.858859000
6	-3.239174000	-2.591313000	-2.038309000	6	4.016407000	-0.851640000	-1.168599000
6	-1.003340000	-3.722667000	2.309814000	1	5.330853000	-1.835545000	-2.589690000
6	-0.196447000	-3.061201000	3.192236000	1	3.002109000	0.398897000	0.286217000
6	1.715849000	1.584769000	3.417139000	7	2.885287000	-1.650774000	-1.463520000
6	1.621784000	2.696129000	2.628050000	6	1.755584000	-1.657567000	-0.597345000
6	-0.661794000	3.843914000	-1.689676000	6	2.907663000	-2.545277000	-2.625570000
6	-1.449144000	3.176330000	-2.583596000	1	1.158490000	-2.555527000	-0.760680000
6	-2.347364000	0.830795000	-2.706378000	1	2.033633000	-1.578227000	0.452045000
6	-2.089426000	-3.112217000	0.130226000	1	0.697232000	-0.295755000	-1.739816000
6	0.769054000	-0.741132000	3.274297000	1	3.619838000	-3.371977000	-2.496743000
6	0.461091000	3.217565000	0.465081000	1	1.913196000	-2.973755000	-2.767476000
1	-2.851787000	1.082734000	-3.633026000	1	3.179084000	-2.000786000	-3.537505000
1	-2.517916000	-4.108363000	0.090741000	1	-4.628087000	-0.590471000	0.169703000
1	1.253708000	-0.986146000	4.213370000	1	-2.920029000	3.293587000	0.594320000
1	0.850074000	4.228453000	0.528764000	7	-3.076555000	4.239771000	0.270221000
1	-3.858620000	-1.362624000	-3.761876000	7	-5.398952000	-1.041266000	-0.307117000
1	-3.715568000	-3.551144000	-2.177438000	1	-2.420140000	4.836517000	0.755126000
1	-1.375615000	-4.735093000	2.372884000	1	-4.020095000	4.602300000	0.249538000
1	0.222273000	-3.425287000	4.119355000	1	-5.427290000	-2.001628000	0.007561000
1	2.252443000	1.466487000	4.347417000	1	-6.302603000	-0.588035000	-0.317885000

Table S20 Cartesian Coordinates for Various Reaction Species in C–H Hydroxylation of p-Cl-DMA by Cpd I

I. For ^4RC

26	-2.378685000	-0.258944000	0.095413000	6	4.276460000	0.820150000	0.608992000
7	-2.974823000	-2.124344000	0.588174000	6	-0.683382000	4.232814000	-0.089752000
7	-1.815902000	0.046951000	2.008232000	6	-4.159809000	0.617093000	0.002220000
7	-2.055317000	1.689813000	-0.304324000	6	-4.139263000	-0.738950000	0.154098000
7	-3.203148000	-0.495682000	-1.731407000	6	-0.536578000	-4.189856000	0.704506000
6	-3.544261000	-3.072950000	-0.259315000	6	0.825967000	-4.158834000	0.794949000
6	-2.755772000	-2.779297000	1.796128000	6	2.534896000	-2.321739000	0.744635000
6	-1.756785000	-0.895787000	3.022083000	6	2.446272000	2.515145000	0.329424000
6	-1.304213000	1.219526000	2.549175000	6	-2.390511000	2.393689000	-0.075761000
6	-1.504333000	2.632595000	0.541702000	6	-2.310574000	-2.434437000	0.432879000
6	-2.249257000	2.331404000	-1.515081000	1	3.314274000	-3.066360000	0.868010000
6	-3.237465000	0.442850000	-2.751296000	1	3.197790000	3.297390000	0.328158000
6	-3.726631000	-1.658663000	-2.267659000	1	-3.165100000	3.136734000	-0.231394000
6	-3.705519000	-4.326239000	0.443716000	1	-3.060035000	-3.218725000	0.445217000
6	-3.218181000	-4.146485000	1.705834000	1	5.157358000	-1.187468000	0.850900000
6	-1.202032000	-0.301789000	4.219889000	1	5.106788000	1.510849000	0.623002000
6	-0.927118000	1.003631000	3.929750000	1	1.326496000	5.131611000	0.023754000
6	-1.345969000	3.892779000	-0.152520000	1	-1.366801000	5.058154000	-0.224274000
6	-1.805921000	3.706359000	-1.424416000	1	-5.014689000	1.262595000	-0.135500000
6	-3.801099000	-0.145891000	-3.946293000	1	-4.973946000	-1.424454000	0.164489000
6	-4.102199000	-1.444482000	-3.648146000	1	-1.192175000	-5.047651000	0.738081000
6	-3.885612000	-2.857361000	-1.582212000	1	1.509005000	-4.986525000	0.917684000
6	-2.176896000	-2.213418000	2.918209000	8	0.172032000	-0.134244000	-1.423011000
6	-1.160230000	2.416985000	1.870113000	16	-0.379179000	0.455052000	2.727928000
6	-2.799210000	1.754235000	-2.649997000	1	-1.035999000	-0.727412000	3.015154000
1	-4.312920000	-3.690987000	-2.129425000	17	-0.506807000	6.169922000	-4.848072000
1	-2.059555000	-2.844693000	3.792359000	6	-0.069632000	4.403505000	-5.110782000
1	-0.738619000	3.252972000	2.417782000	6	0.059176000	3.916819000	-6.406998000
1	-2.892921000	2.379940000	-3.531355000	6	0.129050000	3.577127000	-4.008160000
1	-4.133217000	-5.219095000	0.011728000	1	0.394068000	2.575563000	-6.605865000
1	-3.168864000	-4.862587000	2.512865000	1	-0.095363000	4.570084000	-7.257695000
1	-1.053219000	-0.826431000	5.152048000	6	0.464015000	2.236329000	-4.200364000
1	-0.503155000	1.758546000	4.575154000	1	0.025817000	3.967518000	-3.002727000
1	-0.937318000	4.789452000	0.289547000	6	0.599885000	1.700615000	-5.508156000
1	-1.850679000	4.420556000	-2.233437000	1	0.495496000	2.216153000	-7.621605000
1	-3.941845000	0.377828000	-4.880447000	1	0.600054000	1.607566000	-3.329285000
1	-4.538889000	-2.196166000	-4.289220000	7	0.926735000	0.363904000	-5.704321000
8	-0.872996000	-0.715984000	-0.414448000	6	1.267983000	-0.485152000	-4.559843000
16	-4.696938000	0.232575000	1.089342000	6	1.113646000	-0.150473000	-7.057213000
1	-5.456587000	-0.520282000	0.212855000	1	1.387088000	-1.513840000	-4.905572000
17	3.890518000	0.573719000	4.582290000	1	2.205990000	-0.171423000	-4.076573000
6	3.737239000	0.016901000	2.836104000	1	0.486853000	-0.470816000	-3.793805000
6	4.871198000	-0.035799000	2.033526000	1	1.953356000	0.333666000	-7.580734000
6	2.487635000	-0.347041000	2.342075000	1	1.319175000	-1.220843000	-7.005779000
6	4.753541000	-0.459261000	0.707677000	1	0.211238000	-0.010138000	-7.667471000
1	5.839770000	0.245152000	2.430160000				
6	2.363490000	-0.770277000	1.018278000				
1	1.611891000	-0.303734000	2.978067000	26	-2.202150000	-0.095522000	-0.038466000
6	3.496232000	-0.829512000	0.1646435000	7	-2.280009000	-2.125242000	0.247374000
1	5.648145000	-0.498849000	0.099987000	7	-1.674641000	0.142337000	1.898450000
1	1.379326000	-1.035378000	0.651994000	7	-2.166102000	1.878390000	-0.300887000
7	3.376713000	-1.239841000	-1.158563000	7	-2.905202000	-0.351755000	-1.907263000
6	2.094745000	-1.741552000	-1.661210000	6	-2.618197000	-3.082975000	-0.692160000
6	4.568497000	-1.369428000	-1.990799000	6	-2.012187000	-2.805901000	1.422781000
1	2.173334000	-1.892688000	-2.739663000	6	-1.489270000	-0.859559000	2.841766000
1	1.812488000	-2.699297000	-1.197017000	6	-1.370062000	1.334542000	2.528044000
1	1.280636000	-1.034801000	-1.473482000	6	-1.781942000	2.835364000	0.626374000
1	5.270722000	-2.126980000	-1.607727000	6	-2.508460000	2.569259000	-1.452254000
1	4.269456000	-1.663970000	-2.998012000	6	-3.145473000	0.642853000	-2.837916000
1	5.110295000	-0.417015000	-2.066604000	6	-3.144010000	-1.557990000	-2.553623000

II. For ^2RC

26	0.088380000	0.024122000	0.217842000	6	-2.545397000	-4.400752000	-0.094436000
7	2.079832000	0.084916000	0.489374000	6	-2.174547000	-4.229739000	1.209454000
7	0.035552000	2.041193000	0.171179000	6	-1.067866000	-0.271168000	4.095882000
7	-1.935722000	-0.005847000	0.253164000	6	-0.992881000	1.080176000	3.902121000
7	0.106234000	-1.965574000	0.553787000	6	-1.868278000	4.154130000	0.031863000
6	2.930338000	-0.995417000	0.650402000	6	-2.317985000	3.990833000	-1.245250000
6	2.889195000	1.205356000	0.463524000	6	-3.569685000	0.051369000	-4.089121000
6	1.124311000	2.902595000	0.192220000	6	-3.565267000	-1.303167000	-3.915092000
6	-1.080480000	2.843253000	-0.004156000	6	-3.007851000	-2.821057000	-1.998743000
6	-2.788784000	1.075199000	0.055134000	6	-1.642915000	-2.221109000	2.625846000
6	-2.754649000	-1.131822000	0.296618000	6	-1.410293000	2.589811000	1.936335000

6	-2.971815000	2.003106000	-2.627149000	1	5.097835000	-1.334953000	0.140832000
1	-3.243617000	-3.670972000	-2.630460000	1	5.111578000	1.366259000	-0.033660000
1	-1.462944000	-2.881502000	3.467532000	1	1.390756000	5.108246000	-0.109793000
1	-1.143417000	3.442655000	2.550877000	1	-1.315290000	5.103960000	0.003749000
1	-3.202385000	2.671429000	-3.449629000	1	-5.042769000	1.400354000	0.112338000
1	-2.766031000	-5.322604000	-0.612975000	1	-5.058471000	-1.306866000	0.133650000
1	-2.029498000	-4.983869000	1.969434000	1	-1.337580000	-5.041437000	0.270880000
1	-0.864683000	-0.831332000	4.997134000	1	1.369835000	-5.044251000	0.312430000
1	-0.717869000	1.845261000	4.613642000	8	-0.135950000	-0.064239000	-1.718556000
1	-1.621501000	5.072490000	0.544413000	16	0.029814000	0.190105000	2.402565000
1	-2.512480000	4.748356000	-1.990458000	1	-0.634832000	-0.989296000	2.677042000
1	-3.825608000	0.612943000	-4.975812000	17	-0.827200000	6.044689000	-5.791452000
1	-3.819577000	-2.071881000	-4.630468000	6	-0.218492000	4.354674000	-5.465627000
8	-0.545766000	-0.247329000	-0.566548000	6	-0.033268000	3.481068000	-6.535260000
16	-4.428768000	-0.087220000	0.808316000	6	0.040001000	3.962341000	-4.153587000
1	-5.058270000	-0.665373000	-0.277390000	6	0.432853000	2.189229000	-6.288776000
17	5.123167000	0.997058000	4.073167000	1	-0.243657000	3.802060000	-7.547990000
6	4.293410000	0.173206000	2.669547000	6	0.506332000	2.672149000	-3.903834000
6	5.056522000	-0.259416000	1.587469000	1	-0.135316000	4.639922000	-3.327248000
6	2.910884000	0.000642000	2.698755000	6	0.721429000	1.769144000	-4.970496000
6	4.424372000	-0.890726000	0.514955000	1	0.589710000	1.522822000	-7.127483000
1	6.129680000	-0.113529000	1.579974000	1	0.645036000	2.352946000	-2.879881000
6	2.276828000	-0.628769000	1.628019000	7	1.212665000	0.477804000	-4.720693000
1	2.324333000	0.366154000	3.532474000	6	1.763339000	0.136834000	-3.457932000
6	3.026588000	-1.094851000	0.524438000	6	1.015383000	-0.580309000	-5.720174000
1	5.027634000	-1.240128000	-0.313538000	1	2.296080000	-0.813053000	-3.495057000
1	1.198032000	-0.705687000	1.626672000	1	2.384045000	0.931289000	-3.038192000
7	2.388949000	-1.751814000	-0.542803000	1	0.879758000	-0.016397000	-2.617249000
6	1.065940000	-2.232006000	-0.421147000	1	1.717741000	-0.474170000	-6.557058000
6	3.051618000	-1.817416000	-1.852271000	1	1.184045000	-1.547843000	-5.247222000
1	0.789531000	-2.897411000	-1.237245000	1	-0.006446000	-0.557271000	-6.111138000

V. For ⁴Int. Complex

26	0.030088000	0.027365000	-0.011016000	26	-2.281524000	-0.059863000	0.022565000
7	2.042561000	0.027613000	-0.001888000	7	-2.231827000	-2.077875000	0.256377000
7	0.043920000	2.046430000	0.005542000	7	-1.757519000	0.171211000	1.954084000
7	-1.991170000	0.029531000	0.096274000	7	-2.326345000	1.932216000	-0.214987000
7	0.021466000	-1.985205000	0.169952000	7	-2.984052000	-0.306577000	-1.853420000
6	2.869870000	-1.083287000	0.089657000	6	-2.597360000	-3.033259000	-0.680275000
6	2.880867000	1.132123000	-0.049672000	6	-1.896900000	-2.768927000	1.411148000
6	1.150016000	2.877349000	-0.058007000	6	-1.472749000	-0.833953000	2.866798000
6	-1.066844000	2.874291000	0.032008000	6	-1.538242000	1.371476000	2.609699000
6	-2.812695000	1.142137000	0.092394000	6	-2.017478000	2.886659000	0.738842000
6	-2.825300000	-1.074060000	0.112990000	6	-2.651345000	2.622572000	-1.370136000
6	-1.089344000	-2.813306000	0.181677000	6	-3.219879000	0.695561000	-2.781873000
6	1.127922000	-2.815534000	0.211040000	6	-3.221888000	-1.509068000	-2.504732000
6	4.254288000	-0.662924000	0.077439000	6	-2.456498000	-4.353677000	-0.106663000
6	4.261351000	0.700008000	-0.011521000	6	-2.024038000	-4.191174000	1.179351000
6	0.722103000	4.260386000	-0.073109000	6	-1.079188000	-0.245035000	4.127926000
6	-0.643558000	4.257999000	-0.014459000	6	-1.121336000	1.111950000	3.970415000
6	-4.200506000	0.723959000	0.108445000	6	-2.138923000	4.208798000	0.161070000
6	-4.208367000	-0.640408000	0.118484000	6	-2.527152000	4.046351000	-1.137169000
6	-0.665235000	-4.196169000	0.244915000	1	-3.641902000	0.107562000	-4.035353000
6	0.700268000	-4.197680000	0.265982000	1	-3.645116000	-1.248099000	-3.862600000
6	2.450805000	-2.400657000	0.181569000	1	-3.052550000	-2.773922000	-1.963664000
6	2.471546000	2.456142000	-0.096107000	1	-1.531955000	-2.196593000	2.620018000
6	-2.389071000	2.460666000	0.071619000	1	-1.658966000	2.634366000	2.051807000
6	-2.411221000	-2.395846000	0.149843000	1	-3.065438000	2.055669000	-2.563559000
1	3.216991000	-3.166529000	0.236652000	1	-3.293653000	-3.624230000	-2.592076000
1	3.241518000	3.219066000	-0.134034000	1	-1.289854000	-2.864870000	3.438941000
1	-3.152467000	3.231110000	0.080762000	1	-1.450307000	3.486488000	2.688963000
1	-3.178847000	-3.161945000	0.166813000	1	-3.289629000	2.724682000	-3.386919000

6	5.100955000	-0.452037000	1.717706000	1	-1.267560000	-0.241133000	-4.579104000
6	2.852275000	0.197196000	2.373954000	7	0.620914000	1.650488000	-4.329006000
6	4.577576000	-1.173214000	0.641861000	6	-0.255968000	1.627300000	-3.181401000
1	6.170268000	-0.422648000	1.888062000	6	1.838449000	2.462618000	-4.292843000
6	2.327919000	-0.516486000	1.295614000	1	0.042641000	2.429124000	-2.501061000
1	2.189522000	0.744449000	3.033178000	1	-1.295740000	1.774036000	-3.482450000
6	3.184613000	-1.222596000	0.423516000	1	0.597943000	0.108439000	-2.131386000
1	5.257499000	-1.712900000	-0.006270000	1	1.759137000	3.363211000	-4.919486000
1	1.265862000	-0.466449000	1.089319000	1	2.026287000	2.778859000	-3.265065000
7	2.646562000	-1.971219000	-0.647345000	1	2.706979000	1.886471000	-4.634511000
6	1.349867000	-2.458622000	-0.612159000				
6	3.478707000	-2.242779000	-1.828168000				
1	1.024438000	-3.042646000	-1.462068000				
1	0.902782000	-2.640596000	0.356886000				
1	-0.109315000	-0.939991000	-0.721628000				
1	4.130117000	-3.113447000	-1.675158000	26	0.479527000	0.418774000	0.149252000
1	2.826498000	-2.444308000	-2.680199000	7	2.296487000	-0.442227000	-0.054127000
1	4.096895000	-1.372682000	-2.062472000	7	1.401126000	2.202287000	0.395524000

VII. For ² Carbinolainline Complex.

26	0.252487000	0.385399000	0.558969000	7	-0.433516000	-1.330535000	-0.236588000
7	1.891711000	-0.391247000	-0.360066000	6	2.534117000	-1.801673000	-0.208645000
7	1.020047000	2.224971000	0.286792000	6	3.545682000	0.153850000	0.076285000
7	-1.536473000	1.209484000	0.984226000	6	2.765527000	2.454031000	0.461263000
7	-0.615807000	-1.421898000	0.484732000	6	0.774624000	3.410158000	0.672738000
6	2.165140000	-1.744635000	-0.561950000	6	-1.566070000	2.650130000	0.494344000
6	3.081531000	0.278205000	-0.650088000	6	-2.570865000	0.726242000	0.031404000
6	2.321075000	2.545565000	-0.094540000	6	-1.793715000	-1.573588000	-0.357132000
6	0.415891000	3.434266000	0.623751000	6	0.192667000	-2.556997000	-0.390135000
6	-1.801435000	2.556028000	1.202232000	6	3.959550000	-2.054477000	-0.195578000
6	-2.714476000	0.538782000	1.286654000	6	4.582280000	-0.850522000	-0.024201000
6	-1.918000000	-1.740816000	0.855954000	6	2.994527000	3.850881000	0.762924000
6	-0.014445000	-2.628726000	0.140405000	6	1.768727000	4.438980000	0.897090000
6	3.523252000	-1.909905000	-1.019820000	6	-2.992582000	2.897396000	0.512368000
6	4.087174000	-0.665691000	-1.073469000	6	-3.610984000	1.713931000	0.222273000
6	2.526055000	3.970100000	0.007499000	6	-2.022864000	-2.984181000	-0.593889000
6	1.352347000	4.517016000	0.449188000	6	-0.799472000	-3.590627000	-0.609201000
6	-3.170790000	2.726765000	1.633740000	6	1.562394000	-2.778371000	-0.367119000
6	-3.733605000	1.483909000	1.685124000	6	3.765848000	1.505984000	0.297482000
6	-2.121371000	-3.166780000	0.763441000	6	-0.596688000	3.618254000	0.717920000
6	-0.948615000	-3.713847000	0.323264000	6	-2.791472000	-0.616117000	-0.242460000
6	1.277948000	-2.782593000	-0.335868000	1	1.902002000	-3.801352000	-0.490634000
6	3.280315000	1.642955000	-0.529537000	1	4.794215000	1.840694000	0.382112000
6	-0.894915000	3.590032000	1.045128000	1	-0.940138000	4.621815000	0.946337000
6	-2.893582000	-0.832920000	1.234206000	1	-3.819650000	-0.945231000	-0.348980000
1	1.617651000	-3.790016000	-0.548880000	1	4.409401000	-3.031075000	-0.301377000
1	4.259346000	2.033802000	-0.784086000	1	5.641512000	-0.647663000	0.040264000
1	-1.234713000	4.595648000	1.266761000	1	3.969834000	4.303652000	0.868885000
1	-3.869149000	-1.224627000	1.499892000	1	1.542413000	5.469014000	1.132363000
1	3.977100000	-2.860682000	-1.257922000	1	-3.446010000	3.855423000	0.722279000
1	5.093504000	-0.399755000	-1.362298000	1	-4.669822000	1.511641000	0.149721000
1	3.452271000	4.474195000	-0.227125000	1	-2.996303000	-3.434979000	-0.722541000
1	1.130396000	5.555969000	0.644404000	1	-0.572200000	-4.636496000	-0.756756000
1	-3.625208000	3.678791000	1.865787000	8	0.637544000	0.710653000	-1.957803000
1	-4.741097000	1.215198000	1.967017000	16	0.481085000	0.021551000	2.404121000
1	-3.048274000	-3.669425000	0.997767000	1	-0.843529000	-0.349081000	2.537850000
1	-0.726517000	-4.752271000	0.125772000	17	-2.245816000	-2.092567000	-7.943586000
8	-0.293513000	0.352953000	-2.464470000	6	-1.456347000	-0.916931000	-6.783817000
16	1.074190000	0.231686000	2.872426000	6	-0.766868000	0.180151000	-7.288137000
1	0.414487000	-0.932432000	3.218292000	6	-1.546304000	-1.144317000	-5.412828000
17	-0.995507000	-1.173399000	-9.421436000	6	-0.166710000	1.079613000	-6.401684000
6	-0.498028000	-0.321893000	-7.876304000	1	-0.699535000	0.342595000	-8.357049000
6	0.552769000	0.587888000	-7.905882000	6	-0.939866000	-0.253135000	-4.526074000
6	-1.170758000	-0.608207000	-6.690703000	1	-2.067034000	-2.015234000	-5.033708000
6	0.930247000	1.238628000	-6.727307000	6	-0.252725000	0.884601000	-5.006966000
1	1.071595000	0.797656000	-8.833639000	1	0.353221000	1.937368000	-6.808589000
6	-0.790110000	0.032254000	-5.511005000	1	-0.963573000	-0.468370000	-3.465552000
1	-1.972911000	-1.336351000	-6.678379000	7	0.332393000	1.804745000	-4.111142000
6	0.260158000	0.981505000	-5.510316000	6	-0.028596000	1.801250000	-2.730245000
1	1.740026000	1.955729000	-6.769534000	6	1.241197000	2.839636000	-4.616106000
1				1	0.235514000	2.754885000	-2.271464000

1	-1.085979000	1.591742000	-2.576699000	1	0.623953000	-1.890527000	1.581308000
1	1.598323000	0.672054000	-2.142707000	1	0.712228000	-0.107152000	1.640244000
1	0.718018000	3.586821000	-5.228784000	1	-0.026352000	-1.433620000	-0.794903000
1	1.699991000	3.355992000	-3.770556000	1	3.668083000	-2.448074000	1.179873000
1	2.041098000	2.398857000	-5.222156000	1	2.134784000	-3.157748000	0.641486000
6	0.864129000	-0.987525000	1.018510000	1	3.291149000	-2.544720000	-0.553965000
6	2.860980000	-2.367678000	0.438696000				

I-1. For $^4\text{RC} + 2\text{NH}_3$ Complex.

26	-1.363221000	0.110862000	-0.045736000	1	-1.537443000	1.676519000	4.966092000
7	-1.795676000	-0.224035000	-1.989634000	1	-4.388694000	4.184352000	1.318568000
7	-0.230799000	-1.558422000	-0.028828000	1	-4.798626000	3.874820000	-1.339928000
7	-1.160259000	0.260729000	1.953853000	8	-0.095255000	1.128315000	-0.350692000
7	-2.716923000	1.607474000	-0.019353000	16	-3.252698000	-1.616069000	0.180906000
6	-2.609909000	0.552209000	-2.812324000	1	-4.254733000	-0.903821000	-0.452116000
6	-1.218772000	-1.179107000	-2.820969000	17	5.998050000	-2.299340000	0.316090000
6	0.130763000	-2.333096000	-1.119372000	6	5.304063000	-0.618254000	0.042164000
6	0.435568000	-2.102568000	1.061693000	6	6.131876000	0.491615000	0.167420000
6	-0.364079000	-0.518861000	2.770259000	6	3.959167000	-0.479888000	-0.289709000
6	-1.714304000	1.228385000	2.773524000	6	5.603725000	1.767755000	-0.041291000
6	-3.056920000	2.396116000	1.069058000	1	7.178558000	0.371714000	0.421320000
6	-3.392944000	2.141997000	-1.101669000	6	3.425490000	0.792295000	-0.498802000
6	-2.557464000	0.052487000	-4.168243000	1	3.324908000	-1.352607000	-0.386479000
6	-1.700241000	-1.009534000	-4.173970000	6	4.236211000	1.950709000	-0.371806000
6	1.036378000	-3.382991000	-0.703432000	1	6.264742000	2.619155000	0.055378000
6	1.220795000	-3.243691000	0.642103000	1	2.373582000	0.876326000	-0.742624000
6	-0.416467000	-0.029428000	4.131434000	7	3.707248000	3.221608000	-0.568074000
6	-1.250768000	1.051297000	4.133319000	6	2.327512000	3.380995000	-1.035764000
6	-3.969963000	3.439798000	0.657479000	6	4.580020000	4.389861000	-0.511410000
6	-4.176710000	3.283793000	-0.683718000	1	2.065532000	4.440547000	-1.007576000
6	-3.343243000	1.650366000	-2.400829000	1	2.193744000	3.018556000	-2.066862000
6	-0.314134000	-2.145989000	-2.419532000	1	1.619287000	2.836789000	-0.403490000
6	0.373584000	-1.621331000	2.357970000	1	5.358769000	4.373376000	-1.290530000
6	-2.595556000	2.218077000	2.364244000	1	3.979806000	5.290209000	-0.652030000
1	-3.927909000	2.169993000	-3.152574000	1	5.081105000	4.469330000	0.462747000
1	0.062610000	-2.823653000	-3.177984000	1	-3.289862000	-2.047167000	2.805477000
1	0.953000000	-2.143533000	3.111730000	1	-2.159564000	-3.773599000	-0.926215000
1	-2.952138000	2.910699000	3.119362000	7	-1.773072000	-4.637375000	-1.285827000
1	-3.107297000	0.473914000	-4.996986000	7	-3.309906000	-2.289998000	3.788043000
1	-1.409870000	-1.631171000	-5.008108000	1	-1.785131000	-4.575471000	-2.294858000
1	1.462147000	-4.123038000	-1.364770000	1	-2.117835000	-5.517161000	-0.926332000
1	1.831993000	-3.843231000	1.300264000	1	-3.775098000	-1.535972000	4.275037000
1	0.118433000	-0.466799000	4.961512000	1	-3.628273000	-3.210100000	4.060393000

II-1. For $^2\text{RC} + 2\text{NH}_3$ Complex.

