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Mechanism of NHC Catalyzed Aza-Morita—Baylis—Hillman Reaction: Insights on a New Substrate-Catalyzed Bimolecular Pathway

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Computational Methods

DFT (Density Functional Theory) calculations of all the stationary points such as reactants, intermediates, transition states, and products were carried out in the solvent phase using the mPW1K functional in conjunction with 6-31+G** basis set[1]. Additional geometry optimizations on the critical transition states were performed in the condensed phase at the M06-2X/6-31G** level of theory. A model system, consisting of a chemically equivalent N-mesyl instead of N-tosyl on the benzaldimine was employed. Also, the real NHC(1,3-bis-(2,6-diisopropylphenyl)imidazole-2-ylidene) was modelled as 1,3-(diphenyl)imidazole-2-ylidene. The solvent effects were incorporated with the continuum solvation model using the SCRF=PCM framework with UAKS radii. Toluene was taken as the continuum solvent dielectric (epsilon = 2.3741) since it was employed as solvent in the experimental study. Fully optimized geometries of all the stationary points were characterized by evaluating the harmonic vibrational frequencies in order to verify that (a) the transition states (TSs) have one and only one imaginary frequency pertaining to the desired reaction coordinate, and (b) all minimum energy structures were verified to possess only positive Hessians. The Intrinsic Reaction Coordinate (IRC) calculations were performed at the same level of theory to further authenticate that the transition states on the energy profile connect to the nearest minima involved in each elementary step of the reaction.[2] The geometries reached at the end of the IRC trajectories were subjected to additional optimization. In a small percentage of TSs 10% displacement of the TS geometry along the direction of the imaginary frequency followed by re-optimization of the corresponding perturbed geometries using 'opt=calcfc' was done. This procedure again was to connect to the reactant and product for the corresponding TS. The enthalpy and Gibbs free energy for all the stationary points were obtained by adding the zero point vibrational energy (ZPVE) and thermal energy corrections obtained by using the standard statistical mechanics approximations at 298.15 K and 1 atm pressure. Single-point calculations were carried out at the $PCM_{(toluene)}$/M06-2X/6-31+G** level of theory with an ultrafine intergration grid (invoked using *integration=grid=ultrafine* option available in Gaussian09 program suite) using the $PCM_{(toluene)}$/mPW1K/6-31+G** optimized geometries.[1] The Gibbs free energies of the stationary points presented in the manuscript are computed with respect to the infinitely separated reactants which include the substrate (cyclopent-2-en-1-one), N-mesylphenylimine and NHC (1,3-(diphenyl)imidazole-2-ylidene). All calculations were carried out using the Gaussian 09 suite of quantum chemical programs.[3]

References:

1 For basis set, See (*a*) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (*b*) P. C. Hariharan, J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213; For mPW1K see ref. (*c*) B. J. Lynch, P. L. Fast, M. Harris, D. G. Truhlar, J. Phys. Chem. A, 2000, **104**, 4811; (*d*) B. J. Lynch, Y. Zhao, D. G. Truhlar, *J. Phys. Chem. A*, 2003, **107**, 1384; For M06-2X see ref. (e) Y. Zhao, D. G. Truhlar, *Theo. Chem. Acc.*, 2008, **120**, 215.

2 For IRC computations, See (a) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154. (b) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.

3 *Gaussian 09, Revision A.02*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009

Table S1. Relative Gibbs Free Energies (in kcal/mol) for Various Elementary Steps Involved in the Conventional and Bimolecular Pathways[a,b]

	L1		L2		L3		L4
TS	**ΔH**	**ΔG**	**ΔH**	**ΔG**	**ΔH**	**ΔG**	**ΔG**
Conventional Pathway							
TS(2-3)	14.7	28.0	9.1	22.4	6.5	20.6	24.3
TS(3-5)	-5.8	21.5	-17.1	10.2	-19.6	10.0	14.0
TS(5-6)[c]	1.9	30.0	-7.5	20.6	-11.4	17.3	24.3
Bimolecular Pathway							
TS(5-8)	-22.1	23.0	-46.3	-1.2	-54.1	-6.4	4.5
TS(8-9)	-23.9	21.8	-48.8	-3.1	-58.0	-9.7	2.6
TS(9-10)	-32.8	13.2	-57.5	-11.5	-65.9	-17.3	-5.8
TS(10-11)	-11.0	34.2	-36.4	8.9	-45.4	2.7	14.6
TS(11-6)	-34.4	-6.8	-44.3	-16.6	-48.6	-19.5	-12.8
TS(6-7)	-14.8	13.1	-27.1	0.8	-33.2	-3.1	4.6

[a]L1= $PCM_{(toluene)}$/mPW1K/6-31+G**; L2= $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G**; L3= $PCM_{(toluene)}$/M06-2X/6-31G**; L4= $PCM_{(toluene)}$/M06-2X/mPW1K/6-31+G** (reported as the standard state of 1mol.L^{-1} at 298.15 K, as per the guidelines provided in Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*; 2nd Ed.; Wiley 2004.)

[b]Calculated with respect to the infinitely separated reactants.

[c]Optimized with BONDI as radii followed by single point with UAKS radii to maintain consistency.

Table S2. Gibbs Free Energies of Activation (in kcal/mol) for Various Elementary Steps Involved in the Conventional and Bimolecular Pathways[a,b]

	L1		L2		L4
TS	**ΔH**	**ΔG**	**ΔH**	**ΔG**	**ΔG**
Conventional Pathway					
TS(2-3)	15.8	22.9	12.3	19.4	19.4
TS(3-5)	3.2	6.8	-2.7	0.8	0.8
TS(5-6)[c]	41.6	41.1	42.9	42.4	42.4
Bimolecular Pathway					
TS(5-8)	12.5	17.4	2.3	7.2	7.2
TS(8-9)	11.9	10.8	12.6	11.4	11.4
TS(9-10)	2.1	2.8	1.2	2.0	2.0
TS(10-11)	24.3	23.8	23.2	22.7	22.7
TS(11-6)	0.2	0.4	0.7	1.0	1.0
TS(6-7)	20.7	20.7	18.0	18.0	18.0

[a]L1= $PCM_{(toluene)}$/mPW1K/6-31+G**; L2= $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G**; L4= $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G** (in the standard state of 1mol.L^{-1} at 298.15 K, instead of 1atm as per the guidelines provided in Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*; 2nd Ed.; Wiley 2004.))

[b]Calculated with respect to the respective pre-reacting complexes as obtained through IRC.

[c]Optimized with BONDI as radii followed by single point with UAKS radii to maintain consistency.

Conformational Sampling for TS(3-5) in Conventional Pathway

Although there is no chiral entity present in the reaction system and the racemic product formed has only one chiral centre, there are many transition states along the pathway that are diastereomeric. A conformational analysis is first performed for the first stereogenerating transition state **TS(3-5)** taking into account the possibility of both *re*- and *si*- face additions to the prochiral electrophile *N*-mesylbenzaldimine (**4**). Different conformers, arising as a result of rotations along the newly forming C-C bond formation, in the staggered orientation for each such conformer is considered for each mode of addition. The most stable conformer thus chosen, and important transition states for the subsequent steps are calculated for each mode of addition. The pathway with the lowest overall barrier decides the configuration carried forward in the Bimolecular pathway.

Table S3. Relative Gibbs Free Energies (in kcal/mol) of Various Conformers of **TS(3-5)** for both *si*- and *re*- face additions to the prochiral electrophile N-mesylbenzaldimine.[a,b] Highlighted entries indicate the most preferred conformer for each prochiral approach

TS	L3
***re*- face addition**	
C1-TS(3-5)$_{re}$	22.2
C2-TS(3-5)$_{re}$	23.3
C3-TS(3-5)$_{re}$	19.8*
***si*- face addition**	
C1-TS(3-5)$_{si}$	30.4
C2-TS(3-5)$_{si}$	19.4
C3-TS(3-5)$_{si}$	24.4

[a]L3= mPW1K/6-31+G**
[b]Calculated with respect to the infinitely separated reactants.
*Forward IRC gives a conformationally blocked isomer.

Table S4. Relative Gibbs Free Energies of Important Transition States in the Conventional Pathway Taking into Account the Most Stable Conformer in Each Prochiral Mode of Addition for **TS(3-5)**. Highlighted Entries Indicates the Most Preferred Pathway [a,b]

***re* face addition**		***si* face addition**	
TS	**L3**	**TS**	**L3**
C1-TS(3-5)$_{re}$	22.2	**C2-TS(3-5)$_{si}$**	19.4
TS(5-6)''	30.1	**TS(5-6)'**	35.3

[a]L3= mPW1K/6-31+G**
[b]Calculated with respect to the infinitely separated reactants.

Conformational Sampling in the Bimolecular Pathway for TS(5-8)

A similar conformational analysis is performed for the first stereogenerating transition state **TS(5-8)** taking into account the possibility of both *re*- and *si*- face additions to the prochiral electrophile *N*-mesylbenzaldimine (**4**). Rotation is performed along the newly developing N-C bond to get three conformers in staggered orientations for each mode of addition. The most stable configuration from Table S2 is used in the present analysis.

Table S5. Relative Gibbs Free Energies of Various Conformations of **TS(5-8)** for Both *si*- and *re*- face Additions to the Prochiral Electrophile N-mesylbenzaldimine. Highlighted Entries Indicate the Most Preferred Conformer for Each Prochiral Approach [a,b]

TS	L3
***re* face addition**	
C1-TS(5-8)$_{re}$	34.5
C2-TS(5-8)$_{re}$	24.1
C3-TS(5-8)$_{re}$	27.9
***si* face addition**	
C1-TS(5-8)$_{si}$	31.9
C2-TS(5-8)$_{si}$	22.8
C3-TS(5-8)$_{si}$	36.8

[a]L3= mPW1K/6-31+G**
[b]Calculated with respect to the infinitely separated reactants.

The most stable conformation is thus chosen, and important subsequent transition states of the Bimolecular pathway are calculated for each mode of addition. The pathway with the lowest overall barrier decides the configuration as used in the main paper.

Table S6. Energies of Important Transition States in the Bimolecular Pathway Taking into Account the Most Stable Conformation in Each Prochiral Mode of Addition for **TS(5-8)** and the Most Stable Configuration from Table S2. Highlighted entry indicates the most preferred pathway. [a,b]

***re*- face**		***si*- face**	
TS	**L1**	**TS**	**L1**
C2-TS(5-8)$_{re}$	33.5	**C2-TS(5-8)$_{si}$**	23.0
TS(8-9)'	39.8	**TS(8-9)**	21.8
TS(9-10)'	4.2	**TS(9-10)**	13.2
TS(10-11)'	28.6	**TS(10-11)**	34.2
TS(11-6)'	2.2	**TS(11-6)**	-6.8
TS(6-7)'	20.9	**TS(6-7)**	13.1

[a]L1= PCM$_{(toluene)}$/mPW1K/6-31+G**

[b]Calculated with respect to the infinitely separated reactants.

Direct and Water-Assisted Proton Transfers

TS(5-11) : Direct Keto-Enol Tautomerisation
TS(5-11)$_w$: Water Assisted Keto-Enol Tautomerisation (One water molecule only)
TS(5-6) : Direct Proton Transfer to Nitrogen
TS(5-6)$_w$: Water Assisted Proton Transfer to Nitrogen (One water molecule only)

Table S7. Relative Gibbs Free Energies (in kcal/mol) for Various Proton Transfer Steps[a,b]

TS	L1	L2
TS(5-11)[c]	67.2	55.4
TS(5-11)$_w$	43.1	25.5
TS(5-6)[c]	30	20.6
TS(5-6)$_w$	23.3	10.1

[a]L1= PCM$_{(toluene)}$/mPW1K/6-31+G**; L2= PCM$_{(toluene)}$/M06-2X//mPW1K/6-31+G**
[b]Calculated with respect to the infinitely separated reactants.
[c]Optimized with BONDI as radii followed by single point with UAKS radii to maintain consistency.