26	1.391600000	0.084283000	-0.132160000	6	3.199270000	2.489275000	1.515369000
7	1.632955000	0.609544000	1.793756000	6	0.153192000	-1.043526000	2.863118000
7	0.225837000	-1.461509000	0.437988000	6	-0.236709000	-2.473811000	-1.760263000
7	1.386722000	-0.638583000	-2.023344000	6	2.881751000	0.999758000	-3.096462000
7	2.781133000	1.443575000	-0.674002000	1	3.736769000	3.276842000	2.033003000
6	2.390834000	1.660988000	2.280063000	1	-0.265533000	-1.374519000	3.807471000
6	1.006548000	0.052197000	2.892892000	1	-0.799964000	-3.241397000	-2.279764000
6	-0.210084000	-1.744007000	1.725630000	1	3.310851000	1.327211000	-4.037526000
6	-0.395281000	-2.386755000	-0.385239000	1	2.720312000	2.502909000	4.334161000
6	0.597691000	-1.671940000	-2.518518000	1	1.024086000	0.529712000	5.085642000
6	2.030578000	-0.089718000	-3.129936000	1	-1.588743000	-3.296825000	2.577583000
6	3.229980000	1.712432000	-1.955202000	1	-1.821186000	-4.076938000	-0.002757000
6	3.378053000	2.389902000	0.144501000	1	0.279020000	-2.515092000	-4.571237000
6	2.232075000	1.765075000	3.714485000	1	2.028502000	-0.592191000	-5.315316000
6	1.377067000	0.770048000	4.093498000	1	4.621448000	3.250309000	-2.811284000
6	-1.113897000	-2.874158000	1.704530000	1	4.804221000	4.078900000	-0.239826000
6	-1.231805000	-3.267653000	0.402250000	8	0.121179000	1.103296000	-0.400712000
6	0.774998000	-1.784218000	-3.949715000	16	3.221181000	-1.741681000	0.020585000
6	1.658292000	-0.814071000	-4.325148000	1	4.102823000	-1.219948000	-0.908197000
6	4.131350000	2.843816000	-1.938751000	17	-6.254977000	-2.179531000	0.307849000
6	4.223313000	3.261714000	-0.641610000	6	-5.476031000	-0.524946000	0.118224000

6	-6.276241000	0.580694000	-0.147962000	1	-2.007764000	3.265021000	1.004387000
6	-4.095326000	-0.400641000	0.246107000	1	-1.649377000	2.728192000	-0.641335000
6	-5.684199000	1.837769000	-0.289091000	1	-5.202328000	4.637607000	0.291046000
1	-7.350276000	0.472268000	-0.242907000	1	-3.873837000	5.301582000	-0.680297000
6	-3.498012000	0.852587000	0.106395000	1	-5.126197000	4.321954000	-1.456886000
1	-3.481903000	-1.269354000	0.453491000	1	1.828463000	-3.955522000	-0.464020000
6	-4.280283000	2.004593000	-0.170562000	1	3.773789000	-1.748144000	2.622541000
1	-6.323507000	2.687451000	-0.490383000	7	3.982974000	-1.831176000	3.609532000
1	-2.421212000	0.924749000	0.195402000	7	1.337975000	-4.832483000	-0.587172000
7	-3.688740000	3.253855000	-0.317289000	1	4.571458000	-1.048005000	3.859437000
6	-2.257079000	3.424706000	-0.055885000	1	4.308222000	-2.717983000	3.969962000
6	-4.519041000	4.431621000	-0.548160000	1	1.146582000	-4.934242000	-1.574661000
1	-1.966715000	4.441445000	-0.327629000	1	1.708650000	-5.667741000	-0.154664000

III-1. For $^4TS_H + 2NH_3$ Complex.

26	-1.362825000	0.026982000	-0.051310000	1	-2.592841000	2.990957000	-4.183095000
7	-1.254711000	-1.456914000	1.360743000	1	-4.885136000	-1.705645000	-3.530714000
7	-0.096566000	1.150530000	1.053548000	1	-4.656108000	-3.709451000	-1.725199000
7	-1.497777000	1.486947000	-1.399190000	8	-0.063690000	-0.735693000	-0.932275000
7	-2.760738000	-1.037287000	-1.033914000	16	-3.047198000	0.966340000	1.347057000
6	-1.918195000	-2.670893000	1.340927000	1	-4.047779000	0.045453000	1.101910000
6	-0.508710000	-1.436360000	2.526790000	17	6.966326000	1.562258000	-0.217741000
6	0.489124000	0.801966000	2.263289000	6	5.660574000	0.312851000	-0.484896000
6	0.402277000	2.395987000	0.721127000	6	5.927021000	-0.785655000	-1.298952000
6	-0.797367000	2.683857000	-1.404067000	6	4.417008000	0.483950000	0.120313000
6	-2.302229000	1.503616000	-2.527346000	6	4.931051000	-1.742202000	-1.502700000
6	-3.391090000	-0.676092000	-2.210895000	1	6.898159000	-0.900567000	-1.764457000
6	-3.206030000	-2.317288000	-0.728747000	6	3.419969000	-0.469683000	-0.082557000
6	-1.566888000	-3.438857000	2.518179000	1	4.212017000	1.356259000	0.728413000
6	-0.700447000	-2.677002000	3.250136000	6	3.666467000	-1.604178000	-0.888426000
6	1.368520000	1.866410000	2.699425000	1	5.152927000	-2.602144000	-2.122118000
6	1.316237000	2.847540000	1.748664000	1	2.437960000	-0.302106000	0.338508000
6	-1.159734000	3.457256000	-2.574787000	7	2.668434000	-2.577621000	-1.071528000
6	-2.087370000	2.732989000	-3.263880000	6	1.526392000	-2.620251000	-0.241071000
6	-4.271760000	-1.740889000	-2.642114000	6	2.739005000	-3.477861000	-2.230289000
6	-4.155041000	-2.752244000	-1.731833000	1	0.960797000	-3.542736000	-0.360677000
6	-2.816147000	-3.077288000	0.363114000	1	1.736864000	-2.386279000	0.803450000
6	0.302367000	-0.391167000	2.945640000	1	0.668766000	-1.670943000	-0.577913000
6	0.085046000	3.109265000	-0.426931000	1	3.471111000	-4.279880000	-2.069694000
6	-3.188150000	0.508925000	-2.903296000	1	1.758722000	-3.929192000	-2.385187000
1	-3.263587000	-4.059620000	0.471872000	1	3.013081000	-2.923603000	-3.132832000
1	0.831091000	-0.514921000	3.884831000	1	-3.189432000	3.460839000	0.434457000
1	0.553740000	4.078078000	-0.560926000	1	-1.804893000	1.088241000	3.695974000
1	-3.755403000	0.660316000	-3.815215000	7	-1.362547000	1.208813000	4.598525000
1	-1.952019000	-4.422143000	2.746644000	7	-3.245066000	4.434765000	0.163938000
1	-0.234128000	-2.913665000	4.195577000	1	-1.329396000	0.300508000	5.041247000
1	1.939713000	1.851446000	3.616396000	1	-1.683350000	1.948915000	5.207998000
1	1.834717000	3.795281000	1.734043000	1	-3.766972000	4.477626000	-0.700873000
1	-0.753106000	4.428873000	-2.814794000	1	-3.533535000	5.119459000	0.849576000

IV-1. For $^2TS_H + 2NH_3$ Complex.

26	-1.304079000	0.140323000	-0.158103000	6	1.409699000	1.992706000	2.599668000
7	-1.418648000	-1.186299000	1.350896000	6	1.436248000	2.924552000	1.599951000
7	-0.028183000	1.256467000	0.938894000	6	-0.724505000	3.384960000	-2.902892000
7	-1.276871000	1.533034000	-1.626645000	6	-1.603057000	2.640499000	-3.634728000
7	-2.727744000	-0.875670000	-1.170129000	6	-4.160428000	-1.606486000	-2.837121000
6	-2.242614000	-2.301800000	1.411365000	6	-4.250655000	-2.500025000	-1.808291000
6	-0.721511000	-1.154090000	2.550040000	6	-3.131997000	-2.706774000	0.429265000
6	0.492012000	0.952188000	2.185781000	6	0.181547000	-0.174383000	2.933950000
6	0.539615000	2.462666000	0.561351000	6	0.315845000	3.128649000	-0.633359000
6	-0.519424000	2.690035000	-1.647435000	6	-2.844324000	0.496370000	-3.217301000
6	-1.949794000	1.482841000	-2.834379000	1	-3.704370000	-3.609435000	0.614272000
6	-3.206102000	-0.592952000	-2.439393000	1	0.656642000	-0.280935000	3.903114000
6	-3.348748000	-2.046183000	-0.770589000	1	0.841683000	4.064510000	-0.788601000
6	-2.038899000	-2.991331000	2.666958000	1	-3.305484000	0.589004000	-4.194642000
6	-1.100633000	-2.287092000	3.366425000	1	-2.561865000	-3.889052000	2.963297000

1	-0.703688000	-2.492223000	4.350103000	1	5.084159000	-3.005582000	-1.735241000
1	1.943502000	2.000798000	3.538975000	1	2.350478000	-0.432489000	0.418935000
1	1.998444000	3.846136000	1.557232000	7	2.535821000	-2.777278000	-0.882819000
1	-0.250473000	4.318312000	-3.169501000	6	1.319202000	-2.690890000	-0.157255000
1	-1.994788000	2.841903000	-4.621164000	6	2.637972000	-3.738112000	-1.989097000
1	-4.684149000	-1.616128000	-3.782014000	1	0.712602000	-3.587589000	-0.281527000
1	-4.862761000	-3.387779000	-1.742117000	1	1.471078000	-2.449542000	0.896928000
8	-0.042834000	-0.665002000	-1.002119000	1	0.623265000	-1.765486000	-0.569858000
16	-3.053014000	1.452482000	0.876945000	1	3.310621000	-4.567752000	-1.735744000
1	-3.981299000	1.378728000	-0.143312000	1	1.648011000	-4.145468000	-2.194744000
17	7.021952000	1.109621000	0.148893000	1	3.007516000	-3.247299000	-2.894668000
6	5.660018000	-0.063006000	-0.171919000	1	-1.776160000	3.714997000	1.448146000
6	5.913373000	-1.210343000	-0.920945000	1	-3.403374000	0.176494000	3.184475000
6	4.388408000	0.213215000	0.326983000	7	-3.538523000	-0.236939000	4.098594000
6	4.874250000	-2.108544000	-1.166564000	7	-1.326050000	4.574258000	1.737760000
1	6.907074000	-1.406317000	-1.304446000	1	-4.079632000	-1.081221000	3.970103000
6	3.347816000	-0.682559000	0.083686000	1	-3.864332000	0.345529000	4.858003000
1	4.196117000	1.122385000	0.882971000	1	-1.214813000	5.148552000	0.913178000
6	3.578518000	-1.864418000	-0.657556000	1	-1.689857000	5.074092000	2.537716000

V-1. For $^4\text{IM} + 2\text{NH}_3$ Complex.

26	-1.394937000	0.064146000	-0.107689000	1	-2.663717000	2.972082000	-4.282187000
7	-1.190940000	-1.431962000	1.252295000	1	-4.691262000	-1.852085000	-3.716021000
7	-0.224282000	1.247665000	1.027033000	1	-4.477732000	-3.814349000	-1.863240000
7	-1.594767000	1.536417000	-1.456505000	8	0.002520000	-0.587490000	-1.046879000
7	-2.711786000	-1.067313000	-1.136980000	16	-3.177964000	0.942440000	1.179590000
6	-1.831659000	-2.661993000	1.238512000	1	-4.222712000	0.370892000	0.479978000
6	-0.440414000	-1.393845000	2.417836000	17	6.697287000	1.950689000	-0.095859000
6	0.404481000	0.905747000	2.215412000	6	5.585014000	0.525116000	-0.380009000
6	0.170542000	2.541983000	0.731395000	6	6.114986000	-0.658927000	-0.886487000
6	-1.000761000	2.785946000	-1.411987000	6	4.226982000	0.651399000	-0.094521000
6	-2.336137000	1.495686000	-2.624965000	6	5.268624000	-1.750653000	-1.094502000
6	-3.300384000	-0.745828000	-2.350290000	1	7.172736000	-0.737119000	-1.106413000
6	-3.122312000	-2.357535000	-0.831115000	6	3.378541000	-0.435546000	-0.308550000
6	-1.446784000	-3.422500000	2.407220000	1	3.823890000	1.587351000	0.272651000
6	-0.589677000	-2.643069000	3.131868000	6	3.892408000	-1.655675000	-0.798750000
6	1.200740000	2.020484000	2.679620000	1	5.691425000	-2.677427000	-1.463228000
6	1.055315000	3.027978000	1.767588000	1	2.311807000	-0.315339000	-0.164826000
6	-1.369064000	3.541873000	-2.590778000	7	3.035141000	-2.763878000	-0.982209000
6	-2.189262000	2.747349000	-3.338135000	6	1.855431000	-2.894507000	-0.267059000
6	-4.119858000	-1.849179000	-2.799265000	6	3.399844000	-3.805789000	-1.952759000
6	-4.012021000	-2.839584000	-1.864110000	1	1.269499000	-3.784770000	-0.449948000
6	-2.724528000	-3.097188000	0.271593000	1	1.791080000	-2.408090000	0.697982000
6	0.311077000	-0.316741000	2.861936000	1	0.398754000	-1.467159000	-0.803906000
6	-0.187811000	3.261501000	-0.397581000	1	4.094418000	-4.538592000	-1.521045000
6	-3.128177000	0.440817000	-3.045721000	1	2.494137000	-4.329675000	-2.264504000
1	-3.142849000	-4.091188000	0.385731000	1	3.861131000	-3.355079000	-2.834915000
1	0.854141000	-0.433573000	3.793211000	1	-2.689948000	3.555457000	1.081736000
1	0.203289000	4.267935000	-0.496331000	1	-2.530240000	0.141699000	3.632111000
1	-3.656139000	0.552402000	-3.986235000	7	-2.302859000	-0.089042000	4.591206000
1	-1.804888000	-4.415834000	2.635550000	7	-2.520012000	4.552543000	1.123538000
1	-0.107347000	-2.871583000	4.071099000	1	-2.524789000	-1.066061000	4.726491000
1	1.788602000	2.016363000	3.585841000	1	-2.635131000	0.511936000	5.333191000
1	1.499708000	4.012497000	1.779815000	1	-2.805968000	4.944090000	0.236384000
1	-1.035882000	4.547839000	-2.799973000	1	-2.848554000	5.073801000	1.925080000

VI-1. For $^4\text{Carbinolaniline} + 2\text{NH}_3$ Complex.

26	1.658942000	0.329268000	0.197049000	6	2.268538000	2.655859000	-1.692736000
7	0.714625000	-0.598795000	1.740365000	6	1.561332000	3.360348000	0.547799000
7	1.679073000	-1.422302000	-0.792320000	6	0.814610000	2.316476000	2.357952000
7	2.114695000	1.286841000	-1.516334000	6	-0.076520000	-1.039664000	3.881217000
7	1.296107000	2.098761000	1.070555000	6	0.068131000	-2.243855000	3.250380000
6	0.339159000	-0.017309000	2.952009000	6	1.711810000	-3.697881000	-1.252982000
6	0.573406000	-1.974850000	1.926053000	6	2.172638000	-3.053845000	-2.368622000
6	1.404026000	-2.685207000	-0.272427000	6	2.895394000	1.729496000	-3.658661000
6	2.153499000	-1.640204000	-2.083978000	6	2.748741000	2.931720000	-3.028391000
6	2.505536000	0.704791000	-2.716072000	6	1.262845000	4.373771000	1.531249000

6	0.803450000	3.730757000	2.646544000	6	-5.401049000	-1.597582000	-0.652044000
6	0.379392000	1.336648000	3.236196000	1	-7.539837000	-1.694724000	-0.392781000
6	0.890931000	-2.944173000	0.990007000	6	-4.441504000	0.632522000	-0.668346000
6	2.533853000	-0.653660000	-2.979575000	1	-5.838862000	2.251663000	-0.422111000
6	2.018296000	3.622125000	-0.733515000	6	-4.262466000	-0.768534000	-0.763880000
1	0.043881000	1.654910000	4.216917000	1	-5.307362000	-2.674002000	-0.717637000
1	0.736783000	-3.981333000	1.266766000	1	-3.578679000	1.285713000	-0.672098000
1	2.877638000	-0.969714000	-3.958232000	7	-2.984901000	-1.315618000	-0.968096000
1	2.183497000	4.658424000	-1.006549000	6	-1.891664000	-0.474238000	-1.396311000
1	-0.423926000	-0.848489000	4.885910000	6	-2.782382000	-2.760729000	-0.850214000
1	-0.136060000	-3.230850000	3.638953000	1	-1.094038000	-1.113308000	-1.784039000
1	1.590752000	-4.759805000	-1.095820000	1	-2.215254000	0.217822000	-2.177099000
1	2.500143000	-3.485922000	-3.302884000	1	-1.025814000	-0.098034000	0.405747000
1	3.236959000	1.537283000	-4.665182000	1	-3.280841000	-3.319910000	-1.655754000
1	2.945633000	3.920478000	-3.416078000	1	-1.713346000	-2.976470000	-0.897498000
1	1.383780000	5.435319000	1.372503000	1	-3.161851000	-3.135133000	0.108353000
1	0.473773000	4.162123000	3.580295000	1	5.239753000	-0.708342000	-1.190809000
8	-1.360946000	0.414302000	-0.362775000	1	3.746158000	-2.105354000	2.551008000
16	3.962815000	0.054987000	1.014266000	7	3.732019000	-2.954252000	3.102350000
1	4.114132000	1.321053000	1.547353000	7	5.762817000	-1.054775000	-1.985286000
17	-8.486660000	1.054545000	-0.172498000	1	3.312839000	-2.727198000	3.993897000
6	-6.817756000	0.333092000	-0.405404000	1	4.575825000	-3.506190000	3.176358000
6	-6.674117000	-1.048088000	-0.472197000	1	5.942414000	-0.267662000	-2.593824000
6	-5.714397000	1.178139000	-0.498594000	1	6.571743000	-1.639337000	-1.823898000

VII. For ² Carbinolaniline + 2NH₃ Complex.

26	-1.235880000	0.170557000	0.328543000	1	0.364199000	-1.991331000	4.853601000
7	-1.510519000	1.361218000	-1.281093000	1	1.655605000	3.008768000	3.686623000
7	-2.185558000	-1.314559000	-0.663151000	1	1.085888000	4.684176000	1.639791000
7	-0.829553000	-1.076950000	1.857077000	8	0.553534000	-0.396359000	-0.684593000
7	-0.170296000	1.603364000	1.252771000	16	-3.193057000	0.895829000	1.269640000
6	-1.153299000	2.700459000	-1.366329000	1	-2.757757000	0.988749000	2.577972000
6	-2.208474000	1.074604000	-2.448789000	17	7.637228000	0.780782000	-0.023507000
6	-2.789571000	-1.253994000	-1.912465000	6	6.041524000	-0.007862000	-0.450375000
6	-2.481147000	-2.572616000	-0.154994000	6	6.008214000	-0.994410000	-1.429622000
6	-1.312493000	-2.369876000	2.008674000	6	4.880938000	0.399927000	0.202431000
6	-0.105338000	-0.800061000	3.010537000	6	4.789533000	-1.598750000	-1.753053000
6	0.479983000	1.527012000	2.475495000	1	6.917385000	-1.298633000	-1.933954000
6	0.017388000	2.898029000	0.796146000	6	3.661576000	-0.195030000	-0.125423000
6	-1.619249000	3.252939000	-2.620760000	1	4.917111000	1.185602000	0.947275000
6	-2.265198000	2.251324000	-3.288734000	6	3.598820000	-1.217751000	-1.099058000
6	-3.455595000	-2.506652000	-2.198628000	1	4.781769000	-2.376110000	-2.506243000
6	-3.269159000	-3.317360000	-1.114912000	1	2.756130000	0.168237000	0.343406000
6	-0.873121000	-2.912533000	3.277089000	7	2.372427000	-1.843860000	-1.408052000
6	-0.125613000	-1.947747000	3.891567000	6	1.250119000	-1.708869000	-0.536614000
6	1.090255000	2.802733000	2.789248000	6	2.275009000	-2.723330000	-2.578075000
6	0.800972000	3.648635000	1.757035000	1	0.527548000	-2.502567000	-0.730490000
6	-0.444628000	3.409713000	-0.408184000	1	1.535969000	-1.710913000	0.514011000
6	-2.788425000	-0.149008000	-2.752266000	1	0.385852000	-0.180482000	-1.624835000
6	-2.077460000	-3.061495000	1.079460000	1	2.851856000	-3.649567000	-2.448818000
6	0.520361000	0.406044000	3.292330000	1	1.229180000	-2.994669000	-2.735196000
1	-0.226816000	4.450977000	-0.621268000	1	2.636241000	-2.217870000	-3.481096000
1	-3.307714000	-0.237902000	-3.700511000	1	-4.905265000	-0.986114000	0.493605000
1	-2.384714000	-4.068954000	1.340015000	1	-3.732571000	3.057357000	-0.183741000
1	1.058191000	0.486263000	4.231009000	7	-4.014345000	3.854551000	-0.740418000
1	-1.467279000	4.275853000	-2.933578000	7	-5.608824000	-1.643235000	0.180549000
1	-2.747943000	2.293218000	-4.254385000	1	-3.443744000	4.638465000	-0.454034000
1	-4.001475000	-2.717628000	-3.106900000	1	-4.997923000	4.073557000	-0.822465000
1	-3.630449000	-4.324125000	-0.961820000	1	-5.508352000	-2.480337000	0.738479000
1	-1.114101000	-3.902523000	3.636708000	1	-6.565016000	-1.329804000	0.082684000

Table S21 Cartesian Coordinates for Various Reaction Species in C–H Hydroxylation of *p*-CN-DMA by Cpd I

I. For ^4RC

26	-2.346240000	-0.205724000	0.111157000	6	4.346746000	-0.570516000	1.099623000
7	-2.854936000	-2.082739000	0.653449000	6	0.867710000	4.287718000	0.077599000
7	-1.784997000	0.172440000	2.010885000	6	-0.475105000	4.270799000	-0.169637000
7	-2.117510000	1.745670000	-0.338468000	6	-3.994681000	0.704112000	-0.404924000
7	-3.169287000	-0.525622000	-1.704841000	6	-4.006680000	-0.652262000	-0.255872000
6	-3.382165000	-3.078552000	-0.167414000	6	-0.519901000	-4.152560000	0.633562000
6	-2.601425000	-2.696062000	1.877043000	6	0.828202000	-4.139642000	0.853473000
6	-1.675829000	-0.740948000	3.047086000	6	2.559528000	-2.326380000	0.960796000
6	-1.320081000	1.379466000	2.517875000	6	2.578804000	2.509617000	0.531755000
6	-1.606273000	2.733900000	0.480510000	6	-2.202386000	2.455894000	-0.313994000
6	-2.353292000	2.348532000	-1.561817000	1	-2.236218000	-2.372983000	0.193233000
6	-3.254759000	0.385140000	-2.746791000	1	3.312969000	-3.081667000	1.158147000
6	-3.637525000	-1.725602000	-2.209718000	1	3.337457000	3.281792000	0.602434000
6	-3.483077000	-4.319243000	0.568423000	1	-2.948568000	3.210046000	-0.539132000
6	-3.001053000	-4.084682000	1.823518000	1	-2.994380000	-3.146556000	0.132913000
6	-1.134093000	-0.094564000	4.223685000	1	5.177112000	-1.229168000	1.307722000
6	-0.918561000	1.213805000	3.898577000	1	5.186142000	1.469158000	1.075296000
6	-1.516888000	3.983775000	-0.243796000	1	1.528679000	5.140420000	0.127247000
6	-1.978407000	3.745378000	-1.506582000	1	-1.132188000	5.106279000	-0.361644000
6	-3.794400000	-0.259562000	-3.923879000	1	-4.823559000	1.361861000	-0.621113000
6	-4.029517000	-1.563804000	-3.592748000	1	-4.847850000	-1.326149000	-0.326364000
6	-3.736376000	-2.913128000	-1.494035000	1	-1.186791000	-5.001749000	0.604176000
6	-2.040556000	-2.077548000	2.980066000	8	1.485334000	-4.976273000	1.040389000
6	-1.239145000	2.565898000	1.809813000	16	0.440245000	-0.128819000	-1.421183000
6	-2.881980000	1.718623000	-2.678846000	1	-0.493347000	0.477728000	2.655398000
1	-4.124901000	-3.779786000	-2.018339000	6	-1.164560000	-0.709211000	2.884950000
1	-1.889265000	-2.680900000	3.868552000	6	-0.834741000	5.668177000	-4.902373000
1	-0.853556000	3.433834000	2.333898000	6	-0.413273000	4.322890000	-5.112716000
1	-3.012805000	2.318436000	-3.573400000	6	-0.439031000	3.742175000	-6.396982000
1	-3.870057000	-5.241897000	0.161404000	6	0.039737000	3.533440000	-4.033187000
1	-2.915939000	-4.776721000	2.648345000	6	-0.032206000	2.429358000	-6.596499000
1	-0.950839000	-0.5886669000	5.166263000	1	-0.778787000	4.331498000	-7.242310000
1	-0.522222000	2.001703000	4.521798000	6	0.446343000	2.220674000	-4.220131000
1	-1.150442000	4.909960000	0.173760000	1	0.073217000	3.962214000	-3.037573000
1	-2.066432000	4.437704000	-2.330937000	6	0.414282000	1.625358000	-5.511485000
1	-3.965989000	0.233610000	-4.869420000	1	-0.061943000	2.025236000	-7.599685000
1	-4.432123000	-2.351373000	-4.212713000	7	0.772143000	1.650640000	-3.360155000
8	-0.825378000	-0.606740000	-0.399662000	6	0.806060000	0.313456000	-5.707228000
16	-4.686095000	0.187496000	1.095932000	6	1.369321000	-0.473000000	-4.602451000
1	-5.412242000	-0.591378000	0.214015000	6	0.857432000	-0.241464000	-7.059108000
6	3.791207000	0.081286000	4.242514000	1	1.386722000	-1.525733000	-4.891303000
6	3.702309000	-0.253881000	2.859601000	1	2.396902000	-0.163353000	-4.356433000
6	4.858948000	-0.520641000	2.098692000	1	0.767566000	-0.380381000	-3.694963000
6	2.447383000	-0.326512000	2.216136000	1	1.578302000	0.287654000	-7.700622000
6	4.768771000	-0.845003000	0.751049000	1	1.158684000	-1.288219000	-7.001134000
1	5.833233000	-0.471710000	2.573782000	1	-0.125143000	-0.199875000	-7.546327000
6	2.343729000	-0.649506000	0.870576000	7	-1.185254000	6.775881000	-4.715363000
1	1.546320000	-0.125900000	2.785581000				
6	3.507890000	-0.916320000	0.098325000				
1	5.680379000	-1.043596000	0.202787000				
1	1.358859000	-0.692677000	0.420864000				
7	3.411602000	-1.235635000	-1.243675000				
6	2.095345000	-1.315750000	-1.887932000				
6	4.614867000	-1.531891000	-2.018573000				
1	2.233095000	-1.540254000	-2.946771000				
1	1.468823000	-2.099089000	-1.443340000				
1	1.542569000	-0.373834000	-1.800455000				
1	5.159078000	-2.397760000	-1.615163000				
1	4.329911000	-1.761022000	-3.046164000				
1	5.306074000	-0.677754000	-2.040376000				
7	3.852420000	0.360192000	5.384284000				

II. For ^2RC

26	0.206289000	0.050954000	0.203736000	26	-2.201307000	-0.100687000	-0.050457000
7	2.165727000	0.085298000	0.657125000	6	-2.295475000	-2.131524000	0.230734000
7	0.186545000	2.068161000	0.149365000	6	-1.670475000	0.125352000	1.887391000
7	-1.812301000	0.050532000	0.052672000	6	-2.151261000	1.871590000	-0.306030000
7	0.163557000	-1.937353000	0.546056000	6	-2.908708000	-0.346037000	-1.917158000
6	2.981659000	-1.006366000	0.898846000	6	-2.637596000	-3.084314000	-0.712798000
6	2.989450000	1.194114000	0.706994000	6	-2.036212000	-2.818447000	1.405092000
6	1.280945000	2.914590000	0.271576000	6	-1.495660000	-0.880504000	2.829136000
6	-0.897527000	2.886600000	-0.123271000	6	-1.352627000	1.312636000	2.519667000
6	-2.628794000	1.143302000	-0.222230000	6	-1.754518000	2.822583000	0.622765000
6	-2.647281000	-1.064542000	0.016299000	6	-2.493938000	2.570202000	-1.452992000
6	-0.929719000	-2.778788000	0.439768000	6	-3.147772000	0.653195000	-2.843378000
6	1.253097000	-2.758346000	0.793679000	6	-3.153221000	-1.548827000	-2.568767000

6	-1.662974000	-2.239958000	2.610009000	1	3.256150000	3.207310000	-0.111376000
6	-1.381163000	2.569674000	1.930683000	1	-3.139304000	3.229172000	0.050986000
6	-2.966651000	2.011707000	-2.627663000	1	-3.176379000	-3.163787000	0.147364000
1	-3.262623000	-3.660749000	-2.654622000	1	5.102251000	-1.349702000	0.176339000
1	-1.490501000	-2.904000000	3.450388000	1	5.121707000	1.351258000	0.000972000
1	-1.104374000	3.418227000	2.546743000	1	1.407623000	5.099080000	-0.098909000
1	-3.196558000	2.684548000	-3.446599000	1	-1.298950000	5.098440000	-0.008647000
1	-2.801862000	-5.322882000	-0.641110000	1	-5.032539000	1.401234000	0.066397000
1	-2.071728000	-4.997742000	1.944601000	1	-5.052669000	-1.305757000	0.092730000
1	-0.871269000	-0.862961000	4.984701000	1	-1.339021000	-5.045166000	0.269416000
1	-0.694747000	1.812168000	4.606197000	1	1.367940000	-5.052445000	0.329354000
1	-1.575206000	5.058417000	0.547772000	8	-0.124135000	-0.075704000	-1.723560000
1	-2.482656000	4.751168000	-1.983105000	16	0.016511000	0.188566000	2.398250000
1	-3.832642000	0.635032000	-4.979710000	1	-0.634384000	-0.999088000	2.669688000
1	-3.834239000	-2.051117000	-4.646496000	6	-0.723116000	5.693359000	-5.742394000
8	-0.544678000	-0.261496000	-0.580341000	6	-0.242847000	4.374387000	-5.480346000
16	-4.424334000	-0.093360000	0.807698000	6	-0.087229000	3.446717000	-6.530796000
1	-5.053260000	-0.702067000	-0.261630000	6	0.074018000	3.972755000	-4.165640000
6	4.967845000	0.893715000	3.747760000	6	0.379549000	2.162233000	-6.278963000
6	4.312372000	0.229598000	2.667086000	1	-0.331109000	3.742164000	-7.545067000
6	5.041670000	-0.194075000	1.537200000	6	0.543392000	2.691552000	-3.906974000
6	2.921628000	-0.005451000	2.705013000	1	-0.066816000	4.663162000	-3.341906000
6	4.406083000	-0.841183000	0.484080000	6	0.715942000	1.764253000	-4.962878000
1	6.110379000	-0.016358000	1.493739000	1	0.501333000	1.477707000	-7.108444000
6	2.280714000	-0.652847000	1.657122000	1	0.720535000	2.392315000	-2.883317000
1	2.340054000	0.337991000	3.552934000	7	1.208415000	0.479811000	-4.707912000
6	3.014268000	-1.093968000	0.529579000	6	1.766982000	0.144278000	-3.447054000
1	4.996601000	-1.167508000	-0.362313000	6	1.010216000	-0.586148000	-5.700754000
1	1.206077000	-0.767168000	1.686264000	1	2.300905000	-0.804647000	-3.482051000
7	2.373860000	-1.768149000	-0.516885000	1	2.383479000	0.941102000	-3.026778000
6	1.050688000	-2.248787000	-0.383310000	1	0.877913000	-0.014221000	-2.597819000
6	3.030612000	-1.862943000	-1.828980000	1	1.693226000	-0.469340000	-6.551557000
1	0.773194000	-2.928819000	-1.186395000	1	1.206856000	-1.548049000	-5.227653000
1	0.825280000	-2.648189000	0.605977000	1	-0.019805000	-0.584913000	-6.070225000
1	0.179755000	-1.246683000	-0.494214000	7	-1.116693000	6.779722000	-5.957845000
1	3.833651000	-2.610679000	-1.819880000				
1	2.289260000	-2.158376000	-2.571310000				
1	3.449149000	-0.895755000	-2.122783000	26	-2.283899000	-0.059992000	0.021318000
7	5.506726000	1.439117000	4.638779000	7	-2.238800000	-2.078652000	0.243393000

V. For 4IM

26	0.038851000	0.020822000	-0.010994000	6	-2.283899000	-0.059992000	0.021318000
7	2.050160000	0.017586000	0.008566000	6	-2.238800000	-2.078652000	0.243393000
7	0.055856000	2.038830000	0.003875000	6	-1.750394000	0.159327000	1.950642000
7	-1.983064000	0.025740000	0.078573000	6	-2.316437000	1.932435000	-0.207652000
7	0.025713000	-1.991314000	0.173720000	6	-2.995094000	-0.294768000	-1.852512000
6	2.875556000	-1.094748000	0.108016000	6	-2.616692000	-3.028344000	-0.694934000
6	2.891215000	1.120949000	-0.032235000	6	-1.900708000	-2.777126000	1.393337000
6	1.163636000	2.868607000	-0.050675000	6	-1.465294000	-0.851454000	2.857472000
6	-1.054088000	2.868680000	0.021092000	6	-1.525546000	1.355660000	2.612245000
6	-2.803069000	1.139718000	0.066184000	6	-2.000566000	2.881334000	0.749656000
6	-2.819275000	-1.076709000	0.090830000	6	-2.639319000	2.629815000	-1.359442000
6	-1.086660000	-2.817897000	0.178618000	6	-3.227811100	0.712950000	-2.776130000
6	1.130560000	-2.823795000	0.223049000	6	-3.245744000	-1.492880000	-2.507639000
6	4.260272000	-0.676466000	0.105933000	6	-2.478253000	-4.351701000	-0.128327000
6	4.270235000	0.686473000	0.016499000	6	-2.036028000	-4.197330000	1.155476000
6	0.737696000	4.252015000	-0.068470000	6	-1.066446000	-0.270206000	4.120346000
6	-0.628404000	4.251494000	-0.021225000	6	-1.105620000	1.087736000	3.970262000
6	-4.191345000	0.723589000	0.070931000	6	-2.114587000	4.206413000	0.177450000
6	-4.201401000	-0.640748000	0.083516000	6	-2.505489000	4.051674000	-1.120886000
6	-0.665180000	-4.201036000	0.247054000	6	-3.661118000	0.133214000	-4.027528000
6	0.700196000	-4.204806000	0.277377000	6	-3.674533000	-1.223063000	-3.861806000
6	2.454170000	-2.411187000	0.200364000	6	-3.080514000	-2.761103000	-1.973462000
6	2.484715000	2.445636000	-0.079994000	6	-1.528321000	-2.212513000	2.603570000
6	-2.377252000	2.457431000	0.048784000	6	-1.641736000	2.621706000	2.060979000
6	-2.407610000	-2.398824000	0.134909000	6	-3.061531000	2.070867000	-2.553596000
1	3.218843000	-3.178018000	0.261784000	1	-3.331302000	-3.607215000	-2.603661000
6	-2.238800000	-2.078652000	-1.285329000	1	-1.285329000	-2.885840000	3.418040000
6	-1.427826000	3.469787000	-1.427826000	1	-1.427826000	3.469787000	2.701673000
6	-3.283658000	2.744715000	-3.283658000	1	-3.283658000	2.744715000	-3.373508000
6	-2.707125000	-5.268155000	-2.707125000	1	-2.707125000	-5.268155000	-0.652526000
6	-1.831670000	-4.962225000	-1.831670000	1	-1.831670000	-4.962225000	1.890427000
6	-0.794662000	-0.839893000	-0.794662000	1	-0.794662000	-0.839893000	4.996917000
6	-0.872826000	1.849600000	-0.872826000	1	-0.872826000	1.849600000	4.699798000
6	-1.919276000	5.122586000	-1.919276000	1	-1.919276000	5.122586000	0.715164000
6	-2.695875000	4.815853000	-2.695875000	1	-2.695875000	4.815853000	-1.860177000
6	-3.912008000	0.703228000	-3.912008000	1	-3.912008000	0.703228000	-4.910152000
1	-3.938509000	-1.983783000	-3.938509000	1	-3.938509000	-1.983783000	-4.581956000

8	-0.571248000	-0.078278000	-0.555320000	1	0.998942000	0.816227000	-8.778572000
16	-4.496336000	-0.048303000	0.844386000	6	-0.975715000	0.385370000	-5.462782000
1	-5.155382000	-0.040195000	-0.369310000	1	-2.346732000	-0.800096000	-6.604809000
6	4.750481000	1.044066000	3.642476000	1	0.209885000	1.164277000	-5.468603000
6	4.227646000	0.280642000	2.555588000	6	1.826598000	1.878901000	-6.735288000
6	5.093625000	-0.393746000	1.669764000	1	-1.490799000	0.200625000	-4.529522000
6	2.835005000	0.195596000	2.340092000	1	0.662916000	1.787179000	-4.303487000
6	4.586121000	-1.144655000	0.615510000	1	-0.191908000	1.866583000	-3.134521000
1	6.165716000	-0.332619000	1.820750000	7	1.981059000	2.427202000	-4.277698000
6	2.321296000	-0.550863000	1.287759000	6	0.224265000	2.617602000	-2.457897000
1	2.156584000	0.733263000	2.993072000	1	-1.204423000	2.159139000	-3.420326000
6	3.190137000	-1.246705000	0.414769000	1	0.458692000	0.266462000	-2.064018000
1	5.275246000	-1.671491000	-0.032784000	1	2.021725000	3.318045000	-4.920289000
1	1.256606000	-0.535367000	1.092512000	1	2.207589000	2.733404000	-3.255085000
7	2.667045000	-2.030965000	-0.628585000	1	2.764152000	1.732955000	-4.605122000
6	1.370166000	-2.518507000	-0.598059000	7	-1.619701000	-1.174095000	-10.030674000
6	3.518498000	-2.359207000	-1.783460000				
1	1.050840000	-3.119018000	-1.437871000				
1	0.894481000	-2.650171000	0.364418000				
1	-0.139338000	-0.949724000	-0.747527000				
1	4.182503000	-3.206025000	-1.567917000				
1	2.878714000	-2.625481000	-2.626363000				
1	4.123113000	-1.494107000	-2.065938000				
7	5.179150000	1.671764000	4.539632000				

VI. For ⁴ Carbinolainline Complex.

26	0.307385000	0.461448000	0.642341000	7	0.507838000	0.574672000	0.142225000
7	1.810597000	-0.378058000	-0.438921000	7	2.172924000	-0.511567000	-0.204140000
7	1.197953000	2.251978000	0.411577000	7	1.693327000	2.142223000	0.624541000
7	-1.377146000	1.392382000	1.236995000	7	-1.143072000	1.713892000	0.357703000
7	-0.714250000	-1.261219000	0.509031000	6	-0.665725000	-0.936130000	-0.482861000
6	1.962527000	-1.735270000	-0.731044000	6	2.199834000	-1.841774000	-0.596264000
6	3.031915000	0.213574000	-0.768849000	6	3.495892000	-0.146141000	0.006033000
6	2.491632000	2.496019000	-0.043739000	6	3.078664000	2.166388000	0.726728000
6	0.717743000	3.480407000	0.860087000	6	1.255776000	3.388645000	1.051096000
6	-1.516489000	2.739070000	1.552044000	6	-1.175006000	3.021167000	0.824434000
6	-2.585465000	0.798017000	1.579076000	6	-2.469641000	1.338808000	0.175688000
6	-2.013012000	-1.501289000	0.947170000	6	-2.050918000	-0.964718000	-0.574514000
6	-0.237607000	-2.487227000	0.053511000	6	-0.228659000	-2.199389000	-0.852384000
6	3.272891000	-1.976912000	-1.282361000	6	3.569553000	-2.311440000	-0.646285000
6	3.930961000	-0.778521000	-1.304856000	6	4.367569000	-1.267082000	-0.276333000
6	2.816441000	3.892104000	0.122172000	6	3.514690000	3.460722000	1.205122000
6	1.723539000	4.497993000	0.678548000	6	2.392431000	4.213289000	1.405472000
6	-2.835410000	2.987318000	2.088959000	6	-2.547066000	3.472238000	0.927084000
6	-3.494367000	1.791486000	2.104837000	6	-3.343852000	2.436805000	0.526720000
6	-2.339966000	-2.897103000	0.779798000	6	-2.487722000	-2.270373000	-1.021710000
6	-1.246063000	-3.504570000	0.229972000	6	-1.365313000	-3.031560000	-1.191464000
6	1.007671000	-2.712390000	-0.510850000	6	1.093115000	-2.619129000	-0.902721000
6	3.346130000	1.550149000	-0.590485000	1	3.921522000	1.104456000	0.430937000
6	-0.542622000	3.708599000	1.387649000	1	-0.253096000	3.797539000	1.136803000
6	-2.882420000	-0.548038000	1.451060000	1	-0.067321000	2.894276000	0.095275000
1	1.250260000	-3.727789000	-0.803582000	1	-3.962021000	-0.064706000	-0.376011000
1	4.335834000	1.878990000	-0.887894000	1	3.863745000	-3.312665000	-0.925964000
1	-0.784045000	4.721105000	1.691529000	1	5.444370000	-1.243526000	-0.191938000
1	-3.868279000	-0.878555000	1.758503000	1	4.545718000	3.737985000	1.370740000
1	3.634262000	-2.944094000	-1.599484000	1	2.323521000	5.228826000	1.767964000
1	4.937047000	-0.574831000	-1.641333000	1	-2.845665000	4.453312000	1.267425000
1	3.762134000	4.337735000	-0.150024000	1	-4.422503000	2.403284000	0.474244000
1	1.599252000	5.536574000	0.948030000	1	-3.519004000	-2.553954000	-1.174337000
1	-3.194133000	3.954744000	2.408398000	1	-1.297473000	-4.062011000	-1.509265000
1	-4.500397000	1.584538000	2.439186000	8	0.719888000	1.172830000	-1.880364000
1	-3.289475000	-3.339219000	1.043631000	16	0.443912000	-0.140280000	2.315945000
1	-1.123500000	-4.541718000	-0.045451000	1	-0.918788000	-0.348805000	2.414443000
8	-0.386516000	0.604861000	-2.434977000	6	-1.494815000	-2.198655000	-7.408759000
16	1.264111000	0.096543000	2.874550000	6	-1.078320000	-1.125048000	-6.564175000
1	0.423108000	-0.929573000	3.261609000	6	-0.587165000	0.074046000	-7.114990000
6	-1.223785000	-0.669681000	-9.044992000	6	-1.139904000	-1.246075000	-5.160426000
6	-0.743331000	-0.057204000	-7.848616000	6	-0.183682000	1.122848000	-6.294001000
6	0.446149000	0.696905000	-7.852983000	1	-0.527964000	0.182527000	-8.192396000
6	-1.441169000	-0.203695000	-6.630716000	6	-0.732229000	-0.205912000	-4.334608000
6	0.915994000	1.295954000	-6.688860000	1	-1.496637000	-2.168275000	-4.715581000
				6	-0.259759000	1.008797000	-4.887036000

1	0.177292000	2.033416000	-6.753914000	1	1.663471000	1.381779000	-2.028979000
1	-0.738745000	-0.353137000	-3.263220000	1	0.138832000	3.816288000	-5.297184000
7	0.122991000	2.075968000	-4.057927000	1	1.119227000	3.905826000	-3.823935000
6	-0.182901000	2.058816000	-2.659734000	1	1.688352000	2.948884000	-5.202380000
6	0.800268000	3.245295000	-4.632430000	7	-1.839080000	-3.082128000	-8.103554000
1	-0.120290000	3.069916000	-2.254756000				
1	-1.167203000	1.640911000	-2.457450000				

I-1. For $^4\text{RC} + 2\text{NH}_3$ Complex.

26	-1.260203000	0.120612000	-0.072707000	1	-4.248781000	4.336048000	0.887113000
7	-1.474095000	-0.221494000	-2.050901000	1	-4.344536000	4.013663000	-1.799442000
7	-0.209105000	-1.592554000	0.092280000	8	0.075987000	1.081728000	-0.232776000
7	-1.292705000	0.286996000	1.935695000	16	-3.245390000	-1.509834000	-0.074644000
7	-2.541822000	1.674094000	-0.220145000	1	-4.140549000	-0.740639000	-0.794881000
6	-2.147818000	0.579239000	-2.971963000	6	5.764864000	-2.190010000	0.285341000
6	-0.845957000	-1.212717000	-2.799590000	6	5.309417000	-0.846775000	0.140509000
6	0.246903000	-2.395454000	-0.940830000	6	6.217700000	0.231174000	0.108790000
6	0.302665000	-2.147176000	1.258721000	6	3.930892000	-0.562965000	0.025254000
6	-0.634337000	-0.515012000	2.847847000	6	5.770332000	1.538822000	-0.030506000
6	-1.903143000	1.284496000	2.675950000	1	7.281485000	0.035283000	0.194375000
6	-2.976615000	2.489274000	0.813726000	6	3.471130000	0.738844000	-0.114431000
6	-3.056621000	2.224652000	-1.380303000	1	3.217158000	-1.379405000	0.046157000
6	-1.957113000	0.058591000	-4.307444000	6	4.383403000	1.829591000	-0.143802000
6	-1.155273000	-1.040716000	-4.201579000	1	6.500029000	2.337677000	-0.051273000
6	1.057474000	-3.472112000	-0.412193000	1	2.404038000	0.906853000	-0.199049000
6	1.088482000	-3.321348000	0.944379000	7	3.931464000	3.129404000	-0.279578000
6	-0.833391000	-0.009928000	4.189511000	6	2.494500000	3.398650000	-0.408652000
6	-1.617543000	1.102840000	4.083147000	6	4.882278000	4.238070000	-0.333371000
6	-3.785427000	3.566684000	0.287037000	1	2.340696000	4.477346000	-0.465904000
6	-3.833734000	3.404241000	-1.068417000	1	2.070667000	2.937037000	-1.309257000
6	-2.873031000	1.714910000	-2.660401000	1	1.930430000	3.011141000	0.446965000
6	-0.036144000	-2.209815000	-2.285984000	1	5.572352000	4.145031000	-1.184121000
6	0.104160000	-1.649317000	2.534752000	1	4.333112000	5.173827000	-0.444811000
6	-2.685403000	2.305444000	2.156544000	1	5.483257000	4.304369000	0.584355000
1	-3.338238000	2.250426000	-3.481222000	7	6.129096000	-3.302668000	0.405763000
1	0.398629000	-2.912355000	-2.988650000	1	-3.577808000	-1.972395000	2.523650000
1	0.566414000	-2.185628000	3.356548000	1	-2.150569000	-3.705855000	-1.101508000
1	-3.102085000	3.019847000	2.858770000	7	-1.771795000	-4.583512000	-1.434756000
1	-2.384064000	0.492494000	-5.199716000	7	-3.712371000	-2.226579000	3.494263000
1	-0.796221000	-1.686092000	-4.989661000	1	-1.675298000	-4.508023000	-2.438305000
1	1.531210000	-4.235364000	-1.011522000	1	-2.195294000	-5.449126000	-1.129006000
1	1.594215000	-3.935586000	1.674598000	1	-4.188050000	-1.456150000	3.944029000
1	-0.423330000	-0.459951000	5.081579000	1	-4.102540000	-3.132673000	3.715356000
1	-1.979265000	1.746936000	4.871133000				

II-1. For $^2\text{RC} + 2\text{NH}_3$ Complex.

26	-1.295190000	0.115348000	0.128046000	6	-4.092105000	3.334431000	0.557932000
7	-1.905119000	0.265950000	-1.782829000	6	-3.459741000	2.163621000	-1.569566000
7	-0.202378000	-1.511820000	-0.352118000	6	-0.595327000	-1.564002000	-2.782525000
7	-0.916238000	-0.236671000	2.085086000	6	0.687973000	-2.094835000	1.870357000
7	-2.608997000	1.552152000	0.658969000	6	-2.237123000	1.582212000	3.094946000
6	-2.776470000	1.206155000	-2.305004000	1	-4.111609000	2.838593000	-2.114140000
6	-1.475832000	-0.491996000	-2.856007000	1	-0.349837000	-2.071305000	-3.709446000
6	-0.003864000	-2.035379000	-1.623167000	1	1.361870000	-2.752527000	2.408432000
6	0.587070000	-2.269313000	0.497799000	1	-2.492166000	2.085249000	4.021644000
6	-0.016159000	-1.160237000	2.607830000	1	-3.511231000	1.641634000	-4.380412000
6	-1.358787000	0.516801000	3.170597000	1	-1.918663000	-0.442334000	-5.055594000
6	-2.818544000	2.063386000	1.927548000	1	1.239800000	-3.728146000	-2.413333000
6	-3.379276000	2.326227000	-0.195387000	1	1.967209000	-4.010401000	0.177343000
6	-2.890718000	1.035025000	-3.737275000	1	0.707861000	-1.597413000	4.683533000
6	-2.087939000	-0.016027000	-4.077745000	1	-0.930220000	0.441655000	5.370379000
6	0.922658000	-3.145153000	-1.561285000	1	-4.076556000	3.741112000	2.725867000
6	1.290344000	-3.287574000	-0.253964000	1	-4.765263000	4.060922000	0.126908000
6	0.081153000	-0.996170000	4.041540000	8	-0.041976000	1.177819000	-0.039358000
6	-0.745729000	0.032631000	4.387871000	16	-3.062350000	-1.689386000	0.677912000
6	-3.744818000	3.173053000	1.869137000	1	-3.787585000	-0.983529000	1.620167000

6	6.064575000	-1.989311000	-0.208936000	1	2.181092000	3.188317000	-1.899804000
6	5.493678000	-0.685313000	-0.282033000	1	1.711676000	2.664545000	-0.273554000
6	6.283307000	0.468443000	-0.101577000	1	5.347180000	4.423903000	-1.188236000
6	4.114807000	-0.516444000	-0.535076000	1	3.991491000	5.252008000	-0.397611000
6	5.721880000	1.736948000	-0.168631000	1	5.176246000	4.375771000	0.581420000
1	7.346231000	0.363052000	0.089211000	7	6.523388000	-3.071118000	-0.145504000
6	3.542791000	0.745279000	-0.602044000	1	-1.537934000	-3.761473000	1.354824000
1	3.489884000	-1.390445000	-0.682755000	1	-4.057035000	-2.234156000	-1.728210000
6	4.331646000	1.913414000	-0.411801000	7	-4.431389000	-2.519619000	-2.624411000
1	6.365509000	2.595595000	-0.030618000	7	-1.006245000	-4.596267000	1.567500000
1	2.479192000	0.824084000	-0.784224000	1	-5.078563000	-1.802403000	-2.922551000
7	3.769371000	3.175935000	-0.464538000	1	-4.786180000	-3.460231000	-2.731623000
6	2.356954000	3.352548000	-0.825360000	1	-0.643518000	-4.491347000	2.505339000
6	4.619984000	4.361102000	-0.364584000	1	-1.419863000	-5.501211000	1.388290000
1	2.054273000	4.372140000	-0.578779000				

III-1. For $^4 TS_H + 2NH_3$ Complex.

26	-1.280672000	0.024364000	-0.052139000	1	-4.802226000	-1.653833000	-3.556763000
7	-1.177610000	-1.478396000	1.341893000	1	-4.569428000	-3.687054000	-1.785252000
7	-0.016023000	1.130594000	1.072606000	8	0.021736000	-0.726052000	-0.941895000
7	-1.411432000	1.501504000	-1.378283000	16	-2.960861000	0.937861000	1.369417000
7	-2.676828000	-1.024094000	-1.050473000	1	-3.947619000	-0.002478000	1.142247000
6	-1.838764000	-2.693457000	1.301765000	6	6.771793000	1.399770000	-0.331579000
6	-0.437930000	-1.473276000	2.512809000	6	5.758224000	0.413216000	-0.526360000
6	0.563652000	0.767029000	2.281319000	6	5.979749000	-0.683245000	-1.384682000
6	0.487723000	2.378400000	0.756915000	6	4.512887000	0.522790000	0.127846000
6	-0.706351000	2.696157000	-1.367447000	6	4.994916000	-1.645227000	-1.575665000
6	-2.216531000	1.537504000	-2.505904000	1	6.931002000	-0.777432000	-1.896402000
6	-3.308586000	-0.644675000	-2.221123000	6	3.525330000	-0.435572000	-0.057197000
6	-3.120934000	-2.309834000	-0.766347000	1	4.314424000	1.373579000	0.769657000
6	-1.492669000	-3.477073000	2.469934000	6	3.752334000	-1.546013000	-0.905391000
6	-0.631969000	-2.723866000	3.217630000	1	5.201535000	-2.482940000	-2.229214000
6	1.443272000	1.824422000	2.733551000	1	2.560510000	-0.295610000	0.410026000
6	1.398003000	2.816169000	1.793479000	7	2.766803000	-2.525761000	-1.074365000
6	-1.065925000	3.486672000	-2.527498000	6	1.631081000	-2.581269000	-0.233714000
6	-1.997146000	2.775930000	-3.225567000	6	2.835896000	-3.433521000	-2.228965000
6	-4.188309000	-1.702985000	-2.669248000	1	1.076036000	-3.510511000	-0.346968000
6	-4.069578000	-2.729269000	-1.776127000	1	1.842515000	-2.339176000	0.808258000
6	-2.732037000	-3.086334000	0.314087000	1	0.754198000	-1.638375000	-0.575862000
6	0.371725000	-0.433857000	2.948524000	1	3.600043000	-4.207310000	-2.082703000
6	0.175861000	3.106073000	-0.383741000	1	1.868054000	-3.919709000	-2.350788000
6	-3.105411000	0.550817000	-2.895223000	1	3.062846000	-2.878668000	-3.144157000
1	-3.178134000	-4.070967000	0.406125000	7	7.606142000	2.211723000	-0.169202000
1	0.895463000	-0.569461000	3.888868000	1	-3.162938000	3.426110000	0.451062000
1	0.647978000	4.074896000	-0.504869000	1	-1.685079000	1.090774000	3.698492000
1	-3.673170000	0.716721000	-3.804263000	7	-1.231217000	1.222608000	4.593721000
1	-1.877291000	-4.464055000	2.682637000	7	-3.240619000	4.397895000	0.178288000
1	-0.170780000	-2.973067000	4.162329000	1	-1.174573000	0.316624000	5.038812000
1	2.009937000	1.798183000	3.653038000	1	-1.556175000	1.958839000	5.205673000
1	1.918780000	3.762727000	1.792125000	1	-3.776445000	4.428141000	-0.678506000
1	-0.655336000	4.459691000	-2.754557000	1	-3.531066000	5.079591000	0.866077000
1	-2.502040000	3.048584000	-4.140799000				

IV-1. For $^2 TS_H + 2NH_3$ Complex.