Table S8. Gibbs Free Energies of Activation (in kcal/mol) for Various Proton Transfer Steps[a,b]

TS	L1	L2
TS(5-11)[c]	78.3	77.3
TS(5-11)$_w$	47.4	42.6
TS(5-6)[c]	41.1	42.4
TS(5-6)$_w$	18.3	17.5

[a]L1= PCM$_{(toluene)}$/mPW1K/6-31+G**; L2= PCM$_{(toluene)}$/M06-2X//mPW1K/6-31+G**
[b]Calculated with respect to the respective pre-reacting complexes as obtained through IRC.
[c]Optimized with BONDI as radii followed by single point with UAKS radii to maintain consistency.

Potential Side Reactions

Figure S1. Conventional and Bimolecular Pathways for the NHC catalyzed aza-MBH reaction including potential side reactions between **1** and **13** as well as **9** and **12**.

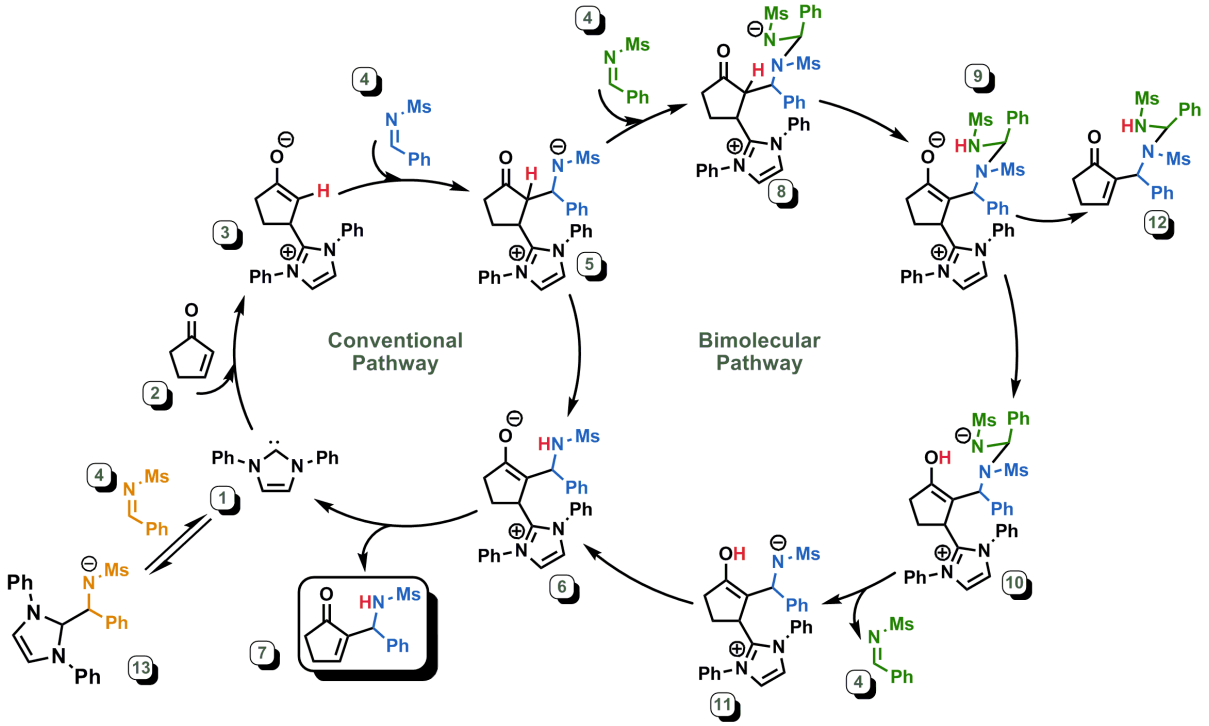

Table S9. Relative Gibbs Free Energies (in kcal/mol) for Potential Side Reactions[a,b]

	L1		L2	
TS	**ΔH**	**ΔG**	**ΔH**	**ΔG**
TS(1-13)	3.1	16.2	-5.0	8.1
TS(9-12)	-9.7	35.5	-34.3	10.9

[a]L1= $PCM_{(toluene)}$/mPW1K/6-31+G**; L2= $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G**
[b]Calculated with respect to the infinitely separated reactants.

Table S10. Gibbs Free Energies of Activation (in kcal/mol) for Potential Side Reactions[a,b]

	L1		L2	
TS	**ΔH**	**ΔG**	**ΔH**	**ΔG**
TS(1-13)	5.4	10.3	-0.5	4.4
TS(9-12)	24.9	23.8	25.1	24.0

[a]L1= $PCM_{(toluene)}$/mPW1K/6-31+G**; L2= $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G**
[b]Calculated with respect to the respective pre-reacting complexes as obtained through IRC.

The Optimized Cartesian coordinates, total electronic energies (in hartree/particle) obtained at the
(a) $PCM_{(toluene)}$/mPW1K/6-31+G (black)**
(b) $PCM_{(toluene)}$/M06-2X//mPW1K/6-31+G (red)**
(c) mPW1K/6-31+G (green)**

The number of imaginary frequencies, along with their values (in cm^{-1}) as applicable, are provided.

Notation for intermediates

For example, **TS(3-5)** gives the intermediate **5** by forward IRC and **TS(5-6)** gives the intermediate **5'** by reverse IRC. These two intermediates differ by a low energy rotational transition state, and only the lower energy intermediate is used for discussions in the main paper.

(I) Conventional Pathway

1

Eelec = -688.1268675, -688.0333541
E = -687.88817
H = -687.874827
G = -687.928554
Nimag = 0

6	-2.762635	1.269734	0.261711
6	-2.402385	-0.049858	0.024462
6	-3.358296	-0.974817	-0.373200
6	-4.679293	-0.579122	-0.520108
6	-5.046675	0.737106	-0.286104
6	-4.082049	1.658089	0.099251
7	-1.056253	-0.449885	0.188306
6	-0.671264	-1.704703	0.627540
6	0.671264	-1.704703	0.627540
7	1.056253	-0.449885	0.188306
6	0.000000	0.353793	-0.092391
6	2.402385	-0.049858	0.024462
6	3.358296	-0.974817	-0.373200
6	4.679293	-0.579122	-0.520108
6	5.046675	0.737106	-0.286104
6	4.082049	1.658089	0.099251
6	2.762635	1.269734	0.261711
1	-1.369122	-2.460947	0.937084
1	1.369122	-2.460947	0.937084
1	5.419111	-1.303194	-0.832578
1	4.358134	2.687211	0.283861
1	-5.419111	-1.303194	-0.832578
1	-4.358134	2.687211	0.283861
1	-2.004389	1.975940	0.565278
1	-6.076167	1.044498	-0.405996
1	-3.071332	-1.994270	-0.589938
1	3.071332	-1.994270	-0.589938
1	2.004389	1.975940	0.565278
1	6.076167	1.044498	-0.405996

2

Eelec = -269.2977579, -269.250661
E = -269.197992
H = -269.191963
G = -269.226617
Nimag = 0

6	1.257242	0.867739	0.000004

6	-0.030213	1.220564	-0.000083
6	-0.869372	0.016879	-0.000043
6	0.050013	-1.186030	0.000077
6	1.465368	-0.614003	0.000113
1	-0.167632	-1.797260	0.878317
1	-0.167543	-1.797364	-0.878112
1	2.045107	-0.919116	0.875792
1	2.045200	-0.919234	-0.875463
8	-2.080708	-0.022862	-0.000097
1	-0.435210	2.222419	-0.000169
1	2.087517	1.562557	-0.000002

4

Eelec = -913.4738793, -913.3692408
E = -913.309017
H = -913.297223
G = -913.346908
Nimag = 0

6	3.710267	1.021776	0.098702
6	2.344922	1.254316	0.075178
6	1.453907	0.186065	-0.012619
6	1.939842	-1.121035	-0.082021
6	3.301759	-1.349268	-0.058984
6	4.186776	-0.279087	0.031896
1	4.399906	1.851358	0.166807
1	1.963589	2.266353	0.124341
1	1.239206	-1.940756	-0.157948
1	3.680655	-2.360274	-0.114679
1	5.252493	-0.463179	0.048182
6	0.029531	0.473846	-0.029315
7	-0.851300	-0.449195	-0.067059
1	-0.262365	1.527261	-0.002121
16	-2.443146	0.055159	-0.125594
8	-3.017501	-0.490510	-1.339683
8	-2.558058	1.487020	0.110063
6	-3.111961	-0.803473	1.259254
1	-4.176779	-0.585874	1.274071
1	-2.938733	-1.865785	1.121797
1	-2.634320	-0.438194	2.162880

PRC(1+2)

Eelec = -957.4281781, -957.2909874
E = -957.089445
H = -957.068483
G = -957.14698
Nimag = 0

6	1.230606	-0.790924	1.935013
6	-0.082354	-1.071204	1.944671
7	-0.448982	-1.244827	0.621769
6	0.589342	-1.083405	-0.235266
7	1.617009	-0.802740	0.605447
1	1.914470	-0.627777	2.747569
1	-0.764961	-1.192490	2.765787
6	-1.974187	2.626723	-1.794769
6	-2.706191	2.768652	-0.686728
6	-1.820601	2.841973	0.478488
6	-0.394155	2.771088	-0.021139
6	-0.503319	2.586243	-1.532281
1	-2.380443	2.535105	-2.794102
1	0.120235	3.692890	0.260413
1	0.122007	1.948199	0.476695
1	0.013835	3.366334	-2.097612
1	-0.086517	1.629637	-1.863097
8	-2.156698	2.939341	1.641164
1	-3.783479	2.809650	-0.614154
6	-1.766024	-1.548635	0.203431
6	-2.850255	-1.011264	0.883322
6	-4.138293	-1.327008	0.477866
6	-4.346904	-2.162247	-0.609113
6	-3.256020	-2.684369	-1.290747
6	-1.965488	-2.386269	-0.885407
1	-2.693994	-0.328450	1.707218
1	-4.979560	-0.903402	1.008969
1	-5.352395	-2.403500	-0.924786
1	-3.408233	-3.337780	-2.138890
1	-1.108601	-2.792388	-1.402047
6	2.932216	-0.533920	0.161499
6	3.733678	0.358994	0.860401
6	5.026359	0.609426	0.424825
6	5.517109	-0.015378	-0.711300
6	4.705256	-0.898457	-1.410119
6	3.417589	-1.165684	-0.975844
1	3.347477	0.873758	1.729027
1	5.645244	1.306661	0.972659
1	6.523771	0.184626	-1.050888
1	5.078811	-1.392913	-2.296345
1	2.779534	-1.855940	-1.507054

TS(2-3)

Eelec = -957.402601, -957.2709827
E = -957.062225
H = -957.043337
G = -957.110482
Nimag = 1(-350.9780)

6	-0.904086	-1.600974	-1.692054
6	0.435775	-1.700648	-1.675707
7	0.863444	-1.052731	-0.536280
6	-0.165416	-0.530865	0.159242
7	-1.254095	-0.891961	-0.557336
1	-1.632539	-1.996767	-2.376114
1	1.116235	-2.199448	-2.342106
6	0.142064	1.171885	1.212933
6	1.357405	1.743319	0.818973
6	1.159277	2.690185	-0.214123
6	-0.335336	2.785069	-0.481801
6	-0.968711	2.067325	0.700835
1	0.020420	0.704025	2.182898
1	-0.644166	3.825193	-0.591790
1	-0.554045	2.277296	-1.427411
1	-1.192803	2.779235	1.500702
1	-1.897609	1.554822	0.466978
8	1.998697	3.359013	-0.827578
1	2.332588	1.470088	1.190849
6	2.220077	-1.017703	-0.122916
6	3.194895	-0.576589	-1.003310
6	4.519087	-0.564938	-0.596409
6	4.861990	-0.984954	0.680975
6	3.876855	-1.425876	1.553041
6	2.551117	-1.452476	1.150221
1	2.914790	-0.208536	-1.980629
1	5.280901	-0.204581	-1.273326
1	5.895636	-0.965060	0.997252
1	4.140322	-1.757533	2.547824
1	1.773344	-1.805440	1.812808
6	-2.596418	-0.688616	-0.151999
6	-3.545998	-0.301137	-1.086045
6	-4.860775	-0.120871	-0.685837
6	-5.222249	-0.316063	0.639253
6	-4.263906	-0.702154	1.565722
6	-2.950175	-0.899731	1.172703
1	-3.254594	-0.117857	-2.111235
1	-5.600802	0.186633	-1.411537
1	-6.247386	-0.168335	0.948947
1	-4.540422	-0.861633	2.598742
1	-2.197714	-1.216488	1.880896