26	0.000000000	0.000000000	0.000000000	6	1.131592570	-2.835303240	0.160277240
7	2.052373000	0.000000000	0.000000000	6	4.266194090	-0.682235040	-0.000268320
7	0.017477170	2.021837200	0.000000000	6	4.265769400	0.684185230	-0.008774780
7	-1.988893180	0.005873930	0.044363470	6	0.710894520	4.232227960	-0.055004030
7	0.019480320	-2.002482200	0.186737650	6	-0.656066290	4.235393460	-0.082471650
6	2.881591340	-1.107849070	0.013250720	6	-4.205675910	0.688009640	0.005273590
6	2.881088480	1.109682520	-0.005707070	6	-4.206177270	-0.671670160	0.109660580
6	1.133783910	2.848255620	-0.009059250	6	-0.658851340	-4.214013250	0.308793390
6	-1.085305350	2.853568200	-0.050377020	6	0.705196270	-4.216219050	0.242535570
6	-2.820858660	1.113762000	-0.025424170	6	2.453541800	-2.427288720	0.073648690
6	-2.821594300	-1.098109680	0.138369500	6	2.456627560	2.430882930	-0.012304830
6	-1.085196980	-2.831730160	0.261138980	6	-2.408539050	2.433532750	-0.072372390

6	-2.408209480	-2.414106580	0.250134260	1	-0.148751360	4.696363230	-3.423867740
1	3.214610550	-3.200431550	0.075002290	6	0.823024100	1.807124400	-4.958044400
1	3.220926560	3.200788530	-0.017594120	1	0.682641930	1.465734520	-7.101469080
1	-3.176482770	3.198177230	-0.114390500	1	0.741092410	2.478264270	-2.894762650
1	-3.175642090	-3.177528400	0.316938020	7	1.376140620	0.555839010	-4.661267820
1	5.114028310	-1.351833870	0.010844830	6	1.930746420	0.277938370	-3.390510980
1	5.113062140	1.354518840	-0.008315520	6	1.260039320	-0.538914670	-5.635915070
1	1.383105480	5.078015770	-0.060447780	1	2.506345950	-0.645643880	-3.381969240
1	-1.323910060	5.084057170	-0.113086360	1	2.471839680	1.117618660	-2.953275820
1	-5.051733470	1.358210250	-0.038578640	1	0.963923600	0.063370010	-2.499303680
1	-5.052822190	-1.340122560	0.166859130	1	1.964330500	-0.409039370	-6.467281360
1	-1.328495060	-5.059056370	0.375660670	1	1.484682400	-1.480019900	-5.134124580
1	1.375193770	-5.063783220	0.247305920	1	0.243543420	-0.593708910	-6.036763830
8	0.010513110	-0.090994370	-1.744323860	7	-1.234848660	6.701001740	-6.111090560
16	0.212321800	0.237835910	2.361500850	1	-2.243511010	0.983209870	3.060714710
1	0.696991980	-1.024437510	2.646623860	1	1.746398760	2.401895720	2.559101160
6	-0.792520980	5.640714870	-5.862275530	7	2.280725720	3.251311400	2.692491510
6	-0.253358670	4.353931070	-5.558888010	7	-3.144235020	1.322366330	3.374522520
6	-0.022396510	3.413095780	-6.583340150	1	3.249256350	3.030272630	2.504843340
6	0.048231010	3.996258440	-4.227734630	1	2.140990240	3.792510220	3.534928220
6	0.502797960	2.159964730	-6.290740280	1	-3.775247960	0.532579780	3.387968810
1	-0.253238220	3.673893020	-7.610135180	1	-3.190795870	1.896695130	4.205244170
6	0.574671290	2.746697610	-3.928692420				

V-1. For $^4\text{IM} + 2\text{NH}_3$ Complex.

26	-1.317901000	0.058034000	-0.110598000	1	-4.575977000	-1.836348000	-3.764212000
7	-1.095779000	-1.460501000	1.220210000	1	-4.350289000	-3.825323000	-1.941717000
7	-0.166873000	1.235683000	1.048409000	8	0.091504000	-0.558062000	-1.059292000
7	-1.529261000	1.549396000	-1.435143000	16	-3.111173000	0.888244000	1.180674000
7	-2.615752000	-1.072199000	-1.164311000	1	-4.146104000	0.318064000	0.465637000
6	-1.723370000	-2.697450000	1.184694000	6	6.465326000	1.855006000	-0.191277000
6	-0.348301000	-1.433949000	2.388592000	6	5.641261000	0.708826000	-0.402673000
6	0.463529000	0.880795000	2.232448000	6	6.184178000	-0.476357000	-0.941174000
6	0.209577000	2.541500000	0.778941000	6	4.265534000	0.743559000	-0.087573000
6	-0.953287000	2.806406000	-1.365852000	6	5.385046000	-1.596499000	-1.140039000
6	-2.263051000	1.518461000	-2.608944000	1	7.238357000	-0.515008000	-1.192422000
6	-3.202627000	-0.737706000	-2.375268000	6	3.461013000	-0.370892000	-0.285684000
6	-3.014089000	-2.371645000	-0.881014000	1	3.825662000	1.656548000	0.298027000
6	-1.331198000	-3.473529000	2.340283000	6	4.012119000	-1.566703000	-0.802898000
6	-0.483912000	-2.697158000	3.079809000	1	5.836009000	-2.499800000	-1.531720000
6	1.241036000	1.998405000	2.720518000	1	2.394657000	-0.296244000	-0.114691000
6	1.083090000	3.020952000	1.827480000	7	3.203818000	-2.705224000	-0.969325000
6	-1.324567000	3.576784000	-2.534151000	6	2.022975000	-2.873720000	-0.263816000
6	-2.128683000	2.783643000	-3.300146000	6	3.623035000	-3.758941000	-1.907615000
6	-4.008593000	-1.842064000	-2.845011000	1	1.466185000	-3.781639000	-0.446943000
6	-3.894691000	-2.845962000	-1.925042000	1	1.913795000	-2.361797000	0.682750000
6	-2.610746000	-3.125617000	0.209800000	1	0.475390000	-1.442400000	-0.828019000
6	0.387182000	-0.355181000	2.854906000	1	4.363230000	-4.431278000	-1.455356000
6	-0.153522000	3.276166000	-0.338508000	1	2.747468000	-4.345909000	-2.189679000
6	-3.040039000	0.461385000	-3.051177000	1	4.048780000	-3.314405000	-2.810322000
1	-3.018732000	-4.125688000	0.306530000	7	7.142946000	2.799578000	-0.014458000
1	0.929080000	-0.481729000	3.785555000	1	-2.653442000	3.508160000	1.134641000
1	0.223375000	4.289699000	-0.417174000	1	-2.465015000	0.048641000	3.620580000
1	-3.564261000	0.581921000	-3.992627000	7	-2.239213000	-0.197621000	4.576181000
1	-1.678650000	-4.474488000	2.551028000	7	-2.495412000	4.506184000	1.196126000
1	-0.000829000	-2.936450000	4.015945000	1	-2.450256000	-1.179555000	4.691887000
1	1.825923000	1.986171000	3.628562000	1	-2.581818000	0.385233000	5.327862000
1	1.512604000	4.011560000	1.860118000	1	-2.781994000	4.911161000	0.315225000
1	-1.003940000	4.590545000	-2.724267000	1	-2.833617000	5.008249000	2.005859000
1	-2.600114000	3.017654000	-4.243417000				

VI-1. For $^4\text{Carbinolaniline} + 2\text{NH}_3$ Complex.

26	1.589959000	0.335494000	0.182548000	6	0.083936000	0.005943000	2.842349000
7	0.525313000	-0.579064000	1.653486000	6	0.356405000	-1.954235000	1.829197000
7	1.639647000	-1.414257000	-0.811566000	6	1.309997000	-2.673579000	-0.315670000
7	2.170844000	1.288065000	-1.494675000	6	2.197099000	-1.637752000	-2.068586000
7	1.178588000	2.110194000	1.025344000	6	2.634555000	0.701352000	-2.666417000

6	2.352382000	2.655544000	-1.660116000	6	-8.247240000	1.001706000	-0.321472000
6	1.491345000	3.369361000	0.522290000	6	-6.954905000	0.418704000	-0.486578000
6	0.614232000	2.334416000	2.277945000	6	-6.784195000	-0.978635000	-0.443420000
6	-0.397887000	-1.011859000	3.743083000	6	-5.816079000	1.228645000	-0.683529000
6	-0.229561000	-2.217518000	3.120384000	6	-5.526163000	-1.549552000	-0.605309000
6	1.664937000	-3.689317000	-1.277113000	1	-7.647134000	-1.617102000	-0.287766000
6	2.210942000	-3.050870000	-2.356629000	6	-4.555785000	0.667329000	-0.839402000
6	3.102301000	1.720765000	-3.578267000	1	-5.926357000	2.307569000	-0.696617000
6	2.927667000	2.924914000	-2.958575000	6	-4.383813000	-0.740644000	-0.818992000
6	1.134838000	4.386536000	1.482220000	1	-5.437463000	-2.627814000	-0.579512000
6	0.595201000	3.748956000	2.563993000	1	-3.690422000	1.311659000	-0.919420000
6	0.116846000	1.359613000	3.127818000	7	-3.123130000	-1.310690000	-1.009948000
6	0.715781000	-2.926900000	0.911727000	6	-2.016801000	-0.501720000	-1.484407000
6	2.657338000	-0.656800000	-2.931620000	6	-2.927110000	-2.747605000	-0.798646000
6	2.042951000	3.625525000	-0.722127000	1	-1.227076000	-1.173406000	-1.831135000
1	-0.277665000	1.681548000	4.085051000	1	-2.336641000	0.136813000	-2.310505000
1	0.531074000	-3.962159000	1.176726000	1	-1.102596000	-0.022895000	0.266193000
1	3.062623000	-0.976701000	-3.885141000	1	-3.453603000	-3.352532000	-1.550342000
1	2.237666000	4.659798000	-0.982985000	1	-1.861645000	-2.974326000	-0.863404000
1	-0.802323000	-0.817566000	4.725570000	1	-3.279021000	-3.052899000	0.194014000
1	-0.466812000	-3.202318000	3.495612000	7	-9.311963000	1.481987000	-0.185651000
1	1.516088000	-4.749376000	-1.131747000	1	5.162794000	-1.046597000	-0.878397000
1	2.593619000	-3.486126000	-3.268127000	1	3.398110000	-1.931609000	2.901327000
1	3.509248000	1.524444000	-4.559332000	7	3.303992000	-2.711419000	3.539952000
1	3.162423000	3.911194000	-3.331207000	7	5.703382000	-1.508094000	-1.599224000
1	1.275557000	5.446756000	1.331311000	1	2.854712000	-2.363249000	4.376042000
1	0.206691000	4.184098000	3.472985000	1	4.107556000	-3.297387000	3.721746000
8	-1.489368000	0.441602000	-0.509146000	1	5.961557000	-0.805125000	-2.278415000
16	3.824528000	0.027982000	1.153824000	1	6.465735000	-2.114729000	-1.329164000
1	4.024881000	1.335684000	1.553560000				

VII. For ²Carbinolaniline + 2NH₃ Complex.

26	-1.124458000	0.098171000	0.317549000	1	2.252052000	0.999590000	4.257564000
7	-1.033314000	1.735444000	-0.858642000	1	2.275718000	3.253476000	2.760550000
7	-2.389586000	-0.732744000	-1.025679000	8	0.461849000	-0.614326000	-0.894722000
7	-1.117191000	-1.597778000	1.410005000	16	-2.861123000	0.998481000	1.506557000
7	0.249448000	0.864502000	1.572788000	1	-2.453690000	0.615409000	2.770436000
6	-0.306092000	2.884429000	-0.584931000	6	7.129937000	0.720362000	-0.126483000
6	-1.751719000	2.002167000	-2.016531000	6	5.925875000	0.050417000	-0.501759000
6	-2.932521000	-0.148518000	-2.163258000	6	5.921603000	-0.884904000	-1.554191000
6	-2.992305000	-1.977804000	-0.909389000	6	4.713079000	0.318504000	0.166227000
6	-1.903574000	-2.718509000	1.178944000	6	4.750131000	-1.541360000	-1.919602000
6	-0.420280000	-1.853670000	2.585776000	1	6.844151000	-1.099505000	-2.082327000
6	0.784097000	0.285690000	2.716074000	6	3.538384000	-0.327794000	-0.197784000
6	0.805669000	2.131975000	1.486026000	1	4.690476000	1.049637000	0.966560000
6	-0.564858000	3.883380000	-1.601964000	6	3.537071000	-1.285281000	-1.240444000
6	-1.454247000	3.339749000	-2.483911000	1	4.788317000	-2.262277000	-2.725689000
6	-3.875614000	-1.056061000	-2.780690000	1	2.615515000	-0.056821000	0.296660000
6	-3.913034000	-2.182249000	-2.008509000	7	2.359636000	-1.965950000	-1.591316000
6	-1.686232000	-3.694853000	2.225877000	6	1.200294000	-1.895937000	-0.754757000
6	-0.772344000	-3.162711000	3.091275000	6	2.325676000	-2.798221000	-2.800553000
6	1.702524000	1.207162000	3.350818000	1	0.524394000	-2.719594000	-0.989277000
6	1.714749000	2.345180000	2.593990000	1	1.452928000	-1.916233000	0.303628000
6	0.548214000	3.065742000	0.492246000	1	0.233789000	-0.417468000	-1.824953000
6	-2.630637000	1.122195000	-2.632038000	1	2.973759000	-3.679771000	-2.709525000
6	-2.763244000	-2.897746000	0.103707000	1	1.304013000	-3.145274000	-2.966260000
6	0.475961000	-0.982479000	3.189101000	1	2.640829000	-2.229076000	-3.682680000
1	1.056572000	4.021339000	0.566650000	7	8.121058000	1.271034000	0.183715000
1	-3.131216000	1.458510000	-3.533610000	1	-4.969560000	-0.107541000	0.320470000
1	-3.313110000	-3.832107000	0.059268000	1	-2.799918000	3.540906000	0.726863000
1	0.958699000	-1.309849000	4.103701000	7	-2.856885000	4.504905000	0.423111000
1	-0.119199000	4.867371000	-1.621190000	7	-5.806884000	-0.455778000	-0.129449000
1	-1.882116000	3.790250000	-3.367741000	1	-2.115593000	5.011315000	0.888037000
1	-4.434974000	-0.841225000	-3.679736000	1	-3.751190000	4.975793000	0.447703000
1	-4.509724000	-3.071738000	-2.150757000	1	-5.935394000	-1.412021000	0.172555000
1	-2.179458000	-4.654663000	2.280570000	1	-6.650521000	0.100310000	-0.095367000
1	-0.369837000	-3.600858000	3.993152000				

Table S22 Cartesian Coordinates for Various Reaction Species in C–H Hydroxylation of p-NO₂-DMA by Cpd I

I. For ⁴RC

26	-2.265256000	-0.500391000	0.283192000	6	-3.547451000	-1.672578000	-2.310642000
7	-3.265267000	-2.208277000	0.684633000	6	-4.424115000	-4.196760000	0.393433000
7	-1.853495000	-0.299113000	2.245643000	6	-4.118685000	-4.055347000	1.717133000
7	-1.533349000	1.347367000	-0.051394000	6	-1.708400000	-0.608333000	4.457370000
7	-2.929611000	-0.580706000	-1.622525000	6	-1.084118000	0.574824000	4.186441000
6	-3.915597000	-3.033994000	-0.231062000	6	-0.427656000	3.378535000	0.081986000
6	-3.312774000	-2.880804000	1.901652000	6	-3.091486000	-0.232695000	-3.993495000
6	-2.078696000	-1.231098000	3.246293000	6	-3.681359000	-1.436879000	-3.731028000
6	-1.159579000	0.742867000	2.848308000	6	-4.023016000	-2.793483000	-1.647604000
6	-0.890310000	2.165368000	0.858102000	6	-2.923982000	-2.299684000	3.056228000
6	-1.487607000	2.015482000	-1.262917000	6	-0.751650000	1.938152000	2.108274000
6	-2.686655000	0.346910000	-2.623755000	1	-1.934779000	1.492049000	-2.580869000
6	-3.606245000	-1.625206000	-2.227820000	1	-4.534379000	-3.544179000	-2.241004000
6	-4.397945000	-4.222531000	0.436310000	1	-3.090907000	-2.894616000	3.947914000
6	-4.025900000	-4.129053000	1.746271000	1	-0.180886000	2.648433000	2.696031000
6	-1.513340000	-0.764772000	4.494780000	1	-1.777007000	2.089065000	-3.472914000
6	-0.944929000	0.451769000	4.250147000	1	-4.954728000	-5.003572000	-0.090525000
6	-0.427357000	3.370345000	0.203956000	1	-4.348533000	-4.723176000	2.534308000
6	-0.798546000	3.278854000	-1.106735000	1	-1.802320000	-1.113897000	5.407162000
6	-3.227820000	-0.126939000	-3.878363000	1	-0.548119000	1.227653000	4.858794000
6	-3.794105000	-1.346261000	-3.634406000	1	0.107219000	4.181703000	0.566868000
6	-4.063080000	-2.767244000	-1.580097000	1	-0.562716000	3.945154000	-2.043418000
6	-2.748299000	-2.434685000	3.083727000	1	-2.998336000	0.276007000	-4.941840000
6	-0.712750000	1.885944000	2.207557000	8	-0.843260000	-1.241458000	-0.067569000
6	-2.024012000	1.553415000	-2.455382000	16	-4.353606000	0.976392000	0.734973000
1	-4.583775000	-3.505725000	-2.180582000	1	-4.548968000	1.505916000	-0.527538000
1	-2.849189000	-3.070991000	3.956406000	7	3.339204000	1.886120000	3.422220000
1	-0.154506000	2.600407000	2.802353000	6	3.394328000	0.976838000	2.311093000
1	-1.913640000	2.186973000	-3.329266000	6	4.542605000	0.917959000	1.507489000
1	-4.944957000	-5.017315000	-0.049392000	6	2.284085000	0.171110000	2.017762000
1	-4.208693000	-4.831630000	2.546000000	6	4.568108000	0.080459000	0.403293000
1	-1.553263000	-1.310150000	5.426117000	1	5.394168000	1.538262000	1.756046000
1	-0.407736000	1.097065000	4.928761000	1	2.297577000	-0.663593000	0.915196000
1	0.105552000	4.168918000	0.698446000	6	1.415756000	0.213664000	2.658507000
1	-0.631967000	3.989587000	-1.902815000	6	3.437194000	-0.719707000	0.061927000
1	-3.175996000	0.413485000	-4.812200000	1	5.460687000	0.054048000	-0.207363000
1	-4.298468000	-2.002619000	-4.328392000	1	1.410381000	-1.243342000	0.698443000
8	-0.834574000	-1.251917000	-0.077512000	7	3.440440000	-1.522173000	-1.056633000
16	-4.541041000	0.433321000	1.022217000	6	2.264715000	-2.341179000	-1.388465000
1	-5.322228000	-0.138133000	0.034771000	6	4.639881000	-1.625642000	-1.890244000
7	3.413203000	1.860789000	3.353349000	1	2.395251000	-2.756261000	-2.388884000
6	3.445831000	1.001868000	2.201918000	1	2.135170000	-3.172050000	-0.681277000
6	4.562120000	1.007555000	1.352439000	1	1.346622000	-1.745727000	-1.376760000
6	2.344171000	0.181625000	1.916316000	1	5.495912000	-2.022010000	-1.327174000
6	4.563690000	0.219523000	0.212140000	1	4.438343000	-2.302026000	-2.721279000
1	5.407658000	1.638518000	1.594678000	1	4.926007000	-0.650836000	-2.306253000
6	2.333823000	-0.604033000	0.778184000	8	2.238932000	2.004117000	4.062772000
1	1.501471000	0.173994000	2.591769000	8	4.380593000	2.552417000	3.721718000
6	3.439953000	-0.594421000	-0.119821000				
1	5.431275000	0.243360000	-0.433622000				
1	1.453053000	-1.196912000	0.570638000				
7	3.418375000	-1.348758000	-1.271126000	26	-2.190340000	-0.113369000	-0.063590000
6	2.248368000	-2.179294000	-1.594384000	7	-2.316166000	-2.143928000	0.209868000
6	4.585966000	-1.386503000	-2.154092000	7	-1.643780000	0.091811000	1.873135000
1	2.352420000	-2.553300000	-2.613873000	7	-2.113992000	1.858004000	-0.307359000
1	2.159753000	-3.038798000	-0.915794000	7	-2.913690000	-0.337033000	-1.924168000
1	1.319497000	-1.604432000	-1.528313000	7	-2.671415000	-3.086932000	-0.739044000
1	5.475058000	-1.773981000	-1.638267000	6	-2.066937000	-2.841868000	1.380746000
1	4.372045000	-2.041766000	-2.998806000	6	-1.484840000	-0.920710000	2.811181000
1	4.826079000	-0.390101000	-2.547773000	6	-1.295865000	1.269572000	2.507698000
8	2.336139000	1.924119000	4.039313000	6	-1.688543000	2.796555000	0.621818000
8	4.450013000	2.538733000	3.642370000	6	-2.460700000	2.570307000	-1.444825000

III. For ⁴TS_H

26	-2.289892000	-0.490549000	0.210723000	6	-3.152325000	0.671176000	-2.841093000
7	-3.283084000	-2.190005000	0.622332000	6	-3.174432000	-1.532761000	-2.583299000
7	-1.946721000	-0.217675000	2.179584000	6	-2.629103000	-4.410692000	-0.152888000
7	-1.571935000	1.368978000	-0.146305000	6	-2.260434000	-4.259158000	1.154262000
7	-2.882589000	-0.6111792000	-1.714713000	6	-1.036585000	-0.352956000	4.065331000
6	-3.902507000	-3.031026000	-0.286427000	6	-0.917320000	0.996003000	3.877580000
6	-3.406688000	-2.803323000	1.854252000	6	-1.752198000	4.122982000	0.041781000
6	-2.240396000	-1.105986000	3.206468000	6	-2.231382000	3.984394000	-1.227323000
6	-1.241831000	0.819885000	2.767841000	6	-3.596681000	0.100209000	-4.094344000
6	-0.921178000	2.200970000	0.760810000	6	-3.605425000	-1.256349000	-3.937105000
6	-1.464855000	2.001251000	-1.384016000				
6	-2.593490000	0.277404000	-2.735047000				

6	-3.055571000	-2.803700000	-2.042970000	6	-2.828050000	1.939647000	-2.648595000
6	-1.680096000	-2.275701000	2.587268000	1	-3.537440000	-3.696474000	-2.577163000
6	-1.304630000	2.529405000	1.923832000	1	-1.412226000	-3.039627000	3.420035000
6	-2.954961000	2.026113000	-2.617281000	1	-1.153260000	3.300132000	2.601336000
1	-3.306689000	-3.642529000	-2.683500000	1	-2.999555000	2.612798000	-3.481470000
1	-1.517332000	-2.946493000	3.424209000	1	-3.074232000	-5.355632000	-0.597634000
1	-1.004082000	3.369165000	2.540764000	1	-2.157771000	-5.085016000	1.934542000
1	-3.185808000	2.707331000	-3.428976000	1	-0.782743000	-0.991447000	4.972703000
1	-2.867607000	-5.323102000	-0.680042000	1	-0.698682000	1.691213000	4.622630000
1	-2.134762000	-5.023137000	1.907741000	1	-1.544841000	4.962390000	0.599403000
1	-0.844103000	-0.923545000	4.962241000	1	-2.311901000	4.674456000	-1.980572000
1	-0.609218000	1.746864000	4.590512000	1	-3.756448000	0.591167000	-4.990820000
1	-1.472063000	5.029363000	0.558342000	1	-3.996216000	-2.077972000	-4.605372000
1	-2.421052000	4.754297000	-1.960875000	8	-0.555255000	-0.234965000	-0.628316000
1	-3.855124000	0.675349000	-4.971465000	16	-4.441001000	0.063043000	0.755036000
1	-3.875787000	-2.013031000	-4.659295000	1	-4.979660000	0.622962000	-0.386677000
8	-0.537712000	-0.293054000	-0.603610000	7	4.897126000	1.029157000	3.740248000
16	-4.406288000	-0.089076000	0.819821000	6	4.254819000	0.332791000	2.640467000
1	-5.043938000	-0.729172000	-0.225947000	6	5.016876000	-0.049456000	1.530583000
7	4.944818000	0.979594000	3.723264000	6	2.881869000	0.065507000	2.700895000
6	4.282283000	0.274354000	2.643585000	6	4.403928000	-0.714258000	0.477206000
6	5.023130000	-0.124487000	1.524839000	1	6.075144000	0.174950000	1.511678000
6	2.908836000	0.013721000	2.729116000	6	2.266098000	-0.600933000	1.651316000
6	4.389502000	-0.797604000	0.489303000	1	2.309140000	0.395503000	3.557221000
1	6.082145000	0.093820000	1.485814000	6	3.018220000	-1.014882000	0.522070000
6	2.272852000	-0.660990000	1.697764000	1	5.005271000	-1.016855000	-0.369683000
1	2.352299000	0.356612000	3.591050000	1	1.196470000	-0.751311000	1.680920000
6	3.002978000	-1.090494000	0.559467000	7	2.405859000	-1.705561000	-0.524193000
1	4.975640000	-1.113224000	-0.363507000	6	1.077046000	-2.191088000	-0.411989000
1	1.203339000	-0.806898000	1.746763000	6	3.084912000	-1.808693000	-1.825443000
7	2.369136000	-1.788474000	-0.468758000	1	0.836884000	-2.898701000	-1.204335000
6	1.047512000	-2.274655000	-0.330343000	1	0.845079000	-2.591887000	0.576205000
6	3.028033000	-1.910356000	-1.778940000	1	0.251573000	-1.263353000	-0.548930000
1	0.777861000	-2.975045000	-1.118068000	1	3.916984000	-2.522135000	-1.783100000
1	0.814837000	-2.647650000	0.666953000	1	2.367357000	-2.155051000	-2.568685000
1	0.170144000	-1.270766000	-0.477862000	1	3.468022000	-0.833650000	-2.141324000
1	3.849857000	-2.636047000	-1.744271000	8	4.187182000	1.359214000	4.738407000
1	2.294048000	-2.250172000	-2.509105000	8	6.139200000	1.273936000	3.652676000
1	3.420423000	-0.943128000	-2.106590000				
8	4.252567000	1.326275000	4.729197000				
8	6.187207000	1.217132000	3.613926000				

IV. $\text{For}^2 \mathbf{T}\mathbf{S}_H$.

26	-2.179477000	-0.214797000	-0.040179000
7	-2.328738000	-2.200780000	0.241795000
7	-1.633957000	-0.000591000	1.890462000
7	-2.133953000	1.791982000	-0.290669000
7	-2.914630000	-0.413334000	-1.911979000
6	-2.788826000	-3.133432000	-0.679282000
6	-2.040465000	-2.910642000	1.399401000
6	-1.426149000	-1.004752000	2.822656000
6	-1.354977000	1.194949000	2.535640000
6	-1.762600000	2.729241000	0.656675000
6	-2.394297000	2.493482000	-1.455263000
6	-3.073111000	0.590575000	-2.854167000
6	-3.264719000	-1.596320000	-2.539650000
6	-2.763211000	-4.454018000	-0.090255000
6	-2.299937000	-4.317651000	1.187502000
6	-1.003810000	-0.424985000	4.079790000
6	-0.962799000	0.929818000	3.903277000
6	-1.790697000	4.053747000	0.069634000
6	-2.176596000	3.908375000	-1.231093000
6	-3.547565000	0.020956000	-4.097349000
6	-3.668724000	-1.325425000	-3.902934000
6	-3.215691000	-2.858611000	-1.968116000
6	-1.600960000	-2.362104000	2.594509000
6	-1.411176000	2.457954000	1.968557000