3

Eelec = -957.4307446, -957.2949845
E = -957.089099
H = -957.070188
G = -957.136608
Nimag = 0

6	-1.111457	-2.279684	-0.738481
6	0.229467	-2.366563	-0.758096
7	0.724069	-1.182952	-0.251332
6	-0.288846	-0.371514	0.075392
7	-1.415757	-1.043987	-0.215666
1	-1.877005	-2.974064	-1.034087
1	0.888559	-3.151481	-1.081572
6	-0.264064	1.015605	0.653689
6	1.062309	1.504703	1.115457
6	1.602745	2.456131	0.277787
6	0.617872	2.718898	-0.860867
6	-0.681416	2.067216	-0.414694
1	-1.034893	0.987203	1.449495
1	0.515311	3.788925	-1.041817
1	1.013929	2.281441	-1.783156
1	-1.316709	2.801314	0.088449
1	-1.267452	1.640107	-1.234943
8	2.714830	3.042689	0.316310
1	1.570600	1.104665	1.980371
6	2.139479	-0.995716	-0.093853
6	2.850779	-0.247841	-1.014069
6	4.225445	-0.157746	-0.884931
6	4.877774	-0.831424	0.138410
6	4.153719	-1.598092	1.038426
6	2.775098	-1.688770	0.922113
1	2.332896	0.282612	-1.799326
1	4.784498	0.455925	-1.576512
1	5.951047	-0.750111	0.238414
1	4.658497	-2.121395	1.838446
1	2.195080	-2.272579	1.623662
6	-2.752299	-0.578780	-0.025598
6	-3.509875	-0.239705	-1.134408
6	-4.820777	0.174759	-0.955381
6	-5.358230	0.250852	0.321181
6	-4.589312	-0.096274	1.423029
6	-3.280993	-0.520609	1.253191
1	-3.074322	-0.294875	-2.122740
1	-5.418671	0.443961	-1.814773
1	-6.378846	0.580191	0.458293
1	-5.008322	-0.041754	2.418028
1	-2.675518	-0.805680	2.102485

PRC(3+4)

Eelec = -1870.9177302, -1870.6810142
E = -1870.410446
H = -1870.378418
G = -1870.47864
Nimag = 0

6	-3.268647	2.102683	-1.759103
6	-3.833386	0.883738	-1.710715
7	-3.131422	0.160499	-0.773768
6	-2.153467	0.912895	-0.247244
7	-2.232584	2.107489	-0.849416
1	-3.498372	2.971994	-2.347918
1	-4.657941	0.456563	-2.251875
6	-1.199042	0.448725	0.792016
6	0.144563	1.101966	0.787436
6	0.607757	1.330594	2.060392
6	-0.468728	0.911962	3.057570
6	-1.728890	0.730637	2.223870
1	-1.142495	-0.653726	0.649894
1	-0.158191	-0.021588	3.535063
1	-0.580946	1.655814	3.847141
1	-2.385896	-0.071019	2.574732
1	-2.307351	1.660138	2.221118
8	1.731659	1.754522	2.458391
1	0.735712	1.231259	-0.107810
6	5.076624	1.486864	0.318490
6	3.986865	0.652749	0.525345
6	3.913581	-0.560014	-0.160621
6	4.927918	-0.931034	-1.049177
6	6.008392	-0.095475	-1.244961
6	6.082658	1.115223	-0.559166
1	5.132313	2.427621	0.848407
1	3.196328	0.956548	1.210249
1	4.851940	-1.872534	-1.575010
1	6.795731	-0.379521	-1.929528
1	6.931533	1.767863	-0.714823
6	2.766697	-1.417083	0.079286
1	2.024121	-1.059357	0.798036
7	2.629451	-2.539320	-0.524628
16	1.264290	-3.417007	-0.182199
8	0.507052	-2.861974	0.929560
8	0.561597	-3.626542	-1.439047
6	1.972538	-4.948902	0.325594
1	2.598271	-5.322812	-0.478113
1	2.550037	-4.782647	1.229634
1	1.146130	-5.627466	0.519244
6	-3.448627	-1.189592	-0.423124
6	-4.506503	-1.422037	0.441027
6	-4.848514	-2.729251	0.750026
6	-4.132679	-3.782941	0.199618
6	-3.073876	-3.533871	-0.661473
6	-2.728924	-2.231077	-0.984195
1	-5.049264	-0.588757	0.865960
1	-5.670675	-2.922381	1.424833
1	-4.397879	-4.801510	0.447223
1	-2.504283	-4.349688	-1.083048

1	-1.899145	-2.029249	-1.647124
6	-1.406403	3.263418	-0.665452
6	-1.557945	4.055282	0.458656
6	-0.793781	5.203693	0.578517
6	0.098414	5.557102	-0.423878
6	0.224289	4.764119	-1.554404
6	-0.534678	3.611662	-1.682465
1	-2.251577	3.768308	1.234841
1	-0.889067	5.817958	1.462676
1	0.699138	6.449929	-0.320667
1	0.921056	5.035067	-2.335172
1	-0.435680	2.974375	-2.550513

TS(3-5)

Eelec = -1870.911446, -1870.6842367
E = -1870.403962
H = -1870.373257
G = -1870.46782
Nimag = 1(-125.7747)

6	-2.213613	2.818940	-1.207638
6	-3.282745	2.046373	-0.956596
7	-2.841941	1.001546	-0.179288
6	-1.523455	1.118202	0.047659
7	-1.135316	2.237150	-0.575550
1	-2.104141	3.725479	-1.774002
1	-4.310123	2.127127	-1.261435
6	-0.738045	0.148975	0.867719
6	0.752481	0.324769	0.930963
6	1.206873	0.299114	2.255030
6	0.054968	-0.136127	3.151932
6	-1.189238	0.215622	2.356036
1	-1.030643	-0.843971	0.457663
1	0.131186	-1.212151	3.336111
1	0.104065	0.362200	4.119207
1	-2.043688	-0.436565	2.553256
1	-1.491032	1.242374	2.593599
8	2.346836	0.514161	2.702785
1	1.346263	0.724925	0.124397
6	4.657070	-1.954841	2.032657
6	3.345060	-2.004009	1.590400
6	3.016921	-1.577001	0.306175
6	4.022396	-1.076158	-0.524280
6	5.327216	-1.014969	-0.076388
6	5.649108	-1.459985	1.202402
1	4.899213	-2.286814	3.032425
1	2.569324	-2.379402	2.243027
1	3.763626	-0.746109	-1.520123
1	6.101019	-0.624740	-0.723477

1	6.672391	-1.412967	1.549643
6	1.648754	-1.721305	-0.168582
1	0.956393	-2.259876	0.474438
7	1.387860	-1.547909	-1.440044
16	-0.051759	-2.014590	-2.009859
8	-0.773807	-2.910012	-1.101897
8	-0.804425	-0.851481	-2.481673
6	0.419459	-2.948792	-3.430580
1	1.011075	-2.311827	-4.079757
1	0.993967	-3.809768	-3.104189
1	-0.495099	-3.261338	-3.926936
6	-3.720016	-0.010701	0.318784
6	-4.642300	0.337749	1.293507
6	-5.526496	-0.621802	1.759545
6	-5.477534	-1.914028	1.254683
6	-4.551094	-2.245145	0.276933
6	-3.669715	-1.289468	-0.206627
1	-4.657711	1.345228	1.686553
1	-6.247547	-0.360959	2.521587
1	-6.163420	-2.663710	1.624472
1	-4.509944	-3.250424	-0.118333
1	-2.945093	-1.536124	-0.968909
6	0.166018	2.829217	-0.665417
6	0.656203	3.576929	0.390156
6	1.892006	4.188512	0.259363
6	2.612980	4.058714	-0.919340
6	2.100604	3.315991	-1.972820
6	0.866554	2.695806	-1.851154
1	0.089358	3.659053	1.306370
1	2.296958	4.755464	1.085492
1	3.580565	4.531886	-1.012857
1	2.664769	3.207781	-2.888533
1	0.460849	2.088313	-2.648613

5

Eelec = -1870.9653798, -1870.7372778
E = -1870.457494
H = -1870.427234
G = -1870.51978
Nimag = 0

6	-1.763556	2.265065	-1.913312
6	-2.794122	1.418988	-1.750631
7	-2.548888	0.714197	-0.596360
6	-1.376598	1.092410	-0.072098
7	-0.906151	2.071350	-0.852641
1	-1.543882	2.980096	-2.684630
1	-3.667405	1.234595	-2.348732
6	-0.853934	0.542842	1.202665

6	0.633089	0.184507	1.283667
6	0.871390	0.108791	2.779659
6	-0.300441	0.721792	3.513230
6	-1.114491	1.420790	2.437400
1	-1.406257	-0.396648	1.345426
1	-0.863487	-0.102901	3.961132
1	0.041296	1.361116	4.325323
1	-2.179008	1.493014	2.676267
1	-0.730034	2.432200	2.269344
8	1.844906	-0.351038	3.318711
1	1.249783	1.041687	0.937023
6	4.197068	-2.973261	1.167998
6	2.855901	-2.618753	1.105133
6	2.459926	-1.412196	0.542774
6	3.441364	-0.567882	0.030732
6	4.781713	-0.911594	0.096141
6	5.166209	-2.118704	0.666745
1	4.482869	-3.918487	1.609864
1	2.104551	-3.291518	1.498129
1	3.147382	0.362528	-0.435115
1	5.530404	-0.239407	-0.302164
1	6.212087	-2.390006	0.715989
6	0.991024	-1.049882	0.448009
1	0.398750	-1.932043	0.879635
7	0.561436	-0.721983	-0.893613
16	0.180794	-1.889149	-1.861221
8	-0.502799	-3.020437	-1.193757
8	-0.549234	-1.315969	-3.002920
6	1.648220	-2.609922	-2.570613
1	2.186658	-1.831899	-3.102566
1	2.264704	-3.016644	-1.775040
1	1.339904	-3.396084	-3.254108
6	-3.474371	-0.223326	-0.034591
6	-4.512480	0.268576	0.742855
6	-5.439606	-0.616522	1.269656
6	-5.319912	-1.976230	1.016045
6	-4.277249	-2.450687	0.233972
6	-3.345118	-1.575053	-0.304679
1	-4.593148	1.331802	0.924674
1	-6.253851	-0.243898	1.875386
1	-6.043003	-2.666725	1.428066
1	-4.180370	-3.508823	0.034794
1	-2.523875	-1.941768	-0.904978
6	0.306868	2.820386	-0.728304
6	0.329815	3.950368	0.073147
6	1.486972	4.712642	0.131225
6	2.593983	4.352007	-0.623262
6	2.547448	3.229665	-1.438810
6	1.399641	2.454509	-1.497803
1	-0.549729	4.234270	0.634188

1	1.517985	5.592937	0.757931
1	3.493797	4.950013	-0.579085
1	3.408914	2.951903	-2.030245
1	1.341996	1.555720	-2.096664

5’

Eelec = -1870.9653799, -1870.7372757
E = -1870.457499
H = -1870.427233
G = -1870.519822
Nimag = 0

6	-2.794584	1.419326	-1.750523
6	-1.763892	2.265210	-1.913380
7	-0.906311	2.071278	-0.852888
6	-1.376760	1.092375	-0.072301
7	-2.549212	0.714386	-0.596367
1	-3.668028	1.235127	-2.348447
1	-1.544263	2.980279	-2.684673
6	-0.854018	0.542776	1.202407
6	0.633051	0.184693	1.283374
6	0.871584	0.109282	2.779322
6	-0.300347	0.722018	3.512945
6	-1.114616	1.420771	2.437123
1	-1.406259	-0.396763	1.345161
1	-0.863165	-0.102806	3.960893
1	0.041261	1.361445	4.325008
1	-2.179118	1.492841	2.676075
1	-0.730337	2.432227	2.268957
8	1.845350	-0.350146	3.318248
1	1.249568	1.041896	0.936502
6	0.991142	-1.049825	0.448003
7	0.561429	-0.722358	-0.893703
1	0.399020	-1.931966	0.879876
16	0.181003	-1.890015	-1.860835
8	-0.501368	-3.021656	-1.192754
8	-0.549972	-1.317617	-3.002320
6	1.648562	-2.609963	-2.570780
1	1.340460	-3.396546	-3.253885
1	2.186210	-1.831736	-3.103236
1	2.265707	-3.016020	-1.775379
6	2.460083	-1.411945	0.542926
6	2.856154	-2.618496	1.105235
6	4.197365	-2.972810	1.168265
6	5.166465	-2.118034	0.667304
6	4.781885	-0.910895	0.096824
6	3.441495	-0.567387	0.031241
1	2.104832	-3.291432	1.497986
1	4.483237	-3.918053	1.610046

1	6.212375	-2.389188	0.716681
1	5.530539	-0.238522	-0.301235
1	3.147469	0.363054	-0.434518
6	-3.474679	-0.223114	-0.034530
6	-3.346233	-1.574699	-0.305678
6	-4.278281	-2.450348	0.233081
6	-5.320109	-1.976020	1.016339
6	-5.439045	-0.616442	1.270994
6	-4.511986	0.268653	0.744071
1	-2.525677	-1.941308	-0.906992
1	-4.181987	-3.508379	0.033079
1	-6.043139	-2.666511	1.428469
1	-6.252656	-0.243915	1.877634
1	-4.592094	1.331782	0.926688
6	0.306753	2.820258	-0.728671
6	0.329852	3.950212	0.072809
6	1.487031	4.712464	0.130705
6	2.593896	4.351843	-0.624003
6	2.547202	3.229528	-1.439578
6	1.399376	2.454381	-1.498370
1	-0.549587	4.234115	0.634011
1	1.518173	5.592734	0.757437
1	3.493721	4.949841	-0.579975
1	3.408555	2.951774	-2.031178
1	1.341632	1.555600	-2.097235

TS(5-6)

Eelec = -1870.9005329, -1870.670304
E = -1870.3912809
H = -1870.3609539
G = -1870.4543069
Nimag = 1(-1810.5403)

6	-3.262908	-1.233933	0.462925
6	-3.331789	0.057941	-0.025649
6	-4.384244	0.480389	-0.823907
6	-5.371764	-0.425609	-1.172907
6	-5.303639	-1.734599	-0.714639
6	-4.257161	-2.132780	0.102650
7	-2.351694	1.027012	0.377234
6	-2.553960	1.823632	1.480526
6	-1.501983	2.654700	1.569312
7	-0.674016	2.356887	0.514214
6	-1.189652	1.352435	-0.207648
6	-0.506504	0.736616	-1.384823
6	0.047183	-0.655676	-1.122649
6	0.046406	-1.368389	-2.377201
6	-0.711000	-0.554300	-3.410937
6	-1.392581	0.557051	-2.631130

6	0.564246	3.034759	0.285263
6	1.637669	2.756068	1.115003
6	2.826887	3.442169	0.917890
6	2.930781	4.386147	-0.093498
6	1.842989	4.656031	-0.912553
6	0.646733	3.982766	-0.721731
6	1.111982	-0.843331	-0.038002
6	2.454352	-1.401847	-0.428468
6	3.445859	-0.532338	-0.874740
6	4.695808	-1.005978	-1.244514
6	4.975325	-2.362601	-1.162371
6	3.994410	-3.234902	-0.711954
6	2.743683	-2.758144	-0.349332
8	0.559916	-2.448627	-2.633091
7	0.295823	-1.701903	0.846094
16	0.243563	-1.397009	2.419329
6	1.429832	-2.452659	3.205517
8	0.655202	-0.020155	2.731393
8	-1.075480	-1.807585	2.903471
1	-1.255132	3.417995	2.280394
1	-3.422733	1.707855	2.098094
1	0.303473	1.429029	-1.630265
1	0.038270	-0.160963	-4.101312
1	-1.392906	-1.171938	-3.989828
1	-1.492305	1.485928	-3.189227
1	-2.386715	0.232372	-2.344231
1	-0.551811	-1.409821	-0.070766
1	1.290925	0.123216	0.435272
1	1.392849	-2.257312	4.272963
1	1.160696	-3.481035	2.991679
1	2.413224	-2.223675	2.808085
1	3.239641	0.528858	-0.927253
1	5.452567	-0.315635	-1.588986
1	5.948359	-2.736398	-1.446358
1	4.200658	-4.293836	-0.650745
1	1.974331	-3.436239	-0.014179
1	1.535965	2.004443	1.885252
1	3.673463	3.230811	1.553288
1	3.860551	4.913929	-0.243996
1	1.922305	5.393577	-1.696648
1	-0.212810	4.188435	-1.342161
1	-4.421313	1.502730	-1.170225
1	-6.191555	-0.109005	-1.799730
1	-6.072189	-2.441535	-0.989118
1	-4.209344	-3.145866	0.471531
1	-2.465136	-1.528512	1.129637

6

Eelec = -1870.9595004, -1870.7295888

E = -1870.450919
H = -1870.420537
G = -1870.514267
Nimag = 0

6	-1.716450	3.032918	-1.309706
6	-0.576208	3.311264	-0.574814
6	-0.554133	4.327148	0.367844
6	-1.707192	5.061631	0.593489
6	-2.859689	4.788109	-0.129864
6	-2.862738	3.779146	-1.081620
7	0.616310	2.570953	-0.844529
6	1.165218	1.613940	-0.079899
7	2.280471	1.225236	-0.712388
6	2.428647	1.936027	-1.881571
6	1.385426	2.779029	-1.968628
6	0.558518	1.069115	1.177652
6	0.187038	-0.374843	1.055063
6	0.906599	-1.181031	1.903267
6	1.871165	-0.343899	2.718265
6	1.503337	1.105650	2.408625
6	-0.842041	-0.865983	0.084487
6	-2.214275	-1.060439	0.704406
6	-3.330805	-0.426341	0.173804
6	-4.590629	-0.608805	0.734640
6	-4.745572	-1.440310	1.831337
6	-3.633149	-2.080843	2.368347
6	-2.378878	-1.889969	1.814489
8	0.847384	-2.441124	2.023529
6	3.250734	0.258993	-0.288801
6	4.427458	0.717546	0.281381
6	5.409843	-0.197894	0.626552
6	5.204039	-1.551240	0.400199
6	4.021375	-1.991851	-0.176797
6	3.035132	-1.085651	-0.533236
7	-0.313114	-2.092520	-0.530542
16	-0.955858	-2.758119	-1.855498
8	0.009310	-3.726642	-2.350583
6	-2.410183	-3.672362	-1.425158
8	-1.373465	-1.666355	-2.725619
1	-0.954818	-0.120810	-0.761355
1	1.112319	3.503683	-2.713784
1	3.261686	1.762681	-2.538462
1	-0.318199	1.722219	1.359641
1	1.771669	-0.582623	3.777650
1	2.894291	-0.594486	2.430104
1	0.944328	1.543399	3.239994
1	2.378083	1.741474	2.241593
1	0.101627	-2.749175	0.145722
1	-3.218570	0.209944	-0.694712

1	-5.448273	-0.105686	0.308135
1	-5.723647	-1.589797	2.268405
1	-3.745572	-2.728941	3.227440
1	-1.508861	-2.378052	2.235242
1	-1.704722	2.241036	-2.046813
1	-3.759517	3.566638	-1.646633
1	-3.757193	5.363911	0.048516
1	-1.702786	5.850300	1.332746
1	0.353945	4.532907	0.917768
1	4.570572	1.776337	0.449585
1	6.331322	0.147276	1.074094
1	5.966801	-2.266051	0.676490
1	3.855779	-3.045993	-0.347388
1	2.106372	-1.419002	-0.972673
1	-2.788670	-4.114730	-2.342881
1	-2.130744	-4.446538	-0.716991
1	-3.140525	-2.997047	-0.992393

6’

Eelec = -1870.9594943, -1870.7296006
E = -1870.450931
H = -1870.420498
G = -1870.514193
Nimag = 0

6	-2.286843	-3.765992	-1.370199
16	-0.858663	-2.825818	-1.831535
8	-1.311027	-1.760800	-2.717169
7	-0.220231	-2.121487	-0.525012
6	-0.775923	-0.901661	0.076208
6	-2.140868	-1.114140	0.706216
6	-3.268775	-0.494448	0.182844
6	-4.520948	-0.686669	0.757533
6	-4.656223	-1.513294	1.860466
6	-3.532029	-2.139567	2.390101
6	-2.285431	-1.938860	1.822694
6	0.243146	-0.377487	1.039504
6	0.541228	1.081851	1.177188
6	1.495861	1.153015	2.399367
6	1.929493	-0.281001	2.696896
6	0.997065	-1.155807	1.883431
6	1.102039	1.667964	-0.081111
7	0.488020	2.586184	-0.844103
6	1.233917	2.834705	-1.976342
6	2.327747	2.057963	-1.894791
7	2.233414	1.345130	-0.721546
6	-0.756245	3.235155	-0.579061
6	-1.822260	2.994139	-1.430284
6	-3.023222	3.650755	-1.209351

6	-3.150290	4.531333	-0.145471
6	-2.073525	4.764924	0.698453
6	-0.865613	4.121988	0.480885
6	3.257347	0.432996	-0.304154
6	4.411923	0.954070	0.256971
6	5.441866	0.091768	0.600770
6	5.304099	-1.271486	0.382221
6	4.142613	-1.775073	-0.186347
6	3.109398	-0.922265	-0.541465
8	0.988830	-2.417590	2.003103
8	0.124631	-3.780188	-2.318072
1	-0.910165	-0.169388	-0.778810
1	0.913783	3.541068	-2.720327
1	3.165418	1.935228	-2.557195
1	-0.368345	1.678222	1.381714
1	1.848740	-0.530206	3.755443
1	2.960607	-0.483258	2.399535
1	0.926989	1.561465	3.238988
1	2.340660	1.826908	2.228045
1	0.226046	-2.754364	0.154256
1	-3.171269	0.138699	-0.689804
1	-5.387885	-0.194500	0.337086
1	-5.628249	-1.669931	2.308405
1	-3.629468	-2.783428	3.254191
1	-1.406360	-2.414685	2.238859
1	-1.713386	2.295428	-2.249355
1	-3.861181	3.465962	-1.866860
1	-4.090036	5.037203	0.027109
1	-2.170268	5.453389	1.526170
1	-0.014685	4.305275	1.122364
1	4.501295	2.019557	0.419949
1	6.346814	0.485731	1.041688
1	6.103523	-1.945116	0.658395
1	4.029985	-2.837257	-0.350124
1	2.195911	-1.304102	-0.973195
1	-2.661625	-4.236512	-2.275328
1	-1.983325	-4.518134	-0.648291
1	-3.030083	-3.099581	-0.945640

TS(6-7)

Eelec = -1870.9247914, -1870.6991391
E = -1870.418052
H = -1870.38762
G = -1870.481247
Nimag = 1(-332.3445)

6	2.800827	-2.780055	2.065627
16	1.287117	-1.878699	2.237900
8	1.631590	-0.546567	2.709206