V. $\text{For}^4 \mathbf{IM}$

26	-2.108483000	-0.758462000	0.489804000
7	-3.011366000	-2.453537000	-0.168676000
7	-1.830179000	-1.621664000	2.309520000
7	-1.134507000	0.905411000	1.119829000
7	-2.434403000	0.114269000	-1.306323000
6	-3.554469000	-2.667786000	-1.425808000
6	-3.290211000	-3.587048000	0.577328000
6	-2.271686000	-2.872855000	2.709454000
6	-1.155109000	-1.077585000	3.382262000
6	-0.552201000	1.098556000	2.356423000
6	-0.972194000	2.087609000	0.416245000
6	-2.068582000	1.394364000	-1.683179000
6	-3.035769000	-0.464892000	-2.412153000
6	-4.169369000	-3.979447000	-1.474154000
6	-4.009869000	-4.543434000	-0.240390000
6	-1.871326000	-3.110851000	4.080057000
6	-1.175085000	-2.007000000	4.493648000
6	0.002770000	2.436771000	2.431914000
6	-0.264967000	3.048757000	1.239051000
6	-2.460891000	1.628882000	-3.057187000
6	-3.054124000	0.481744000	-3.507173000
6	-3.550653000	-1.754338000	-2.470575000
6	-2.951234000	-3.782292000	1.909686000
6	-0.519621000	0.165211000	3.391317000
6	-1.401471000	2.316593000	-0.882088000
6	-4.008067000	-2.064232000	-3.404376000
6	-3.239831000	-4.724983000	2.362726000
6	-0.038225000	0.468154000	4.316364000
6	-1.196880000	3.291530000	-1.311985000
6	-4.665623000	-4.393067000	-2.340151000
6	-4.349758000	-5.510191000	0.101960000
6	-2.100310000	-4.005381000	4.641247000
6	-0.733975000	-1.820655000	5.462745000

1	0.497176000	2.851010000	3.299365000	6	3.997951000	1.526040000	-2.266058000
1	-0.020396000	4.056228000	0.934310000	6	4.860694000	0.775596000	-1.460951000
1	-2.294237000	2.550917000	-3.595147000	6	2.625528000	1.576972000	-1.991431000
1	-3.468906000	0.282833000	-4.484752000	6	4.352608000	0.083602000	-0.368681000
8	-0.239481000	-1.514668000	-0.127929000	6	5.916299000	0.748814000	-1.697683000
16	-4.341621000	0.106722000	1.415412000	1	2.112786000	0.885080000	-0.904383000
1	-4.808227000	0.765289000	0.292044000	6	1.974420000	2.143928000	-2.643409000
7	3.545041000	2.696307000	-3.130085000	1	2.969526000	0.132268000	-0.057787000
6	3.329556000	1.900026000	-1.921233000	1	5.035141000	-0.483268000	0.250119000
6	4.238395000	2.014949000	-0.868767000	6	1.044764000	0.883516000	-0.738962000
6	2.224309000	1.049473000	-1.845175000	7	2.463069000	-0.541298000	1.054061000
6	4.031066000	1.263671000	0.285289000	1	1.103474000	-0.315987000	1.491341000
1	5.084150000	2.682691000	-0.960704000	6	3.320663000	-1.459094000	1.813690000
6	2.010262000	0.293185000	-0.693395000	1	1.000183000	-0.690046000	2.512804000
1	1.535871000	0.985072000	-2.677251000	1	0.852742000	0.744600000	1.467438000
6	2.917338000	0.406797000	0.376789000	1	0.118086000	-1.892623000	0.623406000
1	4.739477000	1.3667037000	1.094881000	1	4.133947000	-0.929778000	2.327219000
1	1.135323000	-0.371343000	-0.645927000	1	2.717924000	-1.966194000	2.569432000
7	2.717444000	-0.371049000	1.589667000	1	3.763594000	-2.221146000	1.161965000
6	1.649944000	-1.110537000	1.803011000	1	3.724818000	2.925210000	-4.116381000
6	3.765774000	-0.278310000	2.642605000	8	5.774530000	2.173577000	-3.638147000
1	1.630639000	-1.669000000	2.732927000	8			
1	0.832214000	-1.288547000	1.026450000				
1	-0.359269000	-2.390560000	-0.547119000				
1	3.816640000	0.742407000	3.027965000				
1	3.501975000	-0.954563000	3.453832000				
1	4.735106000	-0.566929000	2.231789000				
8	4.568889000	3.440064000	-3.176709000				
8	2.698746000	2.601068000	-4.064297000				

VI. For ⁴ Carbinolaniline Complex.

26	-2.347543000	-0.417300000	0.374299000	26	-2.210131000	-0.474877000	0.323955000
7	-2.343607000	-2.398107000	-0.076356000	7	-2.328939000	-2.455101000	-0.085894000
7	-2.514753000	-0.884488000	2.330892000	7	-2.235042000	-0.856559000	2.308077000
7	-1.961298000	1.502819000	0.879077000	7	-1.918566000	1.472985000	0.740729000
7	-1.937350000	0.011235000	-1.544622000	6	-2.048558000	-0.118209000	-1.650935000
6	-2.276793000	-2.956309000	-1.347236000	6	-2.396060000	-3.062219000	-1.335204000
6	-2.623360000	-3.449575000	0.790487000	6	-2.541179000	-3.467348000	0.844176000
6	-2.755579000	-2.143521000	2.871749000	6	-2.436701000	-2.098389000	2.896559000
6	-2.508579000	0.000412000	3.403890000	6	-2.156062000	0.056291000	3.353080000
6	-2.036566000	2.063354000	2.148634000	6	-1.884236000	2.085330000	1.989099000
6	-1.747757000	2.561211000	0.005029000	6	-1.821275000	2.497093000	-0.191288000
6	-1.723537000	1.271202000	-2.088502000	6	-1.923038000	1.128745000	-2.241952000
6	-1.912057000	-0.877665000	-2.611125000	6	-2.121751000	-1.031015000	-2.691944000
6	-2.488793000	-4.384389000	-1.267143000	6	-2.624705000	-4.481599000	-1.180091000
6	-2.703187000	-4.687985000	0.048167000	6	-2.715681000	-4.730902000	0.160714000
6	-2.914351000	-2.037580000	4.303007000	6	-2.473405000	-1.957266000	4.336944000
6	-2.760370000	-0.717955000	4.630841000	6	-2.298603000	-0.631019000	4.618042000
6	-1.842324000	3.494580000	2.065188000	6	-1.747441000	3.517137000	1.830402000
6	-1.666067000	3.801092000	0.745495000	6	-1.710308000	3.770773000	0.488391000
6	-1.569578000	1.166364000	-3.522129000	6	-1.907440000	0.990696000	-3.685424000
6	-1.684930000	-0.157177000	-3.843363000	6	-2.029037000	-0.339742000	-3.962217000
6	-2.069208000	-2.253154000	-2.523394000	6	-2.281070000	-2.401546000	-2.549678000
6	-2.811714000	-3.333283000	2.158840000	6	-2.578734000	-3.303339000	2.221209000
6	-2.284904000	1.367915000	3.321587000	1	-1.982868000	1.425992000	3.206327000
6	-1.637625000	2.456801000	-1.3727578000	1	-1.817471000	2.337810000	-1.570260000
1	-2.038217000	-2.819629000	-3.447648000	1	-2.341473000	-2.997210000	-3.454120000
1	-3.021671000	-4.240388000	2.715224000	1	-2.744827000	-4.191398000	2.822164000
1	-2.318312000	1.936692000	4.244548000	1	-1.943692000	2.027365000	4.108382000
1	-1.473665000	3.370199000	-1.933963000	1	-1.729811000	3.235413000	-2.173375000
1	-2.483742000	-5.052978000	-2.115665000	1	-2.712686000	-5.181619000	-1.998272000
1	-2.907801000	-5.653712000	0.487098000	1	-2.892756000	-5.675473000	0.654555000
1	-3.115258000	-2.870829000	4.960701000	1	-2.620701000	-2.773849000	5.029063000
1	-2.811735000	-0.262011000	5.608953000	1	-2.275113000	-0.148980000	5.584745000
1	-1.853146000	4.165088000	2.912196000	8	-1.694447000	4.222848000	2.646751000
1	-1.502420000	4.771185000	0.299378000	1	-1.619202000	4.725085000	-0.009824000
1	-1.394416000	2.002618000	-4.183075000	1	-1.816708000	1.814140000	-4.378844000
1	-1.621789000	-0.615974000	-4.819174000	16	-2.058857000	-0.823888000	-4.927461000
8	0.089144000	-0.914640000	0.625730000	1	-4.483642000	-0.248788000	0.227541000
16	-4.770430000	-0.086923000	-0.003730000	7	-4.644598000	0.580740000	1.321268000
1	-5.181307000	-0.172976000	1.313502000	6	-4.143414000	1.778593000	-1.854946000
7	4.528716000	2.248046000	-3.404179000	6	-4.890223000	0.855601000	-1.116831000
				6	-2.758959000	1.887454000	-1.676688000

6	4.252177000	0.045245000	-0.185732000	1	0.632006000	-0.911201000	2.292530000
1	5.958267000	0.788695000	-1.277426000	1	0.645480000	0.660935000	1.452827000
6	2.116629000	1.076904000	-0.751702000	1	-0.022670000	-1.781073000	0.085257000
1	2.201012000	2.594342000	-2.276322000	1	3.750888000	-1.357290000	2.290560000
6	2.854453000	0.146195000	0.025679000	1	2.261983000	-2.317268000	2.255910000
1	4.845508000	-0.655831000	0.385538000	1	3.405006000	-2.418323000	0.905494000
1	1.040081000	1.129488000	-0.665023000	8	4.110358000	3.456848000	-3.479765000
7	2.218045000	-0.654880000	0.979002000	8	6.063695000	2.494679000	-2.977072000
6	0.854517000	-0.402937000	1.353887000				
6	2.954638000	-1.741131000	1.640011000				

I-1. For $^4\text{RC} + 2\text{NH}_3$ Complex.

26	-1.361466000	0.209290000	0.019249000	1	-2.682987000	4.502314000	2.748932000
7	-2.705057000	0.124885000	-1.485972000	1	-4.315506000	4.522824000	0.588832000
7	-0.651286000	-1.593399000	-0.535034000	8	-0.235423000	1.066891000	-0.839994000
7	-0.229238000	0.133956000	1.684851000	16	-3.197989000	-1.232335000	1.089795000
7	-2.274417000	1.870483000	0.716769000	1	-4.225856000	-0.308278000	1.051438000
6	-3.663728000	1.084048000	-1.808760000	7	5.094018000	-2.151356000	0.022157000
6	-2.760254000	-0.823158000	-2.502757000	6	4.748382000	-0.818917000	-0.389843000
6	-0.972608000	-2.301003000	-1.682492000	6	5.703350000	0.206559000	-0.325149000
6	0.362765000	-2.314798000	0.082811000	6	3.444215000	-0.543985000	-0.827546000
6	0.719631000	-0.818698000	2.004078000	6	5.347807000	1.501310000	-0.669356000
6	-0.176129000	1.077794000	2.696091000	1	6.707784000	-0.026356000	0.004394000
6	-1.937315000	2.583643000	1.856824000	6	3.078174000	0.745544000	-1.167897000
6	-3.272939000	2.598709000	0.094004000	1	2.727038000	-1.349020000	-0.890894000
6	-4.342180000	0.708355000	-3.029097000	6	4.017903000	1.812990000	-1.081302000
6	-3.785704000	-0.462540000	-3.456290000	1	6.096974000	2.279140000	-0.606034000
6	-0.143207000	-3.483134000	-1.784802000	1	2.054543000	0.927529000	-1.466889000
6	0.681741000	-3.491821000	-0.697468000	7	3.647432000	3.103265000	-1.386150000
6	1.385554000	-0.464238000	3.239029000	6	2.270152000	3.401955000	-1.806965000
6	0.830312000	0.706935000	3.668123000	6	4.635755000	4.183490000	-1.360560000
6	-2.746341000	3.778777000	1.949385000	1	2.135822000	4.484285000	-1.831090000
6	-3.570064000	3.789357000	0.859289000	1	2.054837000	3.002229000	-2.807437000
6	-3.917624000	2.233086000	-1.082089000	1	1.538873000	2.976486000	-1.112818000
6	-1.945857000	-1.937613000	-2.601269000	1	5.455730000	4.002964000	-2.068904000
6	0.999084000	-1.958087000	1.259543000	1	4.148150000	5.118321000	-1.638059000
6	-0.969189000	2.212517000	2.777746000	1	5.069720000	4.309248000	-0.359902000
1	-4.687302000	2.899972000	-1.456146000	8	4.172373000	-3.036291000	0.067811000
1	-2.089145000	-2.586339000	-3.458740000	8	6.299863000	-2.401427000	0.340776000
1	1.797716000	-2.604730000	1.605831000	1	-2.058162000	-1.960845000	3.380135000
1	-0.817702000	2.865167000	3.631180000	1	-3.627239000	-3.567292000	-0.109922000
1	-5.136114000	1.279144000	-3.488094000	7	-3.792917000	-4.489488000	-0.493214000
1	-4.034281000	-1.041041000	-4.333866000	7	-1.651948000	-2.312630000	4.238065000
1	-0.196792000	-4.200384000	-2.590469000	1	-4.336572000	-4.371394000	-1.337378000
1	1.453663000	-4.200803000	-0.438662000	1	-4.136694000	-5.220014000	0.115285000
1	2.168159000	-1.047301000	3.701414000	1	-1.677861000	-1.561006000	4.913720000
1	1.065975000	1.276232000	4.555252000	1	-1.967559000	-3.201082000	4.602981000

II-1. For $^2\text{RC} + 2\text{NH}_3$ Complex.

26	-1.346367000	0.187957000	0.082987000	6	1.413841000	-0.684041000	3.257129000
7	-2.663049000	0.210254000	-1.436834000	6	0.831574000	0.434262000	3.779401000
7	-0.605273000	-1.563731000	-0.588586000	6	-2.773571000	3.587074000	2.272411000
7	-0.239348000	-0.018008000	1.766097000	6	-3.603562000	3.659258000	1.189451000
7	-2.276888000	1.775981000	0.910997000	6	-3.920013000	2.248242000	-0.861562000
6	-3.630297000	1.169544000	-1.683891000	6	-1.926028000	-1.800973000	-2.651989000
6	-2.726189000	-0.675535000	-2.495349000	6	1.082188000	-2.007660000	1.153903000
6	-0.937786000	-2.208488000	-1.773304000	6	-0.976522000	1.987658000	2.994013000
6	0.438697000	-2.292446000	-0.042192000	1	-4.705937000	2.923321000	-1.183668000
6	0.754980000	-0.963957000	2.000715000	1	-2.084867000	-2.404937000	-3.539068000
6	-0.187926000	0.861174000	2.846633000	1	1.912893000	-2.646266000	1.432904000
6	-1.947342000	2.413383000	2.094402000	1	-0.825885000	2.588679000	3.884601000
6	-3.290307000	2.531153000	0.340786000	1	-5.112335000	1.471410000	-3.341880000
6	-4.312526000	0.876620000	-2.925656000	1	-4.005106000	-0.791900000	-4.335516000
6	-3.754409000	-0.264841000	-3.426692000	1	-0.139831000	-4.031593000	-2.809925000
6	-0.083875000	-3.361595000	-1.964649000	1	1.569182000	-4.109584000	-0.705222000
6	0.771775000	-3.408980000	-0.902288000	1	2.216900000	-1.277103000	3.669023000

1	1.063227000	0.939385000	4.705644000	6	2.211105000	3.535455000	-1.609743000
1	-2.717269000	4.254381000	3.119963000	6	4.565340000	4.342159000	-1.149318000
1	-4.362072000	4.397494000	0.973896000	1	2.051357000	4.613650000	-1.563427000
8	-0.219151000	1.111000000	-0.698954000	1	1.993602000	3.195133000	-2.631564000
16	-2.828340000	-1.393227000	1.493406000	1	1.498132000	3.049649000	-0.936499000
1	-3.095237000	-0.533953000	2.543602000	1	5.372031000	4.227112000	-1.886176000
7	5.180267000	-2.048854000	-0.137723000	1	4.051452000	5.281863000	-1.353295000
6	4.799924000	-0.703305000	-0.468284000	1	5.020061000	4.412075000	-0.152564000
6	5.733879000	0.337741000	-0.359944000	8	4.278912000	-2.955682000	-0.130701000
6	3.483609000	-0.433090000	-0.870998000	8	6.395724000	-2.289463000	0.150226000
6	5.345474000	1.641635000	-0.625100000	1	-1.709557000	-3.729435000	2.098422000
1	6.748222000	0.108779000	-0.059275000	1	-4.707839000	-2.088789000	-0.255673000
6	3.084823000	0.865062000	-1.132408000	7	-5.414786000	-2.429354000	-0.895242000
1	2.782605000	-1.248773000	-0.969051000	7	-1.353894000	-4.653434000	2.309459000
6	4.002613000	1.946587000	-0.998586000	1	-6.097434000	-1.692436000	-1.009539000
1	6.078981000	2.431057000	-0.529842000	1	-5.820956000	-3.341755000	-0.738165000
1	2.052861000	1.040777000	-1.405146000	1	-0.689040000	-4.554824000	3.064684000
7	3.599771000	3.243730000	-1.222814000	1	-2.007442000	-5.414142000	2.437209000

III-1. For $^4 TS_H + 2NH_3$ Complex.

26	-1.469502000	0.024700000	-0.100401000	1	-4.977084000	-1.530864000	-3.672222000
7	-1.527352000	-1.423969000	1.352800000	1	-4.941061000	-3.514170000	-1.830901000
7	-0.171973000	1.081907000	1.035585000	8	-0.188826000	-0.845911000	-0.910953000
7	-1.446208000	1.454897000	-1.480820000	16	-3.127316000	1.103662000	1.233362000
7	-2.897524000	-0.959768000	-1.113606000	1	-4.154632000	0.198956000	1.043411000
6	-2.265721000	-2.594443000	1.326440000	7	6.617659000	1.041433000	-0.197303000
6	-0.839286000	-1.422529000	2.555611000	6	5.551988000	0.072907000	-0.365603000
6	0.329813000	0.730255000	2.282559000	6	5.758217000	-1.042157000	-1.186348000
6	0.437278000	2.274225000	0.692038000	6	4.327665000	0.273113000	0.284438000
6	-0.652039000	2.592655000	-1.488422000	6	4.737864000	-1.968928000	-1.350301000
6	-2.209072000	1.508663000	-2.636916000	1	6.713752000	-1.168200000	-1.678038000
6	-3.463438000	-0.579176000	-2.317381000	6	3.306835000	-0.652072000	0.125266000
6	-3.437848000	-2.202720000	-0.804855000	1	4.182734000	1.156995000	0.891056000
6	-2.022925000	-3.353302000	2.535941000	6	3.494444000	-1.799362000	-0.688250000
6	-1.147032000	-2.629238000	3.294930000	1	4.914265000	-2.833886000	-1.975752000
6	1.267864000	1.738665000	2.729032000	1	2.347783000	-0.459849000	0.584413000
6	1.336330000	2.688360000	1.747932000	7	2.476216000	-2.742100000	-0.831900000
6	-0.911715000	3.362577000	-2.688294000	6	1.314686000	-2.708162000	-0.024487000
6	-1.872432000	2.698515000	-3.392206000	6	2.536806000	-3.715901000	-1.933543000
6	-4.397653000	-1.590713000	-2.762498000	1	0.727005000	-3.620390000	-0.103492000
6	-4.378056000	-2.592086000	-1.834103000	1	1.501061000	-2.411587000	1.007584000
6	-3.142599000	-2.964018000	0.315244000	1	0.481546000	-1.749944000	-0.456950000
6	0.023209000	-0.424650000	2.987151000	1	3.280619000	-4.496760000	-1.732983000
6	0.224271000	2.974168000	-0.488159000	1	1.559137000	-4.185272000	-2.039392000
6	-3.154955000	0.575075000	-3.022678000	1	2.786604000	-3.219535000	-2.875921000
1	-3.656828000	-3.913336000	0.421723000	8	6.408095000	2.041388000	0.556005000
1	0.496339000	-0.557411000	3.954336000	8	7.712103000	0.844633000	-0.809980000
1	0.773925000	3.898514000	-0.628143000	1	-3.192240000	3.538433000	0.164128000
1	-3.679533000	0.747733000	-3.956061000	1	-2.396417000	1.594590000	3.743417000
1	-2.481194000	-4.304244000	2.766086000	7	-2.150649000	1.854807000	4.690355000
1	-0.744455000	-2.871618000	4.267746000	7	-3.217735000	4.494484000	-0.167720000
1	1.795386000	1.710518000	3.671368000	1	-2.199148000	1.017477000	5.254843000
1	1.929793000	3.590830000	1.729514000	1	-2.598269000	2.657720000	5.111175000
1	-0.419992000	4.291995000	-2.935738000	1	-3.737616000	4.498392000	-1.034800000
1	-2.325035000	2.973252000	-4.333744000	1	-3.485361000	5.229819000	0.472422000

IV-1. For $^2 TS_H + 2NH_3$ Complex.

26	-1.421301000	0.121638000	-0.199513000	6	-0.406792000	2.549726000	-1.749322000
7	-1.683402000	-1.131092000	1.352224000	6	-1.858090000	1.385954000	-2.955254000
7	-0.123741000	1.195811000	0.911046000	6	-3.266858000	-0.583551000	-2.536684000
7	-1.238165000	1.444415000	-1.718954000	6	-3.578585000	-1.951091000	-0.818893000
7	-2.865393000	-0.840259000	-1.235301000	6	-2.483634000	-2.833152000	2.708221000
6	-2.584182000	-2.186606000	1.418482000	6	-1.532745000	-2.162298000	3.423517000
6	-1.041953000	-1.092676000	2.582721000	6	1.277480000	1.916825000	2.610183000
6	0.318438000	0.915773000	2.194231000	6	1.407466000	2.801973000	1.576767000
6	0.533478000	2.351064000	0.514998000	6	-0.508319000	3.201184000	-3.039678000

6	-1.399317000	2.483185000	-3.783009000	6	4.700979000	-2.273523000	-0.999049000
6	-4.266357000	-1.550705000	-2.937542000	1	6.741237000	-1.612393000	-1.231521000
6	-4.460859000	-2.391069000	-1.878685000	6	3.246850000	-0.761307000	0.250113000
6	-3.456780000	-2.572873000	0.414389000	1	4.173011000	1.053911000	0.938896000
6	-0.096057000	-0.156364000	2.971233000	6	3.425135000	-1.980877000	-0.452098000
6	0.407041000	2.978458000	-0.713949000	1	4.869468000	-3.195509000	-1.539374000
6	-2.798693000	0.444718000	-3.340297000	1	2.269877000	-0.477957000	0.614572000
1	-4.095043000	-3.428030000	0.608817000	7	2.365060000	-2.875753000	-0.600850000
1	0.325389000	-0.249584000	3.966142000	6	1.145585000	-2.701134000	0.103748000
1	0.997442000	3.872954000	-0.879773000	6	2.445417000	-3.938650000	-1.615145000
1	-3.207988000	0.524409000	-4.341473000	1	0.523376000	-3.594085000	0.062520000
1	-3.078972000	-3.680826000	3.014975000	1	1.284123000	-2.348054000	1.127036000
1	-1.195991000	-2.350522000	4.432623000	1	0.453517000	-1.803025000	-0.420937000
1	1.768801000	1.932938000	3.572154000	1	3.131325000	-4.735073000	-1.301495000
1	2.028555000	3.684299000	1.524828000	1	1.453389000	-4.368042000	-1.752110000
1	0.037737000	4.089902000	-3.320280000	1	2.783897000	-3.534814000	-2.574108000
1	-1.730981000	2.666639000	-4.794568000	8	6.468987000	1.781331000	0.714547000
1	-4.746392000	-1.568669000	-3.905171000	8	7.793430000	0.406146000	-0.447856000
1	-5.131587000	-3.234784000	-1.806113000	1	-2.130129000	3.947934000	1.402411000
8	-0.186311000	-0.804088000	-0.975554000	1	-3.665859000	0.419963000	3.028493000
16	-3.120207000	1.581520000	0.698548000	7	-3.872127000	0.051353000	3.948485000
1	-4.000619000	1.529806000	-0.364173000	7	-1.796682000	4.842900000	1.738054000
7	6.671866000	0.713885000	0.059810000	1	-4.462644000	-0.759524000	3.822424000
6	5.562399000	-0.205351000	-0.116517000	1	-4.193349000	0.682493000	4.670011000
6	5.761320000	-1.393888000	-0.828201000	1	-1.647684000	5.431142000	0.929419000
6	4.308424000	0.116361000	0.416523000	1	-2.292272000	5.301031000	2.490800000

V-1. For $^4\text{IM} + 2\text{NH}_3$ Complex.

26	-1.527706000	0.108471000	-0.108204000	1	-4.931075000	-1.258196000	-3.844210000
7	-1.448704000	-1.500440000	1.137777000	1	-4.884442000	-3.367123000	-2.141128000
7	-0.273055000	1.106110000	1.112867000	8	-0.191020000	-0.584973000	-1.068415000
7	-1.564934000	1.668041000	-1.364586000	16	-3.199400000	1.020055000	1.215271000
7	-2.919860000	-0.834236000	-1.218259000	1	-4.257859000	0.534511000	0.535202000
6	-2.176579000	-2.659142000	1.031783000	7	6.313873000	1.379282000	-0.145424000
6	-0.724540000	-1.601863000	2.299484000	6	5.404548000	0.268722000	-0.378594000
6	0.304089000	0.635936000	2.267514000	6	5.878944000	-0.889220000	-1.000087000
6	0.243660000	2.359085000	0.902246000	6	4.066012000	0.378562000	0.010394000
6	-0.868344000	2.841799000	-1.236303000	6	5.015577000	-1.951501000	-1.215619000
6	-2.297897000	1.776508000	-2.517699000	1	6.919919000	-0.943249000	-1.293210000
6	-3.466225000	-0.383393000	-2.393397000	6	3.200235000	-0.679801000	-0.204867000
6	-3.426599000	-2.094867000	-1.012791000	1	3.715283000	1.298524000	0.461052000
6	-1.873404000	-3.532831000	2.138400000	6	3.662680000	-1.872545000	-0.809853000
6	-0.973373000	-2.878203000	2.923323000	1	5.402247000	-2.853853000	-1.673520000
6	1.193702000	1.632198000	2.810751000	1	2.149173000	-0.561546000	0.025903000
6	1.155869000	2.699760000	1.965706000	7	2.797876000	-2.951478000	-0.990962000
6	-1.154079000	3.708954000	-2.354441000	6	1.632073000	-3.085488000	-0.272884000
6	-2.039136000	3.049026000	-3.148390000	6	3.142478000	-3.994587000	-1.956707000
6	-4.368521000	-1.372656000	-2.927124000	1	1.032948000	-3.962974000	-0.468679000
6	-4.344951000	-2.431772000	-2.071834000	1	1.552234000	-2.579143000	0.678909000
6	-3.094056000	-2.946619000	0.030901000	1	0.058573000	-1.481390000	-0.771268000
6	0.101826000	-0.618389000	2.826090000	1	3.870608000	-4.703226000	-1.543031000
6	-0.028826000	3.176015000	-0.185830000	1	2.236891000	-4.542642000	-2.219110000
6	-3.185386000	0.830164000	-3.005124000	1	3.554692000	-3.550271000	-2.865375000
1	-3.590983000	-3.910299000	0.067684000	8	5.868584000	2.381140000	0.423847000
1	0.620744000	-0.842392000	3.752057000	8	7.482421000	1.260075000	-0.528512000
1	0.456412000	4.145493000	-0.218564000	1	-2.575842000	3.605733000	1.182964000
1	-3.698505000	1.053966000	-3.934255000	1	-2.544641000	0.112534000	3.628420000
1	-2.312841000	-4.510330000	2.287418000	7	-2.310105000	-0.158760000	4.575097000
1	-0.521066000	-3.207423000	3.849493000	7	-2.352530000	4.590838000	1.250084000
1	1.770471000	1.511282000	3.718052000	1	-2.580620000	-1.126485000	4.686682000
1	1.695575000	3.634734000	2.036177000	1	-2.594751000	0.436001000	5.341490000
1	-0.725831000	4.692881000	-2.492022000	1	-2.635553000	5.023526000	0.381291000
1	-2.491020000	3.377669000	-4.074854000	1	-2.636447000	5.104023000	2.073584000

VI-1. For $^4\text{Carbinolaniline} + 2\text{NH}_3$ Complex.