7	0.590974	-1.712475	0.783884
6	1.043184	-0.727158	-0.201426
6	2.358760	-1.087659	-0.864587
6	3.439688	-0.217090	-0.779507
6	4.654330	-0.529433	-1.377820
6	4.801646	-1.723421	-2.065669
6	3.726046	-2.599010	-2.156439
6	2.514386	-2.284267	-1.563263
6	-0.069923	-0.501375	-1.180166
6	-0.520154	0.739073	-1.609862
6	-1.497913	0.559650	-2.742816
6	-1.864013	-0.921158	-2.701395
6	-0.846111	-1.539811	-1.770994
6	-1.520332	1.599131	0.003290
7	-0.742648	2.297634	0.865099
6	-1.050047	2.010937	2.182609
6	-2.052320	1.117484	2.148547
7	-2.330010	0.891191	0.815724
6	0.251193	3.221055	0.464248
6	1.459937	3.273345	1.145618
6	2.425365	4.185755	0.749051
6	2.194399	5.029018	-0.328319
6	0.986004	4.963634	-1.007045
6	0.007085	4.067343	-0.608416
6	-3.353117	0.020295	0.363722
6	-4.353549	0.516707	-0.458448
6	-5.363731	-0.329977	-0.886094
6	-5.374223	-1.659392	-0.486227
6	-4.371898	-2.142957	0.342515
6	-3.354197	-1.304704	0.771379
8	-0.723972	-2.757549	-1.596929
8	0.392881	-2.707905	3.028133
1	1.205716	0.235011	0.378882
1	-0.550160	2.476448	3.012067
1	-2.604222	0.644905	2.940972
1	0.124212	1.607061	-1.611314
1	-1.816032	-1.409869	-3.676096
1	-2.864119	-1.099830	-2.299860
1	-0.981789	0.807772	-3.674770
1	-2.354893	1.225556	-2.657141
1	0.194617	-2.575442	0.399723
1	3.333317	0.712462	-0.234641
1	5.484922	0.159244	-1.299809
1	5.746562	-1.972057	-2.529408
1	3.831339	-3.530668	-2.696232
1	1.675496	-2.962135	-1.648176
1	1.650977	2.593386	1.965628
1	3.366879	4.226713	1.279234
1	2.952826	5.734760	-0.637227
1	0.796729	5.620973	-1.844439

1	-0.947141	4.020257	-1.114293
1	-4.336615	1.558291	-0.747129
1	-6.147482	0.051471	-1.525934
1	-6.163331	-2.318562	-0.820688
1	-4.370191	-3.180321	0.646379
1	-2.553067	-1.676302	1.396169
1	3.228406	-2.872242	3.060606
1	2.574947	-3.760344	1.657306
1	3.468094	-2.231405	1.408876

7+1

Eelec = -1870.943199, -1870.7082205
E = -1870.437931
H = -1870.405783
G = -1870.507516
Nimag = 0

6	3.873166	-0.738225	2.530344
16	2.128113	-0.457104	2.447487
8	1.928828	0.979957	2.362926
7	1.555227	-1.109721	1.074725
6	1.728922	-0.470141	-0.224181
6	3.116175	-0.625699	-0.816920
6	3.821824	0.504005	-1.215082
6	5.093006	0.390054	-1.762439
6	5.672876	-0.859629	-1.915734
6	4.973782	-1.993371	-1.521607
6	3.704513	-1.878165	-0.977173
6	0.658173	-0.978439	-1.145637
6	-0.083480	-0.260987	-1.997190
6	-1.049515	-1.077656	-2.786237
6	-0.826503	-2.501351	-2.285882
6	0.260476	-2.388637	-1.248519
6	-2.721694	1.231079	-0.183581
7	-1.886677	2.022312	0.536535
6	-1.662473	1.536772	1.814224
6	-2.374459	0.404420	1.913530
7	-3.009002	0.238809	0.693781
6	-1.292854	3.194765	0.016017
6	-0.048474	3.609288	0.473867
6	0.522108	4.765012	-0.039749
6	-0.132833	5.499741	-1.016007
6	-1.372083	5.072738	-1.474149
6	-1.957630	3.928519	-0.958781
6	-3.837932	-0.860709	0.375983
6	-4.918872	-0.684239	-0.478024
6	-5.725808	-1.764967	-0.793426
6	-5.469997	-3.017824	-0.252527
6	-4.391504	-3.185120	0.602830

6	-3.568917	-2.112445	0.913915
8	0.719349	-3.310282	-0.598735
8	1.525930	-1.207264	3.533905
1	1.539709	0.638894	-0.058817
1	-1.042156	2.031821	2.538315
1	-2.499073	-0.268213	2.742175
1	-0.015296	0.813533	-2.114704
1	-0.498938	-3.190692	-3.067414
1	-1.715331	-2.936449	-1.823188
1	-0.859750	-0.969150	-3.857917
1	-2.067441	-0.719171	-2.608380
1	1.490443	-2.129242	1.091777
1	3.376963	1.483151	-1.089942
1	5.630127	1.279368	-2.063307
1	6.663671	-0.951751	-2.339228
1	5.418119	-2.972318	-1.641413
1	3.164328	-2.767293	-0.680267
1	0.482813	3.030199	1.216982
1	1.489301	5.083524	0.324596
1	0.316272	6.398500	-1.415148
1	-1.895225	5.640199	-2.231705
1	-2.924718	3.592668	-1.301494
1	-5.113839	0.297085	-0.884251
1	-6.567232	-1.622628	-1.457742
1	-6.107360	-3.856608	-0.495490
1	-4.176348	-4.157524	1.024126
1	-2.710817	-2.256015	1.556045
1	4.219403	-0.297643	3.461688
1	4.051398	-1.809133	2.527829
1	4.351521	-0.263278	1.679810

7

Eelec = -1182.8088437, -1182.6620322
E = -1182.54295
H = -1182.525434
G = -1182.589446
Nimag = 0

6	0.203837	1.697542	-1.047769
6	0.245426	1.194468	0.250882
6	0.727423	2.007794	1.270512
6	1.161588	3.299346	1.003561
6	1.119313	3.791268	-0.291689
6	0.639083	2.985680	-1.316105
6	-0.220659	-0.212934	0.574059
7	0.410777	-1.258195	-0.221825
16	1.929333	-1.765670	0.078249
8	2.115110	-2.967197	-0.711996
6	-1.709621	-0.358678	0.444954

6	-2.610373	-0.326601	1.432548
6	-4.020439	-0.477843	0.967048
6	-3.894804	-0.639385	-0.544971
6	-2.417160	-0.557317	-0.831154
8	-1.903628	-0.651324	-1.928773
6	3.066995	-0.559635	-0.541304
8	2.086913	-1.807462	1.520765
1	-2.361827	-0.204063	2.479779
1	-4.407866	0.143554	-1.107804
1	-4.273290	-1.596921	-0.909293
1	-4.614641	0.395352	1.251136
1	-4.490191	-1.341562	1.445814
1	0.141638	-1.325839	-1.204932
1	0.049088	-0.436862	1.655130
1	4.065225	-0.937146	-0.334975
1	2.915064	-0.456618	-1.611310
1	2.901930	0.384348	-0.032176
1	0.775448	1.624292	2.281842
1	1.538671	3.916471	1.807800
1	1.459600	4.795615	-0.503814
1	0.600853	3.363201	-2.329067
1	-0.175280	1.079912	-1.850741

(II) Bimolecular Pathway

PRC(4+5)

Eelec = -2784.4352383, -2784.1076807
E = -2783.759256
H = -2783.716383
G = -2783.840051
Nimag = 0

6	5.391186	-2.525052	-1.053860
6	4.247537	-1.921616	-0.524199
6	3.015425	-2.568431	-0.606560
6	2.928289	-3.814631	-1.207650
6	4.066982	-4.413176	-1.724475
6	5.298539	-3.767077	-1.649350
6	4.300485	-0.621924	0.122272
7	5.385215	0.052576	0.192735
16	5.293266	1.540787	0.931093
6	6.572313	1.387004	2.132932
8	5.694330	2.532388	-0.052668
8	4.025500	1.738879	1.616444
8	1.029969	-0.691536	1.910000
6	0.016978	-0.043642	1.833299
6	-0.863014	0.050293	0.604653
6	-1.938237	1.084659	0.999648
6	-1.343757	1.882577	2.172976
6	-0.540391	0.832702	2.924371
6	-2.445134	1.874303	-0.155406
7	-1.830977	2.839545	-0.851291
6	-2.638085	3.251769	-1.884161
6	-3.771022	2.531341	-1.813644
7	-3.638864	1.690946	-0.735244
6	-0.545147	3.432442	-0.621181
6	0.590153	2.824248	-1.126243
6	1.816835	3.440467	-0.922033
6	1.891446	4.646850	-0.242711
6	0.737168	5.256757	0.230032
6	-0.493836	4.650329	0.039379
6	-4.673994	0.789805	-0.330636
6	-4.882854	-0.365340	-1.065819
6	-5.923963	-1.204405	-0.694986
6	-6.730612	-0.887101	0.388377
6	-6.505631	0.276219	1.111979
6	-5.474631	1.128376	0.748636
6	-1.439569	-1.302961	0.063413
7	-0.609800	-1.883473	-0.963006
16	-0.872061	-1.297090	-2.388173
8	-0.309370	0.058588	-2.634794

6	-1.690029	-2.294010	1.178809
6	-0.739534	-3.250689	1.522259
6	-0.965238	-4.134031	2.565723
6	-2.151060	-4.082502	3.286881
6	-3.112820	-3.144580	2.945545
6	-2.882034	-2.262314	1.897638
6	0.036294	-2.397276	-3.430036
8	-2.291107	-1.354199	-2.823590
1	-2.461751	-1.047986	-0.353593
1	-4.654122	2.526315	-2.425856
1	-2.315745	4.009235	-2.575111
1	-2.804454	0.536218	1.384807
1	-1.193164	0.198429	3.534318
1	0.247676	1.225725	3.562579
1	-2.121858	2.353055	2.780415
1	-0.667576	2.664941	1.822169
1	-0.219620	0.443916	-0.198889
1	0.177344	-3.295422	0.954646
1	-0.211537	-4.868513	2.816790
1	-2.327660	-4.775573	4.098315
1	-4.051647	-3.107608	3.482167
1	-3.660024	-1.563528	1.616408
1	-4.221887	-0.613789	-1.887479
1	-6.091787	-2.115758	-1.251513
1	-7.536631	-1.549736	0.672175
1	-7.136141	0.525673	1.953978
1	-5.294806	2.047500	1.289831
1	-1.403613	5.107353	0.404593
1	0.794388	6.202260	0.751043
1	2.854401	5.111973	-0.083868
1	2.718067	2.975413	-1.295446
1	0.505599	1.894018	-1.673616
1	3.368773	-0.249284	0.556658
1	2.124409	-2.094132	-0.212878
1	1.969025	-4.309405	-1.271442
1	3.999272	-5.386386	-2.192130
1	6.181757	-4.237517	-2.058802
1	6.338670	-2.008505	-0.990713
1	6.642449	2.345538	2.640142
1	6.300405	0.602577	2.832307
1	7.499818	1.154267	1.620169
1	-0.082558	-2.037937	-4.447830
1	1.080570	-2.372881	-3.138161
1	-0.373156	-3.396015	-3.323626

TS(5-8)

Eelec = -2784.41364, -2784.1022305
E = -2783.737886
H = -2783.696514

G = -2783.812405
Nimag = 1(-249.7455)

6	3.944670	1.274499	-0.945568
6	3.840876	0.214353	-0.051431
6	4.856627	0.010725	0.878589
6	5.935421	0.877582	0.939805
6	6.025795	1.943248	0.053370
6	5.032398	2.132684	-0.895804
6	2.709533	-0.738962	-0.190405
7	1.295005	0.293329	0.749538
16	0.809352	-0.083525	2.228072
8	0.344590	1.112156	2.957225
6	0.208653	0.920768	-0.002384
6	0.603296	2.285861	-0.547339
6	1.463432	3.078332	0.209433
6	1.775804	4.370957	-0.176915
6	1.233476	4.908512	-1.336036
6	0.370356	4.135929	-2.095355
6	0.057248	2.842129	-1.699769
6	-0.503838	-0.040741	-0.974999
6	-2.035894	0.133878	-1.115160
6	-2.388502	-0.697051	-2.356765
6	-1.241225	-0.397377	-3.307945
6	-0.055495	-0.104788	-2.421401
6	-2.826941	-0.144019	0.113715
7	-3.351861	0.814964	0.893182
6	-3.970468	0.246542	1.979885
6	-3.835736	-1.084991	1.848445
7	-3.139456	-1.311432	0.686806
6	-3.388181	2.222444	0.634628
6	-2.657524	3.078835	1.439754
6	-2.742046	4.444277	1.213340
6	-3.548458	4.935941	0.198230
6	-4.281673	4.064815	-0.595759
6	-4.210431	2.698934	-0.375601
6	-2.923182	-2.644486	0.198002
6	-3.966139	-3.254769	-0.485701
6	-3.807130	-4.558928	-0.920834
6	-2.619261	-5.233848	-0.664609
6	-1.595864	-4.610762	0.031169
6	-1.744330	-3.305422	0.480842
8	1.069047	0.057410	-2.820099
8	-0.187931	-1.169036	2.255607
6	2.256509	-0.660719	3.040270
7	2.912751	-1.951302	0.317594
16	2.110876	-3.196992	-0.305660
8	1.124036	-2.807799	-1.318987
6	3.378979	-4.104879	-1.145239
8	1.629094	-4.060266	0.770289