26	-1.557381000	0.081167000	0.161252000	7	-2.560062000	-1.611355000	0.613450000
7	-2.065858000	-0.164367000	-1.790123000	7	-0.749316000	0.082471000	2.015402000

7	-0.369842000	1.618035000	-0.350555000	8	0.304259000	-1.409101000	-0.588018000
6	-1.743612000	0.685570000	-2.841291000	16	-3.418527000	1.618066000	0.705781000
6	-2.975884000	-1.082521000	-2.304039000	1	-4.275535000	0.687775000	1.263831000
6	-3.390338000	-2.341651000	-0.230942000	7	6.680305000	0.870056000	-0.265468000
6	-2.637189000	-2.228884000	1.857283000	6	5.566914000	-0.054484000	-0.328002000
6	-1.077654000	-0.761732000	3.069516000	6	5.775333000	-1.355668000	-0.796157000
6	0.108018000	1.039374000	2.543671000	6	4.291936000	0.367894000	0.068969000
6	0.438324000	2.363619000	0.497978000	6	4.708239000	-2.243272000	-0.855572000
6	-0.269011000	2.214378000	-1.600523000	1	6.769301000	-1.655509000	-1.101418000
6	-2.441731000	0.271691000	-4.037998000	6	3.222689000	-0.513191000	0.008202000
6	-3.200968000	-0.815685000	-3.707323000	1	4.150685000	1.386907000	0.403809000
6	-4.003468000	-3.423256000	0.503315000	6	3.410269000	-1.846778000	-0.443256000
6	-3.538302000	-3.354990000	1.788443000	1	4.888708000	-3.249246000	-1.209910000
6	-0.392722000	-0.335880000	4.270607000	1	2.233746000	-0.157258000	0.259878000
6	0.335885000	0.773675000	3.947148000	7	2.343862000	-2.745639000	-0.478210000
6	1.048487000	3.449759000	-0.235493000	6	1.081208000	-2.409818000	0.140988000
6	0.613248000	3.356936000	-1.527859000	6	2.507195000	-4.058888000	-1.113467000
6	-0.904266000	1.785206000	-2.756649000	1	0.499618000	-3.326618000	0.264299000
6	-3.588783000	-2.095007000	-1.582500000	1	1.231793000	-1.943283000	1.114616000
6	-1.948697000	-1.837461000	2.997299000	1	-0.001900000	-1.725572000	-1.461749000
6	0.660254000	2.099558000	1.841978000	1	3.211342000	-4.696036000	-0.562525000
1	-0.739746000	2.361399000	-3.660548000	1	1.540676000	-4.565727000	-1.136844000
1	-4.278208000	-2.742700000	-2.113228000	1	2.866450000	-3.960346000	-2.144429000
1	-2.114076000	-2.410745000	3.903100000	8	6.465034000	2.044064000	0.167427000
1	1.313513000	2.774479000	2.384071000	8	7.822602000	0.465117000	-0.644307000
1	-2.361503000	0.765165000	-4.995638000	1	-3.910692000	2.741431000	-1.654605000
1	-3.863725000	-1.386637000	-4.341298000	1	-2.193874000	3.461197000	2.181817000
1	-4.696100000	-4.136192000	0.079980000	7	-1.768224000	4.218437000	2.701641000
1	-3.777319000	-4.000943000	2.620814000	7	-4.102533000	3.239793000	-2.514628000
1	-0.476780000	-0.824830000	5.230286000	1	-1.606938000	3.884540000	3.642184000
1	0.967041000	1.370892000	4.588907000	1	-2.185872000	5.138225000	2.660632000
1	1.720898000	4.178233000	0.193506000	1	-4.629513000	2.617343000	-3.112096000
1	0.860722000	3.994646000	-2.363785000	1	-4.480087000	4.176390000	-2.466046000

VII. For ²Carbinolamine + 2NH₃ Complex.

26	-1.390671000	0.102864000	0.284324000	1	-2.855473000	-4.348764000	2.697559000
7	-2.219818000	0.002824000	-1.561180000	1	0.378469000	-0.930978000	5.135226000
7	-2.159636000	-1.704909000	0.757284000	1	1.440065000	1.469338000	4.481930000
7	-0.429844000	0.114838000	2.053376000	1	1.310645000	4.598771000	0.264011000
7	-0.518393000	1.837865000	-0.247100000	1	0.135186000	4.503597000	-2.170747000
6	-2.169418000	0.959812000	-2.568904000	8	0.246437000	-0.884612000	-0.649611000
6	-3.108608000	-0.971961000	-2.002278000	16	-3.207639000	1.215336000	1.115166000
6	-3.037168000	-2.446646000	-0.023026000	1	-3.311793000	0.547560000	2.320774000
6	-2.008777000	-2.411605000	1.944460000	7	6.861698000	0.628737000	-0.374008000
6	-0.505740000	-0.825993000	3.074968000	6	5.643922000	-0.144960000	-0.519636000
6	0.366402000	1.143440000	2.538029000	6	5.669180000	-1.340068000	-1.244571000
6	0.297037000	2.615631000	0.559192000	6	4.455365000	0.319588000	0.056444000
6	-0.665465000	2.538636000	-1.434349000	6	4.502819000	-2.082263000	-1.384126000
6	-3.018471000	0.560072000	-3.669038000	1	6.600207000	-1.674066000	-1.683455000
6	-3.597756000	-0.627690000	-3.319985000	6	3.287062000	-0.415525000	-0.084462000
6	-3.432150000	-3.644141000	0.688287000	1	4.458098000	1.258678000	0.593715000
6	-2.797423000	-3.623541000	1.898741000	6	3.289777000	-1.642823000	-0.797664000
6	0.271226000	-0.380738000	4.211647000	1	4.541155000	-3.010379000	-1.938228000
6	0.806725000	0.832175000	3.881818000	1	2.364397000	-0.017448000	0.314860000
6	0.676215000	3.825604000	-0.144442000	7	2.122248000	-2.402620000	-0.920740000
6	0.083876000	3.777474000	-1.372565000	6	0.954973000	-2.080965000	-0.147934000
6	-1.430585000	2.132917000	-2.517844000	6	2.091541000	-3.568227000	-1.815088000
6	-3.475861000	-2.108296000	-1.296306000	1	0.270789000	-2.929954000	-0.145760000
6	-1.230839000	-2.008133000	3.021324000	1	1.203026000	-1.805512000	0.875738000
6	0.707417000	2.297081000	1.845375000	1	-0.011263000	-0.958342000	-1.591625000
1	-1.471077000	2.790859000	-3.379210000	1	2.744658000	-4.374411000	-1.457225000
1	-4.175127000	-2.785599000	-1.775545000	1	1.071670000	-3.953845000	-1.861985000
1	-1.205332000	-2.653478000	3.892969000	1	2.402433000	-3.296663000	-2.830241000
1	1.344405000	3.012197000	2.355256000	8	6.813027000	1.707418000	0.292495000
1	-3.152626000	1.128300000	-4.578054000	8	7.921526000	0.191151000	-0.918356000
1	-4.299076000	-1.221849000	-3.887940000	1	-4.991774000	0.881006000	-0.829233000
1	-4.111580000	-4.390267000	0.302017000	1	-2.407581000	3.748688000	0.982401000

7	-2.175881000	4.730873000	0.902201000	1	-2.921315000	5.403475000	0.783644000
7	-5.689532000	0.831773000	-1.561022000	1	-6.091003000	-0.095650000	-1.532239000
1	-1.541357000	4.953096000	1.657263000	1	-6.374618000	1.571343000	-1.637273000

Table S23 Cartesian Coordinates for Various Reaction Species in Carbinolaniline Decomposition Process in Enzymatic Environment and Without Water Assisted

I. For $^4 TS_P$

26	-2.687440000	-0.150729000	0.600015000	26	-2.586121000	-0.112788000	0.655179000
7	-2.097593000	-2.081859000	0.427312000	7	-2.078684000	-2.066901000	0.532002000
7	-2.309313000	-0.216867000	2.591709000	7	-2.276675000	-0.124481000	2.660218000
7	-3.083134000	1.833400000	0.756908000	7	-3.020621000	1.856495000	0.782718000
7	-2.995259000	-0.062722000	-1.387777000	6	-2.839400000	-0.089745000	-1.344648000
6	-2.103721000	-2.844912000	-0.727911000	6	-2.038698000	-2.860830000	-0.601643000
6	-1.701458000	-2.925367000	1.452356000	6	-1.767122000	-2.894851000	1.596979000
6	-1.893385000	-1.324649000	3.319779000	6	-1.947368000	-1.236677000	3.422109000
6	-2.474718000	0.814997000	3.506800000	6	-2.441475000	0.924557000	3.556060000
6	-3.144381000	2.582361000	1.922730000	6	-3.073970000	2.651322000	1.918500000
6	-3.468498000	2.678580000	-0.271028000	6	-3.384063000	2.670066000	-0.277935000
6	-3.389303000	1.046216000	-2.115870000	6	-3.226641000	1.004063000	-2.095473000
6	-2.881334000	-1.106220000	-2.290244000	6	-2.695257000	-1.140045000	-2.231466000
6	-1.685194000	-4.198225000	-0.421306000	6	-1.679256000	-4.218057000	-0.239890000
6	-1.435962000	-4.247778000	0.920758000	6	-1.512631000	-4.239723000	1.115242000
6	-1.800312000	-0.976397000	4.719815000	6	-1.581148000	-0.870136000	4.822869000
6	-2.160058000	0.340315000	4.834873000	6	-2.194776000	0.460529000	4.905024000
6	-3.558037000	3.935802000	1.611679000	6	-3.471228000	3.997096000	1.557524000
6	-3.755113000	3.995352000	0.261208000	6	-3.662451000	4.008411000	0.204754000
6	-3.538392000	0.684997000	-3.510014000	6	-3.329459000	0.627950000	-3.494207000
6	-3.227344000	-0.641526000	-3.617121000	6	-3.001432000	-0.693872000	-3.577871000
6	-2.469905000	-2.397406000	-1.988576000	6	-2.319522000	-2.431839000	-1.891247000
6	-1.602574000	-2.577745000	2.792030000	6	-1.702113000	-2.513476000	2.930909000
6	-2.862076000	2.114513000	3.198059000	6	-2.801793000	2.221509000	3.211209000
6	-3.603846000	2.318970000	-1.603817000	1	-3.476152000	2.278737000	-1.606798000
1	-2.432609000	-3.112444000	-2.803554000	1	-2.254489000	-3.163574000	-2.689788000
1	-1.292245000	-3.350997000	3.487226000	1	-1.456181000	-3.283778000	3.655087000
1	-2.957815000	2.815233000	4.020889000	1	-2.895475000	2.947218000	4.012504000
1	-3.919069000	3.089469000	-2.299418000	1	-3.776204000	3.034804000	-2.325273000
1	-1.608220000	-4.995456000	-1.146587000	1	-1.583016000	-5.035207000	-0.940485000
1	-1.116096000	-5.094053000	1.511774000	1	-1.252776000	-5.078396000	1.745438000
1	-1.506904000	-1.659210000	5.504474000	1	-1.660745000	-1.554281000	5.627267000
1	-2.214792000	0.941547000	5.731141000	1	-2.260742000	1.078591000	5.789141000
1	-3.687170000	4.721248000	2.342493000	1	-3.591411000	4.811045000	2.258234000
1	-4.078237000	4.839054000	-0.331471000	1	-3.969318000	4.834193000	-0.421151000
1	-3.842931000	1.366463000	-4.291168000	1	-3.618791000	1.299216000	-4.290062000
1	-3.226107000	-1.259383000	-4.503422000	16	-2.969027000	-1.323266000	-4.455624000
16	-3.226107000	-4.503422000	-4.809701000	16	-4.809701000	-0.701677000	0.921488000
16	-5.108020000	-0.794822000	0.886607000	1	-5.139571000	0.197823000	1.918162000
1	-5.076197000	-1.114524000	2.232040000	8	-5.672578000	0.331005000	0.322270000
8	-0.543343000	0.362861000	0.219217000	1	-5.662822000	2.275196000	-1.581963000
1	5.955181000	1.869626000	-1.493980000	6	-4.797133000	1.881110000	-1.060412000
6	5.045778000	1.592844000	-0.971291000	6	-4.178553000	0.710512000	-1.514320000
6	4.436768000	0.359468000	-1.229115000	6	-4.294866000	2.546096000	0.064924000
6	4.477432000	2.471916000	-0.041050000	6	-3.058022000	0.202644000	-0.847653000
6	3.260902000	0.001794000	-0.560351000	1	-4.560856000	0.195895000	-2.389263000
1	4.870437000	-0.321819000	-1.953291000	6	-3.178537000	2.041079000	0.739230000
6	3.304542000	2.118982000	0.633932000	1	-4.769598000	3.455558000	0.417535000
1	4.944417000	3.430599000	0.158484000	6	-2.562911000	0.871430000	0.276346000
6	2.699466000	0.883767000	0.368775000	1	-2.565403000	-0.698431000	-1.197928000
1	2.776660000	-0.948290000	-0.760564000	1	-2.788359000	2.553828000	1.612895000
1	2.862001000	2.799235000	1.354969000	7	-1.395180000	0.324790000	0.963886000
7	1.470226000	0.493867000	1.054386000	6	-0.150135000	1.232210000	1.079979000
6	0.212958000	1.396490000	0.840083000	6	-1.718273000	-0.432556000	2.215976000
6	1.671487000	0.047304000	2.468779000	1	-0.158751000	1.355812000	2.118386000
1	-0.174812000	1.742268000	1.802408000	1	0.331795000	2.187627000	0.585205000
1	0.476761000	2.234375000	0.188491000	1	0.512449000	-0.269079000	0.275723000
1	0.659919000	-0.229613000	0.434568000	1	2.160040000	0.230417000	2.965837000
1	2.053649000	0.867637000	3.083568000	1	0.794907000	-0.871760000	2.598721000
1	0.712399000	-0.298485000	2.858636000	1	2.428263000	-1.224341000	1.970299000
1	2.390402000	-0.774297000	2.478004000				

III. For 4 Formaldehyde Complex

26	-2.830786000	-0.063130000	0.484748000
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II. For $^2 TS_P$

7	-1.788804000	-1.755616000	0.162847000	26	-2.624294000	0.015523000	0.494025000
7	-2.123117000	-0.009945000	2.382937000	7	-1.628416000	-1.716465000	0.231239000
7	-3.618128000	1.772744000	0.744737000	7	-2.090915000	-0.013371000	2.444043000
7	-3.237260000	0.055077000	-1.485917000	7	-3.500168000	1.815201000	0.743971000
6	-1.725812000	-2.476757000	-1.023219000	7	-3.049269000	0.111156000	-1.468640000
6	-1.057970000	-2.484643000	1.094089000	6	-1.548922000	-2.434089000	-0.952236000
6	-1.365693000	-0.985513000	3.020654000	6	-0.942061000	-2.460581000	1.180547000
6	-2.453020000	0.920503000	3.362232000	6	-1.365556000	-0.993599000	3.112168000
6	-3.738995000	2.463519000	1.945398000	6	-2.496723000	0.893965000	3.416116000
6	-4.276724000	2.540916000	-0.206620000	6	-3.695976000	2.472694000	1.949719000
6	-3.936580000	1.059929000	-2.136622000	6	-4.111336000	2.598347000	-0.223650000
6	-2.979438000	-0.913814000	-2.443870000	6	-3.713762000	1.119553000	-2.145098000
6	-0.951915000	-3.680288000	-0.824755000	6	-2.773955000	-0.866856000	-2.407844000
6	-0.536390000	-3.683272000	0.478019000	6	-0.791120000	-3.650392000	-0.738458000
6	-1.208094000	-0.648985000	4.418320000	6	-0.412195000	-3.664527000	0.574113000
6	-1.882064000	0.523004000	4.628926000	6	-1.302671000	-0.682330000	4.523884000
6	-4.483304000	3.683718000	1.735953000	6	-2.004291000	0.477480000	4.711111000
6	-4.810526000	3.733580000	0.409426000	6	-4.434507000	3.699334000	1.727012000
6	-4.114084000	0.713814000	-3.530943000	6	-4.685508000	3.779139000	0.387286000
6	-3.527559000	-0.504186000	-3.719408000	6	-3.854974000	0.766526000	-3.543991000
6	-2.288378000	-2.094955000	-2.231147000	6	-3.280189000	-0.460268000	-3.705099000
6	-0.856159000	-2.128795000	2.420326000	6	-2.087346000	-2.048080000	-2.170902000
6	-3.206776000	2.066525000	3.162578000	6	-0.806128000	-2.120411000	2.520758000
6	-4.418652000	2.217167000	-1.547480000	6	-3.239525000	2.044298000	3.187961000
1	-2.162090000	-2.762500000	-3.076373000	6	-4.198314000	2.285402000	-1.571891000
1	-0.277991000	-2.806769000	3.039045000	1	-1.944977000	-2.718259000	-3.012133000
1	-3.387981000	2.704085000	4.021018000	1	-0.260150000	-2.805854000	3.160702000
1	-4.959010000	2.915061000	-2.177581000	1	-3.476590000	2.662337000	4.047615000
1	-0.754293000	-4.415022000	-1.591546000	1	-4.707631000	2.990801000	-2.219740000
1	0.066100000	-4.421851000	0.986572000	1	-0.584853000	-4.386104000	-1.502372000
1	-0.667667000	-1.248690000	5.136568000	1	0.162838000	-4.414592000	1.097718000
1	-1.997508000	1.071742000	5.552422000	1	-0.803324000	-1.289673000	5.265339000
1	-4.717413000	4.399470000	2.510474000	1	-2.185814000	1.007300000	5.635275000
1	-5.366239000	4.497481000	-0.114644000	1	-4.717192000	4.394503000	2.504368000
1	-4.626067000	1.330944000	-4.254756000	1	-5.216107000	4.551374000	-0.150663000
1	-3.461039000	-1.083134000	-4.628895000	1	-4.336443000	1.385344000	-4.287217000
16	-4.961334000	-1.187548000	1.084391000	1	-3.193681000	-1.047240000	-4.608016000
1	-4.414927000	-2.390055000	1.493144000	16	-4.605152000	-1.067376000	0.904183000
8	-0.620071000	1.139654000	-0.227785000	1	-4.114982000	-2.060643000	1.731300000
1	5.648113000	-0.074467000	-1.755330000	8	-0.824680000	1.021790000	-0.017571000
6	4.875845000	0.051809000	-1.004056000	1	5.319962000	-0.023608000	-1.993083000
6	3.635672000	-0.588405000	-1.143824000	6	4.574609000	0.076032000	-1.211253000
6	5.101017000	0.854411000	0.117881000	6	3.380564000	-0.656855000	-1.271067000
6	2.639477000	-0.431481000	-0.182014000	6	4.791573000	0.936145000	-0.131246000
1	3.441885000	-1.213820000	-2.010026000	6	2.418947000	-0.534965000	-0.269008000
6	4.111663000	1.020637000	1.093778000	1	3.195795000	-1.327835000	-2.104155000
1	6.055733000	1.356751000	0.243320000	6	3.836257000	1.068125000	0.883458000
6	2.864688000	0.378303000	0.954031000	1	5.711435000	1.509788000	-0.069417000
1	1.677803000	-0.920497000	-0.306295000	6	2.638067000	0.331356000	0.823323000
1	4.312059000	1.645393000	1.956544000	1	1.493127000	-1.098562000	-0.328517000
7	1.838849000	0.544167000	1.894073000	1	4.028287000	1.738353000	1.713366000
6	-0.013157000	1.989182000	0.441401000	7	1.633469000	0.466590000	1.803788000
6	2.060604000	1.185891000	3.185458000	6	-0.146095000	1.813513000	0.672290000
1	-0.389693000	2.333445000	1.413253000	6	1.904851000	1.114952000	3.087960000
1	0.901413000	2.465042000	0.068108000	1	-0.465328000	2.115356000	1.673333000
1	1.089048000	-0.133826000	1.857769000	1	0.717811000	2.319281000	0.235813000
1	2.308257000	2.247069000	3.059762000	1	0.970797000	-0.300298000	1.845678000
1	1.141616000	1.118300000	3.771333000	1	2.076035000	2.189324000	2.952045000
1	2.875644000	0.716772000	3.758391000	1	1.034022000	0.986353000	3.733761000
				1	2.785449000	0.693734000	3.594815000

IV. For ² Formaldehyde Complex.

Table S24 Cartesian Coordinates for Various Reaction Species in Carbinolaniline Decomposition Process in Enzymatic Environment and With Water Assisted

I. For ⁴Carbinolaniline + H₂O Complex.

26	-3.078939000	0.583409000	0.140063000
7	-2.503507000	-1.329993000	-0.215022000
7	-3.378005000	0.129274000	2.075162000
7	-3.374746000	2.542707000	0.548640000
7	-2.636978000	1.063077000	-1.771504000
6	-2.075615000	-1.859075000	-1.422925000
6	-2.520176000	-2.379460000	0.690292000
6	-3.310854000	-1.129049000	2.655621000
6	-3.762617000	1.000981000	3.080539000
6	-3.754207000	3.082917000	1.768139000
6	-3.385912000	3.591734000	-0.359910000
6	-2.753014000	2.313259000	-2.365492000
6	-2.227223000	0.193148000	-2.775691000
6	-1.784808000	-3.268408000	-1.261649000
6	-2.062122000	-3.589525000	0.042098000
6	-3.675614000	-1.041576000	4.052667000
6	-3.952153000	0.270753000	4.314903000
6	-3.982132000	4.506118000	1.623889000
6	-3.757493000	4.819080000	0.313830000
6	-2.424453000	2.218770000	-3.769461000
6	-2.099001000	0.914080000	-4.021539000
6	-1.955646000	-1.157951000	-2.614801000
6	-2.911107000	-2.293725000	2.018634000
6	-3.930949000	2.372256000	2.944395000
6	-3.101422000	3.488759000	-1.712690000
1	-1.630465000	-1.709778000	-3.490516000
1	-2.889357000	-3.204301000	2.607375000
1	-4.239545000	2.927235000	3.823751000
1	-3.154072000	4.394399000	-2.307206000
1	-1.446111000	-3.921449000	-2.053397000
1	-1.987239000	-4.553972000	0.523542000
1	-3.706844000	-1.881084000	4.731830000
1	-4.256338000	0.716829000	5.250593000
1	-4.286805000	5.162193000	2.426339000
1	-3.839885000	5.782330000	-0.168415000
1	-2.440599000	3.049245000	-4.460326000
1	-1.798484000	0.469582000	-4.959376000
16	-5.491445000	0.126173000	-0.325477000
1	-5.468766000	0.314429000	-1.695315000
1	5.709179000	0.885409000	1.498145000
6	4.831448000	0.844604000	0.859969000
6	4.890937000	0.178080000	-0.368026000
6	3.656006000	1.462890000	1.291575000
1	5.806692000	-0.300042000	-0.697643000
6	3.739391000	0.144616000	-1.162538000
6	2.483868000	1.443099000	0.496218000
1	3.654209000	1.964738000	2.249904000
6	2.553220000	0.757530000	-0.746180000
1	3.758319000	-0.358511000	-2.125306000
7	1.316695000	2.085522000	0.935123000
1	1.690519000	0.708645000	-1.398757000
6	1.258149000	2.624141000	2.298376000
1	1.439293000	1.849450000	3.055181000
1	1.990519000	3.428295000	2.439779000
1	0.260799000	3.031218000	2.468300000
1	1.547498000	-1.267373000	0.140737000
8	0.632349000	-1.386485000	0.457434000
1	0.211526000	-2.185366000	0.089167000
1	-0.284673000	-0.002605000	0.638699000
8	-0.774148000	0.873141000	0.681874000
6	0.058886000	1.978178000	0.227969000
1	-0.537152000	2.869564000	0.417356000

II. For ²Carbinolaniline + H₂O Complex.

1	0.240911000	1.907487000	-0.846208000
26	-2.839216000	0.651839000	0.064581000
7	-2.265658000	-1.227166000	-0.432843000
7	-3.169135000	-0.004326000	1.947099000
7	-3.338492000	2.536985000	0.575654000
7	-2.438881000	1.311048000	-1.802820000
6	-1.849658000	-1.638743000	-1.689698000
6	-2.294894000	-2.365971000	0.356466000
6	-3.079449000	-1.297481000	2.432595000
6	-3.624907000	0.773002000	2.998854000
6	-3.760513000	2.945083000	1.829184000
6	-3.384292000	3.661476000	-0.235030000
6	-2.608636000	2.592327000	-2.310568000
6	-1.996185000	0.532447000	-2.860608000
6	-1.596219000	-3.066445000	-1.679604000
6	-1.872995000	-3.515537000	-0.419821000
6	-3.476556000	-1.330742000	3.826935000
6	-3.810995000	-0.054700000	4.176016000
6	-4.070878000	4.361039000	1.804722000
6	-3.840855000	4.802114000	0.532430000
6	-2.256276000	2.615204000	-3.714631000
6	-1.876564000	1.347197000	-4.053103000
6	-1.710966000	-0.826157000	-2.805999000
6	-2.666763000	-2.403282000	1.696865000
1	-3.886147000	2.133869000	2.949600000
1	-3.045753000	3.689871000	-1.581614000
1	-1.375351000	-1.297969000	-3.723805000
1	-2.664954000	-3.367780000	2.194468000
1	-4.238680000	2.603351000	3.862231000
1	-3.133333000	4.637346000	-2.102871000
1	-1.265541000	-3.636608000	-2.535916000
1	-1.815267000	-4.525911000	-0.040731000
1	-3.495937000	-2.220797000	4.439173000
1	-4.159385000	0.308640000	5.132040000
1	-4.424083000	4.925913000	2.655450000
1	-3.966658000	5.799127000	0.135364000
16	-2.301154000	3.491825000	-4.344699000
1	-1.550847000	0.980710000	-5.015966000
1	-5.022060000	0.148519000	-0.481422000
6	-5.306237000	1.273519000	-1.232376000
6	5.563971000	0.594576000	1.169186000
6	4.595894000	0.464978000	0.694774000
1	4.404163000	-0.563963000	-0.233485000
6	3.558127000	1.339254000	1.026004000
6	5.214123000	-1.239119000	-0.486912000
6	3.144184000	-0.707026000	-0.825815000
6	2.284824000	1.210792000	0.425398000
1	3.744117000	2.128953000	1.742566000
7	2.091826000	0.155133000	-0.502029000
1	2.969096000	-1.500431000	-1.546529000
6	1.246165000	2.099233000	0.754910000
1	1.125136000	0.000558000	-0.967300000
6	1.360691000	2.945175000	1.948517000
1	1.606791000	2.350859000	2.837061000
1	2.126999000	3.721042000	1.824049000
8	0.401791000	3.434757000	2.124187000
1	1.064621000	-1.209658000	1.388736000
1	0.261691000	-0.929963000	1.867495000
8	-0.387418000	-1.657244000	1.944654000
6	-0.460382000	0.326405000	1.164368000
1	-0.930401000	1.052344000	0.641897000

6	-0.012611000	2.054935000	0.070335000
1	-0.526047000	3.010462000	0.160678000
1	0.132810000	1.824731000	-0.985611000

III. For $^4 TS_P + H_2O$ Complex.

26	-2.806689000	0.547743000	-0.082249000
7	-2.627920000	-1.421495000	-0.484436000
7	-3.214213000	0.089538000	1.961171000
7	-2.963787000	2.523599000	0.356118000
7	-2.236309000	1.031648000	-2.053406000
6	-2.322624000	-1.965711000	-1.721408000
6	-2.851930000	-2.466955000	0.396919000
6	-3.348456000	-1.177717000	2.484759000
6	-3.550268000	0.990702000	2.948370000
6	-3.340002000	3.073275000	1.577031000
6	-2.785282000	3.571412000	-0.540287000
6	-2.140819000	2.293046000	-2.590876000
6	-1.968136000	0.124350000	-3.050603000
6	-2.357562000	-3.414229000	-1.610821000
6	-2.680741000	-3.720506000	-0.318163000
6	-3.754708000	-1.073123000	3.878605000
6	-3.879624000	0.261548000	4.163972000
6	-3.396810000	4.516107000	1.437869000
6	-3.057144000	4.819897000	0.146818000
6	-1.777002000	2.182916000	-3.997552000
6	-1.671384000	0.847591000	-4.280490000
6	-2.012207000	-1.261923000	-2.888377000
6	-3.167936000	-2.356395000	1.754875000
6	-3.597778000	2.374958000	2.761693000
6	-2.395759000	3.467300000	-1.879717000
1	-1.790571000	-1.864163000	-3.764331000
1	-3.316183000	-3.290374000	2.289143000
1	-3.883136000	2.976861000	3.619470000
1	-2.298736000	4.402409000	-2.423190000
1	-2.158091000	-4.095877000	-2.425271000
1	-2.796348000	-4.699829000	0.124010000
1	-3.939168000	-1.910619000	4.536883000
1	-4.183084000	0.713602000	5.097908000
1	-3.665259000	5.198500000	2.231948000
1	-2.995997000	5.797012000	-0.311161000
1	-1.633639000	3.016705000	-4.670289000
1	-1.425605000	0.388039000	-5.227416000
16	-5.101407000	0.393319000	-0.684042000
1	-5.445423000	1.716811000	-0.479970000
1	4.326093000	3.419475000	-0.721787000
6	3.835309000	2.467446000	-0.548690000
6	4.164519000	1.352999000	-1.329278000
6	2.867188000	2.360958000	0.455142000
1	4.913945000	1.439118000	-2.109180000
6	3.521232000	0.130978000	-1.104917000
6	2.236894000	1.130569000	0.676974000
1	2.610723000	3.232421000	1.048400000
6	2.553626000	0.011580000	-0.100883000
1	3.767531000	-0.733549000	-1.712166000
7	1.200624000	0.993257000	1.721569000
1	2.039169000	-0.925281000	0.082858000
6	1.573491000	1.590710000	3.042248000
1	2.577700000	1.259743000	3.310839000
1	1.547903000	2.683071000	3.006430000
1	0.859205000	1.241930000	3.791347000
1	0.957109000	-0.170996000	1.868376000
8	0.315748000	-1.277383000	1.566778000
1	-0.074895000	-1.945207000	2.152058000
1	-0.428836000	-0.553327000	0.875790000
8	-0.768087000	0.500055000	0.429645000
6	-0.193061000	1.492524000	1.249591000
1	-0.767243000	1.664896000	2.167485000

1	-0.054977000	2.426862000	0.702800000
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IV. For $^2 TS_P + H_2O$ Complex.

26	-2.753361000	0.514804000	-0.063596000
7	-2.804269000	-1.493431000	-0.304740000
7	-3.292200000	0.333088000	1.879367000
7	-2.624391000	2.511686000	0.208173000
7	-2.148404000	0.687589000	-1.979353000
6	-2.545224000	-2.217438000	-1.457024000
6	-3.184399000	-2.415735000	0.656248000
6	-3.605346000	-0.854501000	2.524656000
6	-3.502270000	1.345324000	2.806562000
6	-2.918038000	3.242356000	1.351582000
6	-2.287824000	3.437026000	-0.767077000
6	-1.873869000	1.874222000	-2.633832000
6	-1.967274000	-0.320382000	-2.909471000
6	-2.755461000	-3.629215000	-1.208585000
6	-3.148976000	-3.752003000	0.093857000
6	-4.008795000	-0.577994000	3.888235000
6	-3.945313000	0.776501000	4.061818000
6	-2.749180000	4.656228000	1.087160000
6	-2.361198000	4.775784000	-0.217682000
6	-1.506363000	1.601733000	-4.011262000
6	-1.564142000	0.249011000	-4.180972000
6	-2.149958000	-1.674852000	-2.671376000
6	-3.548005000	-2.123520000	1.963752000
6	-3.321512000	2.701159000	2.565521000
6	-1.934574000	3.143588000	-2.076842000
6	-1.979364000	-2.358509000	-3.496304000
1	-3.827124000	-2.958282000	2.598793000
1	-3.526685000	3.388693000	3.379606000
1	-1.694356000	3.980850000	-2.724122000
1	-2.624167000	-4.408408000	-1.945690000
1	-3.405676000	-4.652022000	0.634304000
1	-4.307958000	-1.330861000	4.603565000
1	-4.182107000	1.350169000	4.946604000
1	-2.917225000	5.440896000	1.811043000
1	-2.147583000	5.678234000	-0.772446000
1	-1.246949000	2.358656000	-4.737539000
1	-1.361898000	-0.325118000	-5.073761000
16	-4.954413000	0.665416000	-0.742242000
1	-5.392746000	1.575914000	0.201131000
1	3.543680000	4.405295000	0.508992000
1	3.216814000	3.417297000	0.202192000
1	3.518061000	2.941787000	-1.079486000
6	2.487099000	2.623142000	1.092736000
6	4.082347000	3.560951000	-1.769063000
6	3.084902000	1.670077000	-1.470418000
1	2.067721000	1.348441000	0.693930000
6	2.248543000	3.004770000	2.079918000
6	2.356841000	0.865454000	-0.586740000
1	3.308004000	1.300653000	-2.465625000
6	1.283444000	0.492824000	1.609470000
1	2.003736000	-0.118503000	-0.874155000
6	1.825923000	0.420594000	3.002636000
1	2.896954000	0.218971000	2.955229000
6	1.655187000	1.353210000	3.546876000
1	1.321954000	-0.395003000	3.525952000
1	1.230685000	-0.614946000	1.151185000
8	0.682295000	-1.538639000	0.402025000
1	0.567524000	-2.491690000	0.534730000
1	-0.279002000	-0.751950000	0.257641000
1	-0.799063000	0.297136000	0.443461000
1	-0.225445000	0.846097000	1.608226000
8	-0.634634000	0.408606000	2.526389000
6	-0.331799000	1.931592000	1.620774000
1	1.664896000	2.167485000	

V. For ⁴ Formaldehyde + H₂O Complex.

26	-3.266142000	0.611783000	-0.140609000	7	-2.612950000	-1.411523000	-0.347450000
7	-2.756565000	-1.325223000	-0.361300000	7	-3.219990000	0.326821000	1.878978000
7	-2.944956000	0.454852000	1.849555000	7	-2.732648000	2.588560000	0.251919000
7	-3.485500000	2.603626000	0.066274000	6	-2.145438000	0.853619000	-1.981580000
7	-3.261522000	0.833918000	-2.147046000	6	-2.294645000	-2.087025000	-1.514530000
6	-2.680192000	-2.034564000	-1.554451000	6	-2.917846000	-2.380897000	0.594655000
6	-2.509737000	-2.244208000	0.651067000	6	-3.448818000	-0.894119000	2.496487000
6	-2.703098000	-0.712576000	2.562802000	6	-3.495039000	1.299932000	2.829879000
6	-3.103994000	1.456005000	2.798519000	6	-3.058253000	3.267716000	1.416165000
6	-3.553087000	3.317566000	1.258206000	6	-2.475599000	3.556720000	-0.704369000
6	-3.701552000	3.530307000	-0.947692000	6	-1.973369000	2.070260000	-2.612351000
6	-3.508020000	1.998013000	-2.858871000	6	-1.890193000	-0.117436000	-2.931853000
6	-3.125248000	-0.171703000	-3.093703000	6	-2.380387000	-3.515696000	-1.293271000
6	-2.365046000	-3.416908000	-1.281631000	6	-2.764099000	-3.698128000	0.007231000
6	-2.259620000	-3.546391000	0.078799000	6	-3.866254000	-0.678021000	3.867457000
6	-2.700028000	-0.430271000	3.982094000	6	-3.893942000	0.672894000	4.073057000
6	-2.945676000	0.905802000	4.126804000	6	-2.993476000	4.696962000	1.185059000
6	-3.818943000	4.709872000	0.980847000	6	-2.635205000	4.874689000	-0.121273000
6	-3.909759000	4.840830000	-0.377368000	6	-1.600030000	1.856841000	-3.999754000
6	-3.526456000	1.713899000	-4.278234000	6	-1.548041000	0.507988000	-4.196353000
6	-3.291446000	0.377064000	-4.422736000	6	-1.953703000	-1.486948000	-2.719288000
6	-2.857734000	-1.502842000	-2.823555000	6	-3.302099000	-2.143289000	1.908283000
6	-2.494987000	-1.965423000	2.010176000	6	-3.409305000	2.670590000	2.620252000
6	-3.381079000	2.786702000	2.527558000	1	-2.121671000	3.319160000	-2.025416000
6	-3.714425000	3.251838000	-2.305986000	1	-1.731621000	-2.137130000	-3.559121000
1	-2.774282000	-2.179979000	-3.666524000	1	-3.518191000	-3.009432000	2.525874000
1	-2.308373000	-2.790218000	2.689279000	1	-3.653462000	3.322655000	3.452629000
1	-3.474521000	3.462461000	3.370703000	1	-1.953630000	4.186155000	-2.656270000
1	-3.899281000	4.076681000	-2.985385000	1	-2.184645000	-4.266910000	-2.045106000
1	-2.252355000	-4.181274000	-2.036711000	1	-2.949183000	-4.628115000	0.526099000
1	-2.047492000	-4.438136000	0.650767000	1	-4.111580000	-1.466239000	4.565074000
1	-2.538316000	-1.169160000	4.753519000	1	-4.166608000	1.208264000	4.971450000
1	-3.024295000	1.477352000	5.040141000	1	-3.205814000	5.450097000	1.930526000
1	-3.919675000	5.476555000	1.735232000	1	-2.495161000	5.802875000	-0.656738000
1	-4.099042000	5.735901000	-0.951908000	1	-1.410822000	2.646939000	-4.712292000
1	-3.698860000	2.451444000	-5.048455000	16	-1.309556000	-0.029992000	-5.102693000
1	-3.232268000	-0.198723000	-5.334763000	1	-4.922807000	0.589074000	-0.726168000
16	-5.684614000	0.067378000	0.002281000	1	-5.429529000	1.408560000	0.265326000
1	-6.167636000	1.344385000	-0.214988000	6	-4.047188000	3.933515000	0.104895000
1	5.404447000	2.829503000	2.515216000	6	-3.601599000	2.959177000	-0.065008000
6	4.881010000	2.191656000	1.808988000	6	-3.852800000	2.267410000	-1.255539000
6	5.491133000	1.838882000	0.601399000	1	-2.769626000	2.401754000	0.911612000
6	3.598897000	1.729963000	2.127772000	6	-4.496344000	2.704742000	-2.011522000
1	6.486203000	2.198844000	0.362026000	6	-3.267259000	1.014971000	-1.470553000
6	4.800759000	1.008547000	-0.293767000	6	-2.199909000	1.144465000	0.686813000
6	2.901883000	0.899379000	1.227833000	6	-2.572813000	2.951572000	1.825331000
1	3.148439000	2.013693000	3.072064000	1	-2.435111000	0.445581000	-0.500823000
6	3.522558000	0.540934000	0.008649000	7	-3.450394000	0.479049000	-2.395497000
1	5.263911000	0.718674000	-1.232269000	1	-1.290654000	0.544251000	1.686136000
7	1.595174000	0.447205000	1.481453000	6	-1.964837000	-0.518446000	-0.656477000
1	2.994064000	-0.116546000	-0.675518000	1	-1.749576000	0.667178000	3.109754000
6	1.030787000	0.491340000	2.830877000	1	-2.800776000	0.384336000	3.179844000
1	1.671194000	-0.013281000	3.570125000	1	-1.619085000	1.693009000	3.457747000
1	0.880469000	1.524202000	3.165952000	1	-1.141582000	0.000237000	3.722782000
1	0.057273000	-0.001200000	2.815611000	8	-1.168271000	-0.483644000	1.452694000
1	1.288872000	-0.343908000	0.899629000	1	-0.411513000	-1.716966000	0.692602000
8	0.593937000	-1.320442000	-0.497413000	1	-0.066133000	-2.623506000	0.732737000
1	0.129056000	-2.176150000	-0.505473000	8	-0.278426000	-1.041763000	0.374862000
1	-0.007305000	-0.603232000	-0.810958000	6	-0.749848000	0.527530000	0.399901000
8	-0.713383000	1.055599000	-0.480679000	1	-0.218763000	1.094005000	1.524030000
6	0.117710000	1.833946000	0.045497000	1	-0.696619000	0.791569000	2.467215000
1	-0.153152000	2.450096000	0.910141000	1	-0.102196000	2.184730000	1.484955000
1	1.083539000	2.039517000	-0.424770000				

I+1. For ⁴ Carbinolaniine+H₂O+2NH₃ Complex.

26	-1.062115000	0.053788000	0.328338000
7	-0.437711000	1.982773000	0.414671000
7	-1.656632000	0.336274000	-1.570882000

VI. For ² Formaldehyde + H₂O Complex.

26	-2.701024000	0.594447000	-0.060329000
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7	-1.418554000	-1.929797000	0.150506000	1	-6.376254000	-1.625576000	-0.839091000
7	-0.330074000	-0.258328000	2.184733000				
6	0.172117000	2.612094000	1.488968000	<i>II+I. For ² Carbinolaniline+H₂O+2NH₃ Complex.</i>			
6	-0.593659000	2.946651000	-0.569133000	26	-0.947662000	-0.049235000	0.298746000
6	-1.679419000	1.536146000	-2.267019000	7	-0.293946000	1.864663000	0.169486000
6	-2.192553000	-0.616654000	-2.421352000	7	-1.536455000	0.077668000	-1.630112000
6	-1.982333000	-2.571951000	-0.941642000	7	-1.529843000	-1.976316000	0.406776000
6	-1.289606000	-2.892540000	1.141740000	7	-0.291344000	-0.186569000	2.204631000
6	-0.353487000	-1.448162000	2.900965000	6	0.299814000	2.586416000	1.193526000
6	0.230502000	0.692355000	3.030323000	6	-0.425803000	2.741927000	-0.895297000
6	0.435202000	3.996801000	1.157047000	6	-1.506161000	1.181199000	-2.465157000
6	-0.040248000	4.203316000	-0.112234000	6	-2.143407000	-0.936842000	-2.351593000
6	-2.255902000	1.328653000	-3.577383000	6	-2.129061000	-2.693528000	-0.614267000
6	-2.570341000	0.002230000	-3.673179000	6	-1.469103000	-2.830385000	1.497951000
6	-2.185933000	-3.972918000	-0.634890000	6	-0.397631000	-1.268765000	3.068260000
6	-1.761544000	-4.169975000	0.647968000	6	0.303533000	0.831446000	2.933247000
6	0.188306000	-1.232531000	4.223074000	6	0.560860000	3.942357000	0.750867000
6	0.549495000	0.084658000	4.302041000	6	0.111497000	4.039526000	-0.535202000
6	0.474619000	2.019386000	2.707051000	6	-2.097141000	0.847757000	-3.746775000
6	-1.185371000	2.747454000	-1.808031000	6	-2.488180000	-0.457703000	-3.677107000
6	-2.338504000	-1.967511000	-2.136484000	6	-2.444316000	-4.031529000	-0.153591000
6	-0.799266000	-2.672421000	2.419499000	6	-2.039387000	-4.115334000	1.148405000
1	0.931607000	2.642967000	3.468262000	6	0.150523000	-0.920550000	4.362225000
1	-1.254471000	3.600944000	-2.473626000	6	0.584801000	0.372123000	4.278640000
1	-2.779672000	-2.594800000	-2.903544000	6	0.589146000	2.107270000	2.463315000
1	-0.759798000	-3.520025000	3.095083000	6	-0.984101000	2.426039000	-2.130152000
1	0.892609000	4.713421000	1.824339000	6	-2.406064000	-2.217452000	-1.889338000
1	-0.040233000	5.119332000	-0.685355000	6	-0.942843000	-2.502651000	2.740668000
1	-2.391366000	2.104009000	-4.317305000	6	1.055638000	2.797242000	3.158969000
1	-3.015808000	-0.521743000	-4.506270000	1	1.045186000	3.214858000	-2.873052000
1	-2.611382000	-4.694020000	-1.317673000	1	-2.888548000	-2.902958000	-2.578452000
1	-1.768853000	-5.084617000	1.222925000	1	-0.963155000	-3.264537000	3.512811000
1	0.278779000	-1.997146000	4.980980000	1	1.014526000	4.710046000	1.361231000
1	0.991669000	0.607306000	5.137953000	1	0.122980000	4.902394000	-1.185758000
8	1.131000000	-0.317144000	-0.533185000	1	-2.196100000	1.534519000	-4.575010000
16	-3.373359000	0.586237000	1.116137000	1	-2.971866000	-1.053456000	-4.437699000
1	-3.139190000	0.521695000	2.477537000	1	-2.919443000	-4.791532000	-0.757100000
1	7.410067000	-0.497476000	-2.333401000	1	-2.115587000	-4.957190000	1.821455000
6	6.641618000	-0.386600000	-1.574099000	1	0.188522000	-1.586450000	5.212282000
6	6.890653000	0.386778000	-0.435841000	1	1.047043000	0.973858000	5.047898000
6	5.413251000	-1.023986000	-1.761396000	8	0.856389000	-0.683458000	-0.394386000
1	7.846612000	0.879198000	-0.296127000	16	-3.026565000	0.688080000	0.970153000
6	5.875859000	0.508409000	0.520101000	1	-3.210268000	-0.171621000	2.036680000
6	4.378237000	-0.915594000	-0.800205000	1	7.213385000	-0.697525000	-1.895339000
1	5.263005000	-1.609951000	-2.658235000	6	6.323657000	-0.396414000	-1.350591000
6	4.639254000	-0.122098000	0.348969000	6	6.274197000	0.856376000	-0.729934000
1	6.043718000	1.095797000	1.418553000	6	5.242263000	-1.277830000	-1.281842000
7	3.156898000	-1.577794000	-0.993755000	6	7.117424000	1.535988000	-0.786420000
1	3.887885000	-0.002100000	1.119388000	1	5.112410000	1.216765000	-0.037662000
6	2.887941000	-2.235985000	-2.276894000	6	4.068345000	-0.928547000	-0.575832000
1	2.950254000	-1.535263000	-3.119995000	1	5.318078000	-2.242313000	-1.767332000
1	3.589219000	-3.060208000	-2.455472000	6	4.017730000	0.349727000	0.036735000
1	1.876103000	-2.642094000	-2.253405000	1	5.048005000	2.185433000	0.449276000
1	3.509497000	1.829251000	-0.553370000	7	2.986197000	-1.823047000	-0.501371000
8	2.556440000	1.932733000	-0.734909000	1	3.128278000	0.672233000	0.565626000
1	2.198045000	2.767570000	-0.380615000	1	2.743351000	-2.969593000	-1.415084000
1	1.621711000	0.551694000	-0.645903000	6	1.837908000	-1.532122000	0.306043000
6	2.023647000	-1.388900000	-0.114135000	1	3.045149000	-2.655514000	-2.458983000
1	1.405034000	-2.284913000	-0.127436000	1	3.692889000	-3.716588000	-1.182752000
1	2.369650000	-1.224504000	0.908237000	1	1.944925000	-3.442536000	-1.316550000
1	-4.820233000	-1.256783000	-0.143001000	1	2.743351000	1.187815000	-2.004432000
1	-3.853087000	2.896211000	-0.112469000	8	1.878274000	0.825463000	-2.273648000
7	-4.108831000	3.746738000	-0.598271000	1	1.230731000	1.533283000	-2.463154000
7	-5.423832000	-1.899964000	-0.639783000	1	1.253268000	-0.152760000	-1.157097000
1	-3.641714000	4.512177000	-0.131339000	6	1.837908000	-1.532122000	0.306043000
1	-5.083839000	3.924143000	-0.798292000	1	1.309082000	-2.450057000	0.556139000
1	-5.344440000	-2.799449000	-0.185090000	1	2.133812000	-1.027025000	1.226088000

1	-4.440820000	0.456384000	-1.270783000	8	1.377843000	-1.217435000	-2.630348000
1	-2.596570000	3.288359000	1.329663000	1	0.756981000	-1.681990000	-3.213326000
7	-2.502481000	4.291497000	1.427982000	1	0.953336000	-0.659881000	-1.598333000
7	-5.010055000	0.440945000	-2.107766000	6	1.830196000	-1.373763000	0.163005000
1	-2.023904000	4.464767000	2.301518000	1	1.295361000	-2.308435000	0.368592000
1	-3.313421000	4.877608000	1.283164000	1	2.298911000	-0.992567000	1.071867000
1	-5.270833000	-0.521117000	-2.276742000	1	-4.589382000	-0.549924000	-0.672793000
1	-5.777926000	1.093190000	-2.191858000	1	-3.129245000	3.292905000	0.460491000

III+1. For $^4 TS_P + H_2O + 2NH_3$ Complex.

26	-0.871070000	0.094736000	0.373082000	1	-2.721244000	4.818929000	0.861950000
7	-1.330435000	0.824260000	-1.451306000	1	-4.156317000	4.619429000	-0.016173000
7	-1.519125000	-1.842432000	-0.242545000	1	-5.291915000	-1.946630000	-1.133271000
7	-0.391095000	-0.671534000	2.190582000	1	-6.107524000	-0.515811000	-1.530600000
7	-0.065054000	1.956579000	0.946528000				
6	-1.154111000	2.135873000	-1.861255000				
6	-1.935267000	0.131970000	-2.488063000	26	-0.839329000	0.007810000	0.383197000
6	-2.092832000	-2.144480000	-1.458163000	7	-1.895494000	-0.002712000	-1.342536000
6	-1.592824000	-2.968246000	0.549100000	7	-1.309912000	-1.930930000	0.727160000
6	-0.631560000	-1.968346000	2.631902000	7	0.280115000	-0.015098000	2.063777000
6	0.172463000	0.035125000	3.247158000	7	-0.314751000	1.917064000	0.001728000
6	0.470967000	2.273242000	2.171894000	6	-2.083545000	1.044462000	-2.229730000
6	-0.056796000	3.093183000	0.173501000	6	-2.641674000	-1.063188000	-1.829616000
6	-1.671277000	2.271668000	-3.212459000	6	-2.144437000	-2.712779000	-0.058402000
6	-2.148265000	1.048903000	-3.595269000	6	-0.945765000	-2.719857000	1.810411000
6	-2.518064000	-3.536550000	-1.447765000	6	0.441140000	-1.051911000	2.972942000
6	-2.210967000	-4.043595000	-0.212054000	6	0.989463000	1.060816000	2.573560000
6	-0.201149000	-2.075153000	4.013096000	6	0.485464000	2.708718000	0.804692000
6	0.290465000	-0.853527000	4.387821000	6	-0.701954000	2.710029000	-1.063736000
6	0.855091000	3.678830000	2.172606000	6	-2.958435000	0.626118000	-3.306109000
6	0.529459000	4.183562000	0.942357000	6	-3.302343000	-0.672939000	-3.060215000
6	-0.564873000	3.167548000	-1.125091000	6	-2.295123000	-4.022409000	0.542213000
6	-2.271506000	-1.225600000	-2.496593000	6	-1.557053000	-4.026773000	1.692887000
6	-1.170364000	-3.018306000	1.880374000	6	1.280542000	-0.616586000	4.069920000
6	0.579085000	1.373455000	3.234112000	6	1.617941000	0.684564000	3.823737000
1	-0.506463000	4.133021000	-1.618608000	6	0.606422000	4.033341000	0.223860000
1	-2.748988000	-1.594530000	-3.399720000	6	-0.125654000	4.033965000	-0.927687000
1	-1.287929000	-3.965902000	2.397809000	6	-1.524878000	2.308526000	-2.105966000
1	1.009179000	1.751190000	4.156902000	6	-2.752533000	-2.316066000	-1.242103000
1	-1.663361000	3.189913000	-3.782132000	6	-0.123959000	-2.315221000	2.854426000
1	-2.604874000	0.778457000	-4.536716000	6	1.090647000	2.316001000	1.989910000
1	-3.004667000	-4.044067000	-2.268983000	1	-1.754808000	3.037868000	-2.875504000
1	-2.399257000	-5.040951000	0.160107000	1	-3.382128000	-3.044400000	-1.743253000
1	-0.272695000	-2.973547000	4.609799000	1	0.077488000	-3.032600000	3.643299000
1	0.695898000	-0.567209000	5.347969000	1	1.687268000	3.057602000	2.511211000
1	1.302542000	4.201163000	3.006445000	1	-3.266114000	1.257236000	-4.127527000
1	0.661636000	5.194904000	0.584612000	1	-3.949280000	-1.316059000	-3.639768000
8	1.005982000	-0.398711000	-0.435247000	1	-2.897661000	-4.819739000	0.130853000
16	-3.051221000	0.710573000	1.093788000	1	-1.436610000	-4.827841000	2.408286000
1	-2.949793000	0.285218000	2.405431000	1	1.558548000	-1.233135000	4.912849000
1	6.833625000	0.250228000	0.755104000	1	2.228156000	1.343091000	4.425227000
6	6.047334000	0.239816000	0.007555000	1	1.176086000	4.842869000	0.657282000
6	6.032777000	1.198034000	-1.012884000	1	-0.276593000	4.843638000	-1.627149000
6	5.044484000	-0.733005000	0.072276000	8	0.766488000	-0.563247000	-0.720893000
1	6.810459000	1.953266000	-1.059109000	16	-2.699827000	0.745865000	1.532847000
6	5.010826000	1.182506000	-1.968325000	1	-2.583289000	-0.067037000	2.644919000
6	4.032155000	-0.744606000	-0.894881000	1	6.577241000	-0.206103000	0.638621000
1	5.057725000	-1.465409000	0.872642000	6	5.787982000	-0.018314000	-0.081736000
6	4.004189000	0.211669000	-1.915799000	6	5.754613000	1.187361000	-0.792223000
1	4.991068000	1.927512000	-2.756613000	6	4.799939000	-0.985594000	-0.292391000
7	2.952662000	-1.752494000	-0.842492000	1	6.521138000	1.936900000	-0.625105000
1	3.200010000	0.188168000	-2.643039000	6	4.728128000	1.425399000	-1.712749000
6	3.428347000	-3.154603000	-0.623435000	6	3.783542000	-0.740407000	-1.223309000
1	4.250575000	-3.361899000	-1.309792000	1	4.827659000	-1.912180000	0.271300000
1	3.766788000	-3.303980000	0.405319000	6	3.735991000	0.463588000	-1.934024000
1	2.598777000	-3.835026000	-0.827980000	1	4.692758000	2.361793000	-2.259194000
1	2.330779000	-1.700756000	-1.865684000	7	2.718732000	-1.739015000	-1.456431000