1	-0.607123	1.189508	0.749705
1	-4.444460	0.845590	2.735751
1	-4.158894	-1.899490	2.470847
1	-2.231849	1.187445	-1.343434
1	-1.427252	0.499570	-3.906128
1	-1.006053	-1.204612	-3.999637
1	-3.369769	-0.438049	-2.763758
1	-2.387003	-1.762341	-2.117904
1	-0.314072	-1.070725	-0.602422
1	1.894400	2.658441	1.105975
1	2.453575	4.957902	0.428576
1	1.482665	5.914893	-1.644172
1	-0.060713	4.534379	-3.004085
1	-0.619995	2.277915	-2.323491
1	-2.016910	2.680933	2.217078
1	-2.163790	5.120135	1.827221
1	-3.605355	6.001355	0.023485
1	-4.916385	4.447866	-1.382573
1	-4.791338	2.008585	-0.972238
1	-4.881846	-2.710991	-0.674815
1	-4.608076	-5.047068	-1.458477
1	-2.494848	-6.251472	-1.008752
1	-0.666465	-5.122751	0.232707
1	-0.960839	-2.813036	1.039368
1	2.153663	-0.632335	-1.114073
1	3.169316	1.423984	-1.684329
1	5.101408	2.950612	-1.599986
1	6.873584	2.613875	0.094987
1	6.716139	0.712622	1.670209
1	4.806022	-0.844943	1.535841
1	2.925662	-5.010433	-1.538958
1	3.771536	-3.490279	-1.949247
1	4.157917	-4.346625	-0.429466
1	1.933923	-0.931875	4.041520
1	2.639140	-1.522244	2.501637
1	2.980160	0.146296	3.075584

8

Eelec = -2784.4354894, -2784.1262627
E = -2783.759266
H = -2783.71834
G = -2783.83139
Nimag = 0

6	3.789056	-1.825653	0.637430
6	3.576646	-0.722031	-0.184738
6	4.590415	-0.344541	-1.057072
6	5.765769	-1.078495	-1.144656
6	5.954683	-2.193029	-0.341271

6	4.963516	-2.558142	0.559666
6	2.286798	0.084559	-0.047086
7	1.143804	-0.667867	-0.666519
16	0.644987	-0.334419	-2.210008
8	0.033713	-1.563646	-2.721310
6	-0.018981	-1.055214	0.148693
6	0.136996	-2.444200	0.749811
6	0.936647	-3.381777	0.104206
6	1.008906	-4.691539	0.552631
6	0.271781	-5.098251	1.654380
6	-0.544859	-4.179658	2.294742
6	-0.612720	-2.870572	1.842175
6	-0.519670	0.074915	1.069688
6	-2.052652	0.289131	1.116618
6	-2.252666	1.205962	2.330623
6	-1.278170	0.641756	3.352540
6	-0.155739	0.038231	2.545146
6	-2.690145	0.722808	-0.158837
7	-3.359848	-0.106871	-0.974731
6	-3.792716	0.577916	-2.083264
6	-3.392410	1.852514	-1.930260
7	-2.724219	1.929081	-0.733934
6	-3.691875	-1.479048	-0.737108
6	-3.078140	-2.467622	-1.487834
6	-3.444761	-3.788441	-1.275620
6	-4.410565	-4.104542	-0.332214
6	-5.023946	-3.100254	0.404199
6	-4.670709	-1.776441	0.198972
6	-2.245211	3.185438	-0.230943
6	-3.171560	4.036103	0.356255
6	-2.751238	5.277320	0.802116
6	-1.421150	5.651482	0.654509
6	-0.513248	4.792624	0.055885
6	-0.923837	3.547976	-0.404534
8	0.860022	-0.408351	3.007972
8	-0.233492	0.830087	-2.268600
6	2.091192	-0.025669	-3.155205
7	2.382796	1.404358	-0.582487
16	2.666736	2.581372	0.407249
8	1.882214	2.506546	1.657072
6	4.362306	2.526149	0.951138
8	2.543720	3.842918	-0.334862
1	-0.856358	-1.211105	-0.590115
1	-4.340725	0.089652	-2.868183
1	-3.507095	2.716659	-2.558954
1	-2.515378	-0.678878	1.345309
1	-1.722449	-0.164756	3.943284
1	-0.884047	1.377610	4.051609
1	-3.289736	1.212803	2.676555
1	-1.965324	2.231560	2.087911

1	-0.054810	1.024288	0.715719
1	1.510188	-3.073946	-0.756475
1	1.648125	-5.394915	0.036060
1	0.332408	-6.117797	2.009827
1	-1.129039	-4.476932	3.155150
1	-1.263042	-2.187737	2.369069
1	-2.312208	-2.209933	-2.208022
1	-2.961916	-4.570130	-1.844800
1	-4.686497	-5.137050	-0.168705
1	-5.782802	-3.345299	1.134142
1	-5.151630	-0.980201	0.751070
1	-4.201621	3.724072	0.463809
1	-3.460113	5.949251	1.265717
1	-1.091633	6.618250	1.009621
1	0.527509	5.060494	-0.053664
1	-0.225302	2.879024	-0.890122
1	2.036011	0.073291	1.065183
1	3.030932	-2.106313	1.356391
1	5.108662	-3.408718	1.212276
1	6.873130	-2.761141	-0.402644
1	6.540499	-0.769153	-1.833818
1	4.461108	0.549289	-1.650029
1	4.522367	3.362115	1.626078
1	4.542425	1.586952	1.466295
1	5.007329	2.609568	0.082239
1	1.722113	0.075236	-4.173177
1	2.542077	0.891218	-2.792631
1	2.755666	-0.878506	-3.071026

8’

Eelec = -2784.4298727, -2784.1184941
E = -2783.754256
H = -2783.712969
G = -2783.828373
Nimag = 0

6	3.946931	0.149184	-0.399983
6	3.658913	1.492219	-0.239910
6	4.505619	2.348282	0.449637
6	5.654899	1.833667	1.025890
6	5.950062	0.482016	0.896131
6	5.103054	-0.352204	0.182912
7	2.497625	2.047355	-0.873545
6	1.265196	2.170393	-0.368372
7	0.535823	2.809416	-1.293287
6	1.309865	3.068638	-2.400314
6	2.538936	2.590682	-2.135742
6	0.730922	1.679644	0.932040
6	0.635132	0.137312	1.003498

6	1.423755	-0.266254	2.223497
6	2.177652	0.917185	2.775368
6	1.508895	2.148882	2.190089
6	-0.831638	-0.325471	0.814479
6	-1.768369	0.235755	1.871438
6	-2.972393	0.803977	1.461381
6	-3.843946	1.376749	2.371507
6	-3.524498	1.401154	3.721637
6	-2.324154	0.854146	4.144121
6	-1.453699	0.282927	3.225705
8	1.510700	-1.388498	2.658918
6	-0.826566	3.234887	-1.184860
6	-1.133907	4.321988	-0.380883
6	-2.445757	4.763214	-0.320194
6	-3.427401	4.130357	-1.069974
6	-3.101824	3.051155	-1.877762
6	-1.794197	2.592903	-1.939244
7	-0.967596	-1.751269	0.472578
16	-1.827356	-2.837028	1.372316
8	-3.089795	-2.269798	1.814488
6	-0.628952	-2.096394	-0.948017
6	-1.602364	-1.434811	-1.919570
6	-1.162641	-1.060403	-3.185278
6	-2.052217	-0.567836	-4.131364
6	-3.399433	-0.439578	-3.826428
6	-3.848224	-0.814864	-2.567403
6	-2.959144	-1.312515	-1.626100
7	0.727414	-1.764882	-1.240097
16	1.672596	-2.964469	-1.604352
6	1.936959	-3.977398	-0.161801
8	2.990545	-2.400693	-1.939558
8	1.107705	-3.889999	-2.598683
1	1.178404	-0.344741	0.167321
1	-1.131524	0.201481	-0.145810
1	0.909007	3.569372	-3.262775
1	3.440195	2.574764	-2.721650
1	-0.280165	2.093502	0.988656
1	2.180346	0.886333	3.864050
1	3.216053	0.811922	2.451141
1	0.777718	2.550178	2.898081
1	2.216535	2.950505	1.970159
1	-3.234136	0.783969	0.412273
1	-4.775910	1.802596	2.025507
1	-4.204911	1.842614	4.436903
1	-2.060158	0.866176	5.193047
1	-0.529648	-0.138279	3.593663
1	-1.532735	1.744844	-2.557792
1	-3.863954	2.552698	-2.459543
1	-4.449427	4.480339	-1.023888
1	-2.698183	5.606174	0.307645

1	-0.354593	4.816524	0.182877
1	4.268140	3.400519	0.528411
1	6.321986	2.488291	1.569199
1	6.849218	0.082604	1.344845
1	5.334814	-1.401000	0.060726
1	3.305469	-0.505310	-0.978120
1	2.635516	-4.765295	-0.429809
1	2.338035	-3.357903	0.634238
1	0.986826	-4.413684	0.134689
1	-3.334897	-1.612136	-0.656879
1	-4.898518	-0.736759	-2.318582
1	-4.095502	-0.067412	-4.566453
1	-1.690235	-0.298053	-5.114897
1	-0.115474	-1.179366	-3.421293
1	-0.839861	-3.211620	-1.052517
8	-1.885636	-4.070912	0.606237
6	-0.887351	-3.194895	2.821397
1	-1.448193	-3.970799	3.336459
1	0.095418	-3.542299	2.528320
1	-0.809211	-2.310083	3.438449

TS(8-9)

Eelec = -2784.4118198, -2784.1016433
E = -2783.74023
H = -2783.699254
G = -2783.814171
Nimag = 1(-1447.5148)

6	-4.043747	0.245053	0.172443
6	-3.696133	1.559535	-0.059668
6	-4.510660	2.413512	-0.789029
6	-5.691853	1.922765	-1.319144
6	-6.050113	0.596462	-1.107641
6	-5.229752	-0.236867	-0.364374
7	-2.509717	2.098709	0.538825
6	-1.259328	2.106471	0.059766
7	-0.531676	2.835045	0.922251
6	-1.324239	3.259301	1.964397
6	-2.562877	2.798791	1.721827
6	-0.706455	1.454118	-1.165548
6	-0.417457	-0.050011	-1.041987
6	-1.078283	-0.712921	-2.143528
6	-2.077969	0.225946	-2.789023
6	-1.571241	1.615994	-2.442536
6	1.040149	-0.330690	-0.653862
6	2.066856	0.117795	-1.685353
6	3.288633	0.622598	-1.246554
6	4.228639	1.107089	-2.139681
6	3.962846	1.099071	-3.501663

6	2.749151	0.606756	-3.954637
6	1.809293	0.125656	-3.052486
8	-0.942493	-1.879792	-2.496521
6	0.833925	3.245857	0.800273
6	1.186090	4.157727	-0.183747
6	2.493673	4.611166	-0.243241
6	3.426560	4.170256	0.684934
6	3.056404	3.267948	1.670487
6	1.753619	2.796916	1.732972
7	1.207047	-1.699020	-0.121059
16	2.290303	-2.819260	-0.649744
8	3.647039	-2.298247	-0.629425
6	0.482689	-1.944059	1.136986
6	1.044700	-1.117954	2.285158
6	0.201955	-0.582931	3.252243
6	0.721430	0.074243	4.360724
6	2.093093	0.204729	4.518044
6	2.941607	-0.328576	3.556203
6	2.422263	-0.984905	2.450896
7	-0.925275	-1.709025	0.927097
16	-1.871338	-2.997435	1.065680
6	-1.489056	-4.155697	-0.219455
8	-3.244477	-2.550120	0.839626
8	-1.603368	-3.693486	2.325005
1	-0.981923	-0.818206	-0.032620
1	1.236240	0.331948	0.247852
1	-0.928082	3.855223	2.766243
1	-3.482044	2.897929	2.270380
1	0.244251	1.972970	-1.334234
1	-2.123380	0.032479	-3.859554
1	-3.069146	0.021059	-2.380921
1	-0.906780	1.971701	-3.236323
1	-2.366024	2.355851	-2.339549
1	3.506934	0.626463	-0.187376
1	5.171513	1.488004	-1.771624
1	4.695703	1.473893	-4.203266
1	2.528545	0.593289	-5.013576
1	0.873869	-0.259935	-3.429895
1	1.457341	2.084804	2.490895
1	3.781122	2.919597	2.392867
1	4.444513	4.531685	0.638592
1	2.780185	5.316280	-1.010762
1	0.443737	4.512158	-0.885764
1	-4.221359	3.445155	-0.938002
1	-6.333051	2.575680	-1.894765
1	-6.972705	0.215655	-1.523828
1	-5.492773	-1.271260	-0.194602
1	-3.408421	-0.413004	0.745332
1	-2.178964	-4.987811	-0.108108
1	-1.612559	-3.660180	-1.176332