1	2.926896000	0.633202000	-2.635493000	6	-6.462333000	-2.121656000	-0.064742000
6	3.214337000	-3.141341000	-1.624574000	6	-4.989074000	-0.198093000	-0.314390000
1	4.038854000	-3.141908000	-2.338841000	1	-5.832704000	1.686407000	0.349405000
1	3.555788000	-3.561161000	-0.674688000	6	-5.239243000	-1.582302000	-0.461053000
1	2.394678000	-3.751750000	-2.010065000	1	-6.638806000	-3.185866000	-0.189790000
1	2.100297000	-1.421654000	-2.434583000	7	-3.729215000	0.305429000	-0.682484000
8	1.131645000	-0.782399000	-3.041419000	1	-4.470839000	-2.210286000	-0.902484000
1	0.562980000	-1.030652000	-3.785784000	6	-3.517780000	1.740624000	-0.874674000
1	0.685315000	-0.520817000	-1.902919000	1	-4.234839000	2.178804000	-1.585360000
6	1.588625000	-1.662087000	-0.398845000	1	-3.606704000	2.286400000	0.071844000
1	1.057124000	-2.618930000	-0.460607000	1	-2.507173000	1.893953000	-1.256410000
1	2.038374000	-1.536750000	0.586947000	1	-3.178770000	-0.308902000	-1.297145000
1	-4.630442000	0.390630000	-0.262182000	8	-2.032535000	-1.626087000	-1.879766000
1	-2.259754000	3.365915000	1.664261000	1	-1.457954000	-1.666968000	-2.665006000
7	-2.169653000	4.373777000	1.694254000	1	-1.486579000	-1.632724000	-1.057525000
7	-5.393008000	0.328372000	-0.925071000	6	-2.172463000	-0.409611000	1.115616000
1	-1.489522000	4.594052000	2.409113000	1	-2.211052000	0.593364000	1.555125000
1	-3.005602000	4.940766000	1.737082000	1	-3.016820000	-1.073059000	1.323303000
1	-5.663279000	-0.644137000	-0.982518000	1	3.421446000	2.840676000	-1.676464000
1	-6.173595000	0.964841000	-0.837257000	1	4.615324000	-1.248864000	-1.492126000
				7	5.012867000	-1.959533000	-2.093553000
				7	3.389588000	3.600893000	-2.344192000
26	1.299746000	0.086879000	0.293402000	1	5.196387000	-2.771359000	-1.519637000
7	1.150305000	-0.610914000	-1.591039000	1	5.776871000	-1.712263000	-2.707782000
7	0.537597000	1.857527000	-0.316903000	1	3.094485000	4.428552000	-1.844176000
7	1.165923000	0.704770000	2.206164000	1	4.181472000	3.752662000	-2.954102649
7	1.743544000	-1.773534000	0.939207000				
6	1.468060000	-1.890461000	-2.031945000				
6	0.806698000	0.114374000	-2.725162000				
6	0.307236000	2.255520000	-1.627872000				
6	0.314535000	2.981073000	0.467968000				
6	0.839350000	1.981677000	2.650955000				
6	1.479246000	-0.028775000	3.345148000				
6	1.978508000	-2.169561000	2.247078000				
6	1.988555000	-2.889684000	0.151690000				
6	1.304781000	-1.968154000	-3.464399000				
6	0.896585000	-0.731618000	-3.892188000				
6	-0.077787000	3.650129000	-1.658185000				
6	-0.074458000	4.096300000	-0.366947000				
6	0.954951000	2.043842000	4.089321000				
6	1.348380000	0.805803000	4.516661000				
6	2.378560000	-3.560498000	2.277127000				
6	2.385501000	-4.003795000	0.986128000				
6	1.864043000	-2.947940000	-1.225836000				
6	0.425419000	1.448263000	-2.747113000				
6	0.448491000	3.041012000	1.846160000				
6	1.858482000	-1.362331000	3.367050000				
1	2.086276000	-3.891911000	-1.711228000				
1	0.205559000	1.891156000	-3.712411000				
1	0.236005000	3.987544000	2.331137000				
1	2.076719000	-1.805962000	4.332288000				
1	1.490791000	-2.852588000	-4.056241000				
1	0.687838000	-0.409152000	-4.902037000				
1	-0.308600000	4.202726000	-2.557388000	1	-1.207659000	2.861773000	-3.170160000
1	-0.302580000	5.086328000	0.000260000	1	-2.932829000	-3.191369000	-2.002610000
1	0.757290000	2.924874000	4.682413000	1	-0.475151000	-2.813200000	3.895636000
1	1.535331000	0.475461000	5.528096000	1	1.166109000	3.265284000	2.750208000
1	2.619542000	-4.109370000	3.175795000	1	-2.412520000	0.969663000	-4.584962000
1	2.632589000	-4.988209000	0.616393000	1	-3.147330000	-1.586177000	-4.081155000
8	-1.133719000	-0.829962000	0.551951000	1	-2.769256000	-4.849337000	0.026252000
16	3.666526000	0.763086000	-0.033554000	1	-1.728635000	-4.704317000	2.519685000
1	3.993145000	0.918583000	1.300763000	1	0.723508000	-0.913418000	5.308874000
1	-7.984497000	0.710853000	1.044586000	1	1.404951000	1.658750000	4.815922000
6	-7.218561000	0.064229000	0.626482000	1	0.957140000	4.942690000	0.741803000
6	-7.462225000	-1.305172000	0.483860000	1	-0.041472000	4.779560000	-1.769131000
6	-5.996518000	0.621199000	0.232791000	8	0.929095000	-0.515849000	-0.383746000
1	-8.412843000	-1.729534000	0.789274000	16	-2.912044000	0.777907000	1.118669000

1	-3.004385000	-0.004867000	2.254505000	1	2.322955000	-1.832729000	-1.844228000
1	6.672572000	0.254444000	0.673819000	8	1.103086000	-1.305607000	-2.795842000
6	5.866526000	0.243031000	-0.052068000	1	0.424896000	-1.513144000	-3.458940000
6	5.767874000	1.257344000	-1.011466000	1	0.729362000	-0.828639000	-1.979934000
6	4.923243000	-0.789340000	-0.018724000	6	1.690328000	-1.524158000	0.136301000
1	6.499966000	2.057684000	-1.031871000	1	1.171959000	-2.487541000	0.248537000
6	4.720225000	1.239913000	-1.938731000	1	2.233161000	-1.270607000	1.055996000
6	3.887707000	-0.798858000	-0.958650000	1	4.457288000	0.350375000	-1.003837000
1	5.002866000	-1.563824000	0.736096000	1	-2.527194000	3.406174000	1.259013000
6	3.771684000	0.211873000	-1.917399000	7	-2.452882000	4.415599000	1.277588000
1	4.633189000	2.028776000	-2.677915000	7	-5.077175000	0.260720000	-1.799141000
7	2.857510000	-1.858762000	-0.927923000	1	-1.925205000	4.663435000	2.103576000
1	2.947802000	0.189664000	-2.621287000	1	-3.286047000	4.972182000	1.142785000
6	3.387439000	-3.246597000	-0.714624000	1	-5.323267000	-0.716505000	-1.880324000
1	4.238624000	-3.417538000	-1.375077000	1	-5.865267000	0.888664000	-1.881101000
1	3.694698000	-3.374249000	0.324487000				
1	2.589602000	-3.954976000	-0.942496000				

Table S25 Cartesian Coordinates for Various Reaction Species in Carbinolaniline Decomposition Process in Non-enzymatic Environment and Without Water Assisted

I. For Carbinolaniline.

8	-0.027520000	0.505889000	0.042843000	1	2.851678000	2.797511000	1.340494000
1	5.837149000	3.312707000	-0.085636000	7	1.484242000	0.485308000	1.038503000
6	5.091440000	2.524759000	-0.086614000	6	0.168404000	1.403476000	0.839040000
6	5.428608000	1.227031000	-0.481993000	6	1.658268000	0.019597000	2.447597000
6	3.771019000	2.792596000	0.295947000	1	-0.092131000	1.850123000	1.812118000
6	4.473356000	0.205960000	-0.483393000	1	0.453374000	2.190907000	0.122788000
1	6.445372000	0.998238000	-0.787567000	1	0.651636000	-0.210432000	0.458743000
6	2.802077000	1.788383000	0.290689000	1	2.057417000	0.818956000	3.078806000
1	3.484266000	3.798544000	0.587888000	1	0.676470000	-0.294269000	2.809577000
6	3.144069000	0.469095000	-0.087545000	1	2.345606000	-0.829474000	2.466370000
1	4.771428000	-0.792226000	-0.779616000				
1	1.772491000	2.026445000	0.526847000	8	-1.399448000	0.321949000	0.860240000
7	2.175219000	-0.556803000	-0.063499000	1	5.932219000	2.094232000	-1.610863000
6	0.948993000	-0.378544000	0.676048000	6	5.103694000	1.710218000	-1.025645000
6	2.495551000	-1.871081000	-0.622525000	6	4.218460000	0.771940000	-1.575404000
1	0.507321000	-1.366388000	0.846698000	6	4.903422000	2.138630000	0.290227000
1	1.132544000	0.104923000	1.638803000	6	3.152643000	0.276379000	-0.826746000
1	-0.147955000	0.242034000	-0.892966000	1	4.359811000	0.423185000	-2.594035000
1	3.262159000	-2.402704000	-0.039202000	6	3.840690000	1.646873000	1.055428000
1	1.592773000	-2.486029000	-0.633938000	1	5.582714000	2.860234000	0.734423000
1	2.858117000	-1.781406000	-1.653404000	6	2.943473000	0.709660000	0.502534000
				1	2.471886000	-0.450434000	-1.263360000

II. For TSp Complex.

8	-0.624072000	0.363888000	0.378273000	7	1.850916000	0.219401000	1.220542000
1	5.965630000	1.891161000	-1.494582000	6	-0.689088000	1.190309000	0.341945000
6	5.058067000	1.606237000	-0.972854000	6	1.645228000	0.469089000	2.642326000
6	4.464176000	0.364025000	-1.225045000	1	-0.420820000	2.121593000	0.864095000
6	4.475560000	2.482877000	-0.049147000	1	-0.302940000	1.099609000	-0.685776000
6	3.291334000	-0.004126000	-0.557358000	1	1.392134000	-0.596482000	0.842627000
1	4.908424000	-0.316184000	-1.944142000	1	1.591566000	1.545218000	2.843609000
6	3.305543000	2.119078000	0.624982000	1	0.689822000	0.028889000	2.935911000
1	4.929596000	3.448933000	0.145763000	1	2.442087000	0.044755000	3.272256000
6	2.715177000	0.873861000	0.368578000				
1	2.818831000	-0.960925000	-0.753846000				

III. For Formaldehyde Complex.

8	-1.399448000	0.321949000	0.860240000
1	5.932219000	2.094232000	-1.610863000
6	5.103694000	1.710218000	-1.025645000
6	4.218460000	0.771940000	-1.575404000
6	4.903422000	2.138630000	0.290227000
6	3.152643000	0.276379000	-0.826746000
1	4.359811000	0.423185000	-2.594035000
6	3.840690000	1.646873000	1.055428000
1	5.582714000	2.860234000	0.734423000
6	2.943473000	0.709660000	0.502534000
1	2.471886000	-0.450434000	-1.263360000

Table S26 Cartesian Coordinates for Various Reaction Species in Carbinolaniline Decomposition Process in Non-enzymatic Environment and With Water Assisted

I. For Carbinolaniline+H₂O Complex.

8	2.181998000	0.975947000	-1.194642000	7	0.917805000	-0.623260000	0.240967000
1	-4.210793000	0.870087000	-0.358976000	6	1.712080000	-0.714208000	-1.211267000
6	-3.180234000	0.537442000	-0.292556000	6	1.168481000	-1.842107000	1.059150000
6	-2.857045000	-0.637985000	0.390228000	1	2.610773000	-1.281180000	-0.909089000
6	-2.152639000	1.279732000	-0.888386000	1	1.055718000	-1.331525000	-1.835752000
6	-1.530350000	-1.075861000	0.475632000	1	2.300657000	1.179561000	-0.739412000
1	-3.639300000	-1.230332000	0.855372000	1	0.564985000	-1.812331000	1.968593000
6	-0.823391000	0.863012000	-0.803057000	1	0.929571000	-2.747480000	0.494478000
1	-2.383940000	2.197762000	-1.420154000	1	2.227060000	-1.860161000	1.326061000
6	-0.494625000	-0.328784000	-0.119518000	8	2.295521000	1.434665000	0.463595000
1	-1.318640000	-2.001267000	0.996163000	1	3.016378000	1.890823000	0.923633000
1	-0.028310000	1.455927000	-1.239281000				
7	0.875100000	-0.737391000	-0.031284000				
6	1.758542000	-0.392409000	-1.180608000	8	2.214260000	0.646900000	-1.917613000
6	1.166996000	-2.033253000	0.610488000	1	-4.187367000	0.841473000	-0.681580000
1	2.616794000	-1.072878000	-1.129652000	6	-3.181636000	0.523558000	-0.427762000
1	1.231299000	-0.543278000	-2.127728000	6	-2.923916000	-0.805357000	-0.078461000
1	2.587416000	1.200796000	-0.314209000	6	-2.120278000	1.440875000	-0.442927000
1	0.766438000	-2.050107000	1.627765000	6	-1.630244000	-1.224021000	0.252922000
1	0.746998000	-2.889173000	0.060579000	1	-3.734661000	-1.527913000	-0.058574000
1	2.250105000	-2.154044000	0.676722000	6	-0.827076000	1.039228000	-0.115750000
1	1.719541000	0.403577000	1.254712000	1	-2.302909000	2.477278000	-0.711242000
8	2.495559000	0.985684000	1.470901000	6	-0.561751000	-0.304481000	0.235751000
1	2.244964000	1.703188000	2.079243000	1	-1.456818000	-2.259463000	0.523235000
				1	-0.005303000	1.747087000	-0.131351000

II. For TSp Complex.

8	1.920351000	0.535012000	-1.691071000	7	0.757023000	-0.681096000	0.525141000
1	-4.156754000	0.854486000	-0.545925000	6	1.976557000	-0.568447000	-1.769852000
6	-3.129913000	0.546163000	-0.378318000	6	1.066176000	-1.969475000	1.136935000
6	-2.820697000	-0.810658000	-0.232654000	1	2.668949000	-1.238627000	-1.244304000
6	-2.110205000	1.502708000	-0.307290000	1	1.107000000	-1.042148000	-2.240748000
6	-1.497785000	-1.213496000	-0.018009000	1	2.772960000	1.371807000	-0.378468000
1	-3.605283000	-1.558353000	-0.288130000	1	0.507699000	-2.143141000	2.069686000
6	-0.785119000	1.113783000	-0.088644000	1	0.842630000	-2.800376000	0.455612000
1	-2.343636000	2.556106000	-0.421528000	1	2.134070000	-1.995644000	1.366979000
6	-0.486838000	-0.247539000	0.059907000	8	2.689874000	1.399192000	0.607475000
1	-1.270719000	-2.268788000	0.085911000	1	2.751391000	2.308596000	0.944977000
1	0.019194000	1.837305000	-0.023057000				

III. For Formaldehyde+H₂O Complex.

8	2.214260000	0.646900000	-1.917613000
1	-4.187367000	0.841473000	-0.681580000
6	-3.181636000	0.523558000	-0.427762000
6	-2.923916000	-0.805357000	-0.078461000
6	-2.120278000	1.440875000	-0.442927000
6	-1.630244000	-1.224021000	0.252922000
1	-3.734661000	-1.527913000	-0.058574000
6	-0.827076000	1.039228000	-0.115750000
1	-2.302909000	2.477278000	-0.711242000
6	-0.561751000	-0.304481000	0.235751000
1	-1.456818000	-2.259463000	0.523235000
1	-0.005303000	1.747087000	-0.131351000

Table S27 Cartesian Coordinates for Reaction Species in *p*-(Cl, CN, NO₂)-Carbinolaniline Decomposition Process in the Non-enzymatic Environment and with Water Assisted

A. For *p*-Cl-carbinolaniline decomposition

I. For Carbinolaniline+H₂O Complex.

8	2.132860000	0.959949000	-1.304310000	7	0.916989000	-0.629974000	0.244633000
17	-4.905077000	1.084079000	-0.417685000	6	1.715036000	-0.706245000	-1.215581000
6	-3.165229000	0.525658000	-0.314597000	6	1.168425000	-1.856447000	1.050436000
6	-2.859119000	-0.619870000	0.410228000	1	2.618763000	-1.262779000	-0.911399000
6	-2.172222000	1.257862000	-0.962041000	1	1.064528000	-1.328614000	-1.840880000
6	-1.528924000	-1.049014000	0.485913000	1	2.285681000	1.189525000	-0.733398000
1	-3.641650000	-1.182901000	0.904379000	1	0.570080000	-1.834686000	1.963650000
6	-0.844043000	0.838099000	-0.878095000	1	0.926605000	-2.756662000	0.478489000
1	-2.425560000	2.151250000	-1.519977000	1	2.227984000	-1.878547000	1.312619000
6	-0.501788000	-0.326714000	-0.154074000	8	2.272902000	1.435245000	0.471416000
1	-1.313073000	-1.954210000	1.038237000	1	2.977408000	1.907471000	0.940087000
1	-0.058440000	1.416668000	-1.349037000				
7	0.864158000	-0.731833000	-0.072864000				
6	1.737323000	-0.413911000	-1.238475000	8	2.204433000	0.696415000	-1.963966000
6	1.169786000	-2.002384000	0.611177000	17	-4.851078000	1.050794000	-0.860405000
1	2.607266000	-1.076453000	-1.164617000	6	-3.155588000	0.511600000	-0.417634000
1	1.209248000	-0.610400000	-2.176817000	6	-2.931845000	-0.813388000	-0.061444000
1	2.569982000	1.214164000	-0.447250000	6	-2.115623000	1.441597000	-0.442237000
1	0.785415000	-1.984480000	1.634878000	6	-1.638175000	-1.225471000	0.278338000
1	0.745076000	-2.878756000	0.098547000	1	-3.751852000	-1.521489000	-0.043259000
1	2.254047000	-2.117307000	0.665102000	6	-0.827627000	1.032495000	-0.104741000
1	1.759700000	0.461929000	1.194018000	1	-2.308146000	2.470929000	-0.720365000
8	2.563810000	1.023910000	1.333107000	6	-0.564399000	-0.310236000	0.258015000
1	2.406394000	1.726168000	1.988137000	1	-1.473755000	-2.259299000	0.557733000
				1	-0.008125000	1.742171000	-0.121325000

II. For TSP Complex.

8	1.905964000	0.547128000	-1.686678000	7	0.745102000	-0.687640000	0.556984000
17	-4.827253000	1.066279000	-0.658340000	6	2.014836000	-0.528113000	-1.851620000
6	-3.099897000	0.543546000	-0.377327000	6	1.056347000	-1.980398000	1.155967000
6	-2.824362000	-0.811969000	-0.217869000	1	2.700165000	-1.175970000	-1.290744000
6	-2.097753000	1.509703000	-0.324874000	1	1.181358000	-1.026059000	-2.362073000
6	-1.500972000	-1.211882000	-0.000555000	1	2.753097000	1.407989000	-0.399311000
1	-3.620801000	-1.544208000	-0.263938000	1	0.504329000	-2.160450000	2.091510000
6	-0.776984000	1.108882000	-0.102604000	1	0.828808000	-2.807132000	0.470627000
1	-2.338170000	2.557672000	-0.452886000	1	2.125403000	-2.009106000	1.379655000
6	-0.483297000	-0.252208000	0.063578000	8	1.403673000	0.074638000	0.749805000
1	-1.284736000	-2.267486000	0.116416000	1	2.663169000	1.391748000	0.584707000
1	0.028089000	1.832088000	-0.045005000	1	2.826569000	2.265233000	0.977631000

B. For *p*-CN-carbinolaniline decomposition

I. For Carbinolaniline+H₂O Complex.

8	2.143213000	0.974104000	-1.266496000	6	1.166995000	-1.994108000	0.613486000
6	-4.556808000	0.961014000	-0.454831000	1	2.619670000	-1.063790000	-1.153018000
6	-3.199223000	0.525390000	-0.367074000	1	1.248999000	-0.580258000	-2.192219000
6	-2.858204000	-0.611947000	0.388366000	1	2.576668000	1.209797000	-0.403104000
6	-2.171639000	1.227063000	-1.032290000	1	0.777725000	-1.957581000	1.635011000
6	-1.535868000	-1.041274000	0.473238000	1	0.757521000	-2.888664000	0.121303000
1	-3.636650000	-1.165888000	0.901554000	1	2.252304000	-2.091804000	0.675106000
6	-0.849255000	0.810288000	-0.944383000	8	1.737424000	0.494681000	1.272580000
1	-2.417962000	2.109213000	-1.613036000	1	2.575430000	1.004181000	1.368799000
6	-0.505601000	-0.338651000	-0.190638000	7	2.508386000	1.684348000	2.061468000
1	-1.317510000	-1.932509000	1.046640000				
1	-0.062860000	1.379321000	-1.424661000	6	-5.673852000	1.319668000	-0.526301000
7	0.846708000	-0.747794000	-0.106039000	8	1.913648000	0.571597000	-1.674115000
6	1.751418000	-0.400775000	-1.236817000	6	-4.481182000	0.957788000	-0.604581000

6	-3.127438000	0.548940000	-0.383600000	6	-4.237602000	0.721847000	-1.145391000
6	-2.823904000	-0.811758000	-0.186104000	6	-3.005447000	0.338706000	-0.540476000
6	-2.089693000	1.501881000	-0.356633000	6	-2.871974000	-0.906462000	0.109691000
6	-1.505680000	-1.211418000	0.032635000	6	-1.883074000	1.199494000	-0.576661000
1	-3.619320000	-1.547801000	-0.207032000	6	-1.670864000	-1.289139000	0.694819000
6	-0.772906000	1.104787000	-0.132771000	1	-3.725108000	-1.575669000	0.151375000
1	-2.320763000	2.549857000	-0.508010000	6	-0.680030000	0.826589000	0.001591000
6	-0.482513000	-0.254063000	0.064861000	1	-1.973973000	2.168308000	-1.057514000
1	-1.290564000	-2.263571000	0.176515000	6	-0.538436000	-0.433688000	0.652593000
1	0.035105000	1.825030000	-0.094981000	1	-1.603710000	-2.251864000	1.186787000
7	0.913688000	-0.629848000	0.246221000	1	0.170502000	1.500585000	-0.009495000
6	1.717738000	-0.686824000	-1.223924000	7	0.665740000	-0.776605000	1.203306000
6	1.171168000	-1.866991000	1.032681000	6	1.656807000	0.446716000	-2.878185000
1	2.616595000	-1.250100000	-0.920722000	6	0.905657000	-2.031164000	1.896350000
1	1.064622000	-1.296987000	-1.857790000	1	0.720936000	0.262579000	-2.333890000
1	2.299434000	1.194419000	-0.714931000	1	1.637967000	0.318034000	-3.969082000
1	0.575311000	-1.862598000	1.947901000	1	2.838896000	0.929496000	-0.504027000
1	0.934029000	-2.760800000	0.448603000	1	0.259925000	-2.145052000	2.778613000
1	2.231119000	-1.886328000	1.293317000	1	0.744306000	-2.904871000	1.247412000
1	1.492855000	0.245696000	0.667811000	1	1.944873000	-2.046731000	2.231732000
8	2.279477000	1.413890000	0.497552000	1	1.452855000	-0.131493000	1.078628000
1	2.960230000	1.894986000	0.990604000	8	2.729027000	0.958148000	0.476481000
7	-5.592969000	1.291139000	-0.783391000	1	3.186155000	1.724300000	0.860932000
				7	-5.251663000	1.039316000	-1.651152000

III. For Formaldehyde+H₂O Complex.

8 2.695819000 0.792955000 -2.299117000

C. For p-NO₂-carbinolaniline decomposition

I. For Carbinolaniline+H₂O Complex.

8	2.051996000	1.067049000	-0.853619000	6	0.152658000	-0.886426000	-0.329469000
7	-4.701687000	0.849777000	-0.600424000	1	-1.643625000	-2.090437000	-0.349435000
6	-3.326008000	0.413404000	-0.522071000	6	0.663309000	0.416326000	-0.195180000
6	-3.004834000	-0.729254000	0.219371000	1	0.186596000	2.507910000	0.135389000
6	-2.324860000	1.144789000	-1.177428000	7	0.838875000	-1.704140000	-0.508658000
6	-1.684494000	-1.150430000	0.297000000	6	2.106377000	0.582650000	-0.239828000
1	-3.795940000	-1.274987000	0.716982000	6	2.811266000	0.125254000	1.222343000
6	-1.004108000	0.732087000	-1.100143000	1	2.612439000	1.915442000	-0.666119000
1	-2.597695000	2.037341000	-1.725295000	1	3.802324000	0.591472000	1.095355000
6	-0.651512000	-0.437726000	-0.369585000	1	2.216426000	0.653064000	1.975697000
1	-1.455889000	-2.046380000	0.858850000	1	3.136219000	-1.630477000	0.253468000
1	-0.225455000	1.336702000	-1.544948000	1	2.092194000	2.246699000	-1.567500000
7	0.665245000	-0.870188000	-0.315373000	1	2.479631000	2.659546000	0.124592000
6	1.679678000	-0.274154000	-1.190158000	1	3.677800000	1.816499000	-0.882794000
6	1.054265000	-1.948759000	0.597361000	8	2.574841000	-0.250426000	-0.859133000
1	2.542683000	-0.950172000	-1.178265000	1	3.162494000	-1.517210000	-0.974137000
1	1.292621000	-0.217009000	-2.210433000	8	3.761714000	-1.977677000	-1.579000000
1	2.469184000	1.095414000	0.047570000	8	-3.943714000	-1.409368000	-0.087540000
1	0.695403000	-1.754366000	1.614916000	8	-4.258442000	0.776682000	0.234778000
1	0.665253000	-2.925666000	0.278138000				
1	2.143231000	-2.005634000	0.632410000				
1	2.525286000	1.329552000	2.356605000				
8	3.123095000	1.036767000	1.645663000	7	-4.204933000	0.758309000	-1.134972000
1	4.031209000	1.339818000	1.823776000	6	-2.974235000	0.356483000	-0.507463000
8	-4.969368000	1.887163000	-1.283717000	6	-2.906869000	-0.864587000	0.179082000
8	-5.586155000	0.176977000	0.017416000	6	-1.846836000	1.193166000	-0.587289000

II. For TSp Complex.

8	2.781374000	-1.219296000	1.329224000	6	-1.719702000	-1.261980000	0.775606000
7	-3.513021000	-0.227895000	0.042472000	6	-0.558622000	-0.442163000	0.698453000
6	-2.067845000	-0.007937000	-0.034570000	1	-1.680748000	-2.207333000	1.302262000
6	-1.575237000	1.291501000	0.101952000	1	0.212930000	1.447263000	-0.028727000
6	-1.221923000	-1.099581000	-0.247308000	7	0.631914000	-0.801987000	1.254773000
6	-0.199041000	1.501920000	0.024738000	6	1.653756000	0.564095000	-2.952025000
1	-2.263941000	2.109218000	0.266602000	6	0.842061000	-2.040886000	1.988107000

1	0.687926000	0.379451000	-2.462866000	1	1.440020000	-0.186789000	1.099438000
1	1.677481000	0.521436000	-4.049303000	8	2.726875000	0.847773000	0.474517000
1	2.817500000	0.845458000	-0.508486000	1	3.222311000	1.582483000	0.872534000
1	0.199282000	-2.105442000	2.876550000	8	-4.230323000	1.863857000	-1.767866000
1	0.651564000	-2.928182000	1.367542000	8	-5.217249000	-0.007332000	-1.037429000
1	1.882679000	-2.073786000	2.316850000				