1	-0.466287	-4.496924	-0.087701
1	3.098117	-1.401666	1.715659
1	4.014212	-0.245692	3.671868
1	2.498777	0.705403	5.386981
1	0.048986	0.471019	5.109936
1	-0.864657	-0.707584	3.137588
1	0.678763	-3.028200	1.435878
8	2.034391	-4.019667	0.132687
6	1.889963	-3.191496	-2.326444
1	2.456702	-4.090035	-2.557723
1	0.820474	-3.346927	-2.407807
1	2.207089	-2.371066	-2.957991

9

Eelec = -2784.4325127, -2784.1231323
E = -2783.756748
H = -2783.715722
G = -2783.829711
Nimag = 0

6	-3.421208	1.789079	0.240614
6	-2.574410	2.847653	-0.028443
6	-2.999248	3.948570	-0.756701
6	-4.290970	3.966272	-1.256597
6	-5.143856	2.896731	-1.017064
6	-4.711287	1.813521	-0.267469
7	-1.262074	2.870794	0.549305
6	-0.091433	2.487105	0.014633
7	0.849991	2.814272	0.916226
6	0.267661	3.380750	2.028149
6	-1.054257	3.416932	1.795444
6	0.184379	1.780383	-1.283241
6	-0.179190	0.310963	-1.275377
6	-1.235104	0.054934	-2.135089
6	-1.674578	1.341215	-2.815500
6	-0.574248	2.344931	-2.503629
6	0.800772	-0.625194	-0.613886
6	2.138564	-0.685706	-1.356981
6	3.304373	-1.013780	-0.670641
6	4.531614	-1.025132	-1.309939
6	4.620249	-0.696548	-2.655951
6	3.470808	-0.351495	-3.348628
6	2.243281	-0.340757	-2.699268
8	-1.834051	-1.030746	-2.378165
6	2.269893	2.694652	0.797245
6	2.953895	3.487767	-0.111119
6	4.336595	3.416702	-0.157968
6	5.021438	2.577338	0.709346
6	4.324489	1.801515	1.622815

6	2.940100	1.854345	1.669900
7	0.271729	-1.957521	-0.233754
16	0.623002	-3.373442	-1.026566
8	2.018003	-3.740607	-0.846958
6	-0.507208	-2.051710	0.990107
6	0.262218	-1.534665	2.195638
6	-0.292765	-0.648534	3.107671
6	0.411661	-0.277462	4.247863
6	1.673488	-0.795290	4.491156
6	2.230011	-1.690797	3.585170
6	1.529496	-2.056860	2.448277
7	-1.801811	-1.400888	0.854848
16	-3.196205	-2.262803	0.956420
6	-3.401592	-3.168938	-0.541194
8	-4.257021	-1.269811	1.023580
8	-3.032397	-3.199305	2.054247
1	-1.833960	-0.733114	0.079959
1	1.074762	-0.164409	0.393802
1	0.855114	3.709733	2.865729
1	-1.873664	3.782600	2.387537
1	1.270885	1.916840	-1.435550
1	-1.779496	1.155105	-3.884736
1	-2.657335	1.644837	-2.452737
1	0.140772	2.378253	-3.331230
1	-0.933857	3.365934	-2.355656
1	3.246088	-1.278234	0.375477
1	5.421677	-1.295038	-0.757806
1	5.578269	-0.706677	-3.157983
1	3.525521	-0.087952	-4.396522
1	1.346687	-0.063055	-3.238001
1	2.385776	1.247905	2.374118
1	4.855099	1.144678	2.297720
1	6.100786	2.528424	0.671791
1	4.878803	4.025255	-0.867922
1	2.409682	4.155003	-0.765249
1	-2.327342	4.778758	-0.925575
1	-4.630930	4.816551	-1.831163
1	-6.149899	2.911206	-1.413010
1	-5.365207	0.976175	-0.070720
1	-3.091370	0.952205	0.837328
1	-4.376082	-3.647022	-0.487675
1	-3.335221	-2.464155	-1.366372
1	-2.602974	-3.901044	-0.604566
1	1.962052	-2.766109	1.753121
1	3.206482	-2.117310	3.772591
1	2.214336	-0.518726	5.386167
1	-0.040132	0.405315	4.955153
1	-1.290482	-0.272233	2.936026
1	-0.695131	-3.152777	1.212982
8	-0.359888	-4.346572	-0.565456

6	0.330731	-3.082179	-2.737016
1	0.232583	-4.073987	-3.171960
1	-0.584788	-2.493690	-2.823773
1	1.185554	-2.567440	-3.157281

9’

Eelec = -2784.4344534, -2784.1225679
E = -2783.758191
H = -2783.716802
G = -2783.832438
Nimag = 0

6	-5.143928	-1.799483	0.392999
6	-5.500236	-3.096394	0.727206
6	-4.866743	-4.171603	0.119988
6	-3.875642	-3.953066	-0.825642
6	-3.506270	-2.659254	-1.161279
6	-4.139527	-1.595116	-0.540421
7	-3.782733	-0.265362	-0.921638
6	-3.041881	0.607441	-0.222631
7	-2.984114	1.723695	-0.958068
6	-3.671465	1.543944	-2.135381
6	-4.171170	0.296823	-2.116853
6	-2.428147	0.323539	1.114817
6	-0.921451	0.324209	1.131134
6	-0.429997	1.353889	1.893663
6	-1.560539	2.173638	2.478503
6	-2.818842	1.362043	2.197041
6	-0.167464	-0.810295	0.507451
7	0.953725	-0.440236	-0.428660
6	2.330165	-0.201773	0.032866
6	3.365768	-0.949933	-0.778164
6	3.647573	-2.267673	-0.434561
6	4.544377	-3.018223	-1.179874
6	5.177034	-2.450167	-2.276659
6	4.915857	-1.128586	-2.610586
6	4.019481	-0.379687	-1.863839
8	0.778724	1.653482	2.133837
6	-2.359759	2.970673	-0.630392
6	-1.000518	3.138191	-0.824906
6	-0.431423	4.371028	-0.545331
6	-1.221574	5.420137	-0.097936
6	-2.587779	5.243986	0.071242
6	-3.164419	4.011728	-0.194800
6	0.283675	-1.899560	1.473778
6	0.459005	-3.198852	1.000868
6	0.822294	-4.232151	1.850170
6	1.023059	-3.980528	3.200616
6	0.848884	-2.693068	3.685834

6	0.474647	-1.663905	2.831709
16	0.575507	-0.333979	-2.025345
7	2.566714	1.240490	0.094166
16	3.885032	1.862919	0.867625
8	3.709181	3.302931	0.800197
8	5.093984	1.279661	0.315651
6	3.799500	1.397694	2.573209
1	-0.903652	-1.333309	-0.163019
1	-4.761552	-0.246745	-2.831299
1	-3.726289	2.322403	-2.874342
1	-2.839815	-0.666618	1.391763
1	-1.388095	2.323618	3.544832
1	-1.573244	3.163525	2.019066
1	-3.117327	0.807265	3.091073
1	-3.673967	1.977115	1.901117
1	1.756125	1.661855	0.577581
1	0.307509	-3.406231	-0.050915
1	0.944827	-5.233565	1.459440
1	1.307660	-4.782275	3.868402
1	1.002394	-2.484811	4.736271
1	0.338689	-0.662432	3.213767
1	-2.735705	-2.465058	-1.895115
1	-3.385358	-4.790582	-1.302024
1	-5.148237	-5.181721	0.383310
1	-6.276150	-3.265607	1.460633
1	-5.633551	-0.951801	0.852458
1	-0.397119	2.321841	-1.187413
1	0.633858	4.503018	-0.674523
1	-0.769690	6.377880	0.120188
1	-3.205317	6.061873	0.415312
1	-4.226797	3.855786	-0.064828
1	4.611493	1.921367	3.070629
1	2.827706	1.695152	2.954885
1	3.944417	0.324544	2.654740
1	3.157744	-2.712792	0.421532
1	4.755456	-4.040933	-0.898074
1	5.880318	-3.029631	-2.859505
1	5.417827	-0.672677	-3.453042
1	3.819405	0.647892	-2.122315
8	-0.877417	-0.273601	-2.114731
8	1.338419	0.729809	-2.642307
6	1.033224	-1.853512	-2.814324
1	2.329116	-0.647430	1.078186
1	0.695108	-1.766233	-3.843879
1	2.108190	-1.981937	-2.774258
1	0.522505	-2.670956	-2.315985

TS(9-10)

Eelec = -2784.4267378, -2784.1161227

E = -2783.754236
H = -2783.713574
G = -2783.828
Nimag = 1(-390.7475)

6	-5.141338	-1.757584	0.350139
6	-5.511172	-3.055756	0.664637
6	-4.893362	-4.127909	0.036292
6	-3.903608	-3.905731	-0.910058
6	-3.520328	-2.611218	-1.226429
6	-4.139450	-1.550606	-0.585340
7	-3.769559	-0.219195	-0.949612
6	-3.013050	0.633753	-0.245107
7	-2.928556	1.754055	-0.970549
6	-3.615542	1.595774	-2.150481
6	-4.141456	0.358812	-2.141498
6	-2.419077	0.334046	1.096535
6	-0.907609	0.315954	1.117432
6	-0.439947	1.354053	1.847612
6	-1.536985	2.166129	2.468554
6	-2.804242	1.366905	2.183668
6	-0.178759	-0.856008	0.519329
7	0.945034	-0.567820	-0.413840
6	2.319089	-0.286863	0.069693
6	3.356410	-0.929013	-0.834130
6	3.696394	-2.259175	-0.605015
6	4.599512	-2.916609	-1.426920
6	5.182447	-2.240161	-2.489416
6	4.864358	-0.907298	-2.710634
6	3.961975	-0.252625	-1.886123
8	0.787555	1.713374	2.077609
6	-2.286114	2.989444	-0.627703
6	-0.916402	3.126708	-0.764833
6	-0.332516	4.345443	-0.453538
6	-1.117431	5.411261	-0.038943
6	-2.494000	5.266379	0.069044
6	-3.085947	4.047861	-0.223673
6	0.240166	-1.916811	1.530674
6	0.503558	-3.206853	1.072612
6	0.854118	-4.221486	1.947030
6	0.951407	-3.961368	3.308380
6	0.690572	-2.683794	3.776433
6	0.333077	-1.670577	2.894614
16	0.545991	-0.346304	-1.993265
7	2.450656	1.126928	0.335698
16	3.812077	1.732142	0.925597
8	3.524508	3.124913	1.255830
8	4.985829	1.494974	0.087531
6	4.160798	0.912721	2.468367
1	-0.938775	-1.379888	-0.123485

1	-4.740048	-0.167705	-2.861915
1	-3.651083	2.379997	-2.884590
1	-2.828361	-0.658349	1.363945
1	-1.346804	2.286006	3.536065
1	-1.548106	3.169080	2.038478
1	-3.111189	0.812201	3.074666
1	-3.648461	1.996250	1.888984
1	1.507758	1.455747	1.255882
1	0.438245	-3.415189	0.012240
1	1.049597	-5.215893	1.568338
1	1.226335	-4.749675	3.995795
1	0.766104	-2.468000	4.833720
1	0.132926	-0.677513	3.269432
1	-2.749420	-2.412591	-1.958594
1	-3.425551	-4.740966	-1.402607
1	-5.186529	-5.138877	0.283136
1	-6.286705	-3.228238	1.397682
1	-5.621131	-0.911818	0.823394
1	-0.306843	2.301716	-1.096270
1	0.741464	4.446402	-0.526650
1	-0.653511	6.357248	0.203928
1	-3.107484	6.097429	0.388034
1	-4.156166	3.915648	-0.138357
1	5.044417	1.385002	2.888214
1	3.308784	1.039389	3.129690
1	4.361814	-0.138473	2.280607
1	3.244042	-2.787887	0.224572
1	4.853886	-3.949877	-1.232575
1	5.891194	-2.744408	-3.132588
1	5.328417	-0.367400	-3.524792
1	3.722134	0.783914	-2.055785
8	-0.911257	-0.347001	-2.064376
8	1.245477	0.791537	-2.549027
6	1.057219	-1.787021	-2.889556
1	2.358875	-0.879456	1.042182
1	0.696167	-1.644525	-3.905095
1	2.137119	-1.870258	-2.876485
1	0.591275	-2.657262	-2.438833

10

Eelec = -2784.4343721, -2784.1231386
E = -2783.758491
H = -2783.717522
G = -2783.832356
Nimag = 0

6	-4.287744	2.757952	-0.285365
6	-4.298174	4.138780	-0.398299
6	-3.655928	4.921098	0.550864

6	-2.997761	4.324134	1.615561
6	-2.969187	2.943066	1.730789
6	-3.610582	2.174388	0.773720
7	-3.635225	0.755739	0.936849
6	-3.107484	-0.175034	0.126008
7	-3.441727	-1.360666	0.651284
6	-4.161760	-1.174406	1.806640
6	-4.284385	0.150943	1.989336
6	-2.286044	0.118000	-1.094446
6	-0.823777	-0.237686	-0.917772
6	-0.511504	-1.289515	-1.707269
6	-1.661412	-1.739905	-2.557618
6	-2.722453	-0.664584	-2.350762
6	-0.028479	0.665456	-0.011158
7	1.137150	0.089883	0.709298
6	2.494659	0.189887	0.116298
6	3.587709	-0.066178	1.137464
6	4.097597	0.999770	1.871688
6	5.107636	0.804111	2.801470
6	5.626270	-0.468146	3.001077
6	5.140691	-1.532983	2.253363
6	4.134143	-1.331316	1.320306
8	0.603816	-1.953794	-1.851595
6	-3.191387	-2.676986	0.139924
6	-1.998566	-3.315755	0.424061
6	-1.812526	-4.611277	-0.034543
6	-2.813033	-5.253090	-0.749117
6	-4.012788	-4.604078	-1.008858
6	-4.208235	-3.307817	-0.560385
6	0.364918	1.974704	-0.674453
6	0.492151	3.117623	0.111925
6	0.836894	4.335022	-0.451237
6	1.056685	4.426558	-1.819597
6	0.932248	3.295190	-2.609673
6	0.586249	2.076838	-2.041202
16	0.756160	-0.982222	1.898410
7	2.585920	-0.624702	-1.056889
16	3.575767	-0.157445	-2.204744
8	3.963591	1.253888	-2.075437
8	3.033179	-0.572801	-3.499449
6	5.084901	-1.079512	-2.027181
1	-0.740081	0.964143	0.813365
1	-4.776365	0.724728	2.753131
1	-4.513959	-2.009115	2.384908
1	-2.405153	1.203513	-1.267729
1	-1.331229	-1.805476	-3.594962
1	-1.989737	-2.738740	-2.268447
1	-2.713564	0.034007	-3.191962
1	-3.736165	-1.066413	-2.273287
1	1.429461	-1.437804	-1.485574

1	0.322206	3.048229	1.179316
1	0.932994	5.212238	0.174622
1	1.332272	5.373180	-2.264154
1	1.125447	3.350129	-3.672131
1	0.514011	1.193426	-2.660177
1	-2.452987	2.462037	2.550876
1	-2.496826	4.932611	2.355397
1	-3.668956	5.998237	0.459726
1	-4.815707	4.602943	-1.226023
1	-4.801784	2.138202	-1.007103
1	-1.231070	-2.804229	0.980486
1	-0.874475	-5.109803	0.164607
1	-2.658085	-6.261810	-1.106414
1	-4.795560	-5.104271	-1.561754
1	-5.137251	-2.788042	-0.751802
1	5.741519	-0.794927	-2.844742
1	5.538649	-0.834319	-1.072270
1	4.846678	-2.137351	-2.080146
1	3.701709	1.993946	1.704936
1	5.497601	1.644009	3.360563
1	6.415840	-0.626357	3.723332
1	5.549781	-2.524439	2.394532
1	3.752886	-2.153342	0.732007
8	-0.676409	-0.821795	2.139816
8	1.234510	-2.323117	1.617133
6	1.529217	-0.443717	3.400063
1	2.596376	1.286688	-0.154998
1	1.049709	-1.034592	4.176827
1	2.593057	-0.638340	3.377973
1	1.323062	0.611714	3.541163

TS(10-11)

Eelec = -2784.3964317, -2784.0869679
E = -2783.7201
H = -2783.678762
G = -2783.794409
Nimag = 1(-177.5120)

6	-3.145190	-2.827116	-1.367639
6	-3.917411	-1.897516	-0.689951
6	-4.917792	-2.287655	0.186878
6	-5.131572	-3.639279	0.405852
6	-4.359653	-4.582257	-0.258601
6	-3.372088	-4.176844	-1.144236
7	-3.717982	-0.506909	-0.960489
6	-3.106294	0.400441	-0.186133
7	-3.180332	1.565081	-0.836992
6	-3.819345	1.386834	-2.039556
6	-4.156109	0.088199	-2.119968

6	-2.502738	0.116451	1.155104
6	-0.991171	0.212516	1.185134
6	-0.622467	1.224585	1.985047
6	-1.769533	1.935402	2.627990
6	-2.977602	1.071650	2.274227
6	-0.183187	-0.845081	0.476837
6	0.308050	-1.950059	1.408484
6	0.729538	-3.150014	0.834382
6	1.172656	-4.200707	1.618368
6	1.203032	-4.074702	3.002357
6	0.780502	-2.891612	3.584840
6	0.331300	-1.839639	2.793642
8	0.581431	1.669655	2.326190
6	-2.681779	2.843505	-0.427050
6	-3.589932	3.789543	0.023366
6	-3.131583	5.052287	0.364015
6	-1.780388	5.351537	0.250125
6	-0.886898	4.394369	-0.208541
6	-1.334919	3.129382	-0.559820
7	0.905364	-0.346676	-0.380015
16	0.503683	-0.379610	-1.917748
8	-0.786678	0.295798	-2.164934
6	1.753321	0.577359	-2.707472
8	0.534417	-1.731212	-2.517495
6	2.809725	-0.171677	0.572054
7	2.856326	1.083098	0.952025
16	3.418810	2.323543	0.051488
6	4.325502	3.225204	1.268872
8	2.280044	3.148699	-0.336860
8	4.332912	1.944682	-1.018141
1	-0.937817	-1.393645	-0.173604
1	-4.654153	-0.473929	-2.888311
1	-3.951224	2.201146	-2.728149
1	-2.817697	-0.919470	1.384713
1	-1.610094	2.008697	3.705052
1	-1.841882	2.957289	2.250056
1	-3.269162	0.461664	3.133465
1	-3.851037	1.662235	1.987264
1	1.321057	1.398803	1.734217
1	0.706579	-3.249573	-0.243465
1	1.495419	-5.120897	1.149814
1	1.552124	-4.892903	3.617510
1	0.800230	-2.779041	4.660696
1	0.005131	-0.922227	3.261946
1	-2.371481	-2.494029	-2.048758
1	-2.768673	-4.909223	-1.661907
1	-4.529676	-5.635925	-0.085827
1	-5.905239	-3.954377	1.091954
1	-5.519108	-1.540795	0.687157
1	-4.638991	3.538146	0.103375

1	-3.828733	5.798839	0.718181
1	-1.422707	6.335715	0.520241
1	0.167131	4.616008	-0.292593
1	-0.660558	2.370902	-0.927946
1	4.683536	4.130011	0.785381
1	3.656504	3.466088	2.088571
1	5.159022	2.620439	1.611531
1	1.524145	0.543075	-3.768889
1	1.705666	1.594352	-2.334378
1	2.729730	0.145251	-2.519349
1	2.329281	-0.805830	1.306550
6	3.827381	-0.908001	-0.229907
6	5.169442	-0.649012	0.047007
6	6.169504	-1.419037	-0.521385
6	5.845230	-2.459116	-1.380123
6	4.512850	-2.729383	-1.650967
6	3.508998	-1.970206	-1.068958
1	5.432998	0.152455	0.720435
1	7.204311	-1.200861	-0.295666
1	6.626109	-3.054688	-1.833223
1	4.245289	-3.535686	-2.320209
1	2.477184	-2.186200	-1.293112

11+4

Eelec = -2784.4229008, -2784.1005229
E = -2783.749
H = -2783.705902
G = -2783.831185
Nimag = 0

6	-3.410067	3.132444	0.550670
6	-4.196054	2.205688	-0.111443
6	-4.958424	2.553785	-1.214998
6	-4.919313	3.861316	-1.672035
6	-4.130059	4.800962	-1.023045
6	-3.379073	4.437917	0.084829
7	-4.259579	0.862915	0.377953
6	-3.578879	-0.190244	-0.092404
7	-3.975665	-1.248513	0.623367
6	-4.906351	-0.855411	1.556889
6	-5.085434	0.469068	1.405350
6	-2.545898	-0.113681	-1.171932
6	-1.160232	-0.374718	-0.641686
6	-0.668130	-1.505580	-1.165562
6	-1.578473	-2.171468	-2.139784
6	-2.707502	-1.149721	-2.313259
6	-0.458657	0.515179	0.338210
6	0.027263	1.818072	-0.283264
6	0.388947	2.872889	0.554600

6	0.861588	4.065632	0.032994
6	0.983422	4.228956	-1.342740
6	0.632830	3.185382	-2.183699
6	0.157584	1.989885	-1.655367
8	0.505826	-2.057529	-0.880588
6	-3.577726	-2.619143	0.476587
6	-4.410606	-3.469456	-0.234623
6	-4.073531	-4.809506	-0.337734
6	-2.918573	-5.280098	0.272444
6	-2.106186	-4.415338	0.991134
6	-2.431854	-3.071149	1.106145
7	0.662204	-0.200277	0.953060
16	0.523709	-0.387731	2.509112
8	-0.690175	-1.130898	2.927659
6	1.914367	-1.413288	2.881370
8	0.677835	0.862438	3.282889
6	3.663716	0.672863	-0.728903
7	3.525262	-0.130168	-1.712148
16	4.474843	-1.460794	-1.994799
6	3.340062	-2.388959	-2.968470
8	4.752804	-2.212318	-0.781648
8	5.603751	-1.074903	-2.831429
1	-1.238109	0.833247	1.136399
1	-5.711829	1.169798	1.926651
1	-5.339099	-1.559444	2.244347
1	-2.639219	0.913616	-1.573901
1	-1.062689	-2.379308	-3.078670
1	-1.924569	-3.130233	-1.747325
1	-2.589808	-0.618019	-3.261198
1	-3.696655	-1.613763	-2.326103
1	0.858138	-1.504179	-0.122350
1	0.322083	2.735141	1.626738
1	1.143441	4.869227	0.700892
1	1.356540	5.158381	-1.751394
1	0.736456	3.294271	-3.255227
1	-0.095429	1.172469	-2.317489
1	-2.826266	2.835527	1.410913
1	-2.758102	5.166739	0.585871
1	-4.099059	5.819630	-1.383960
1	-5.506173	4.145361	-2.534282
1	-5.571252	1.809617	-1.705148
1	-5.309238	-3.085566	-0.698450
1	-4.712145	-5.482846	-0.892186
1	-2.653834	-6.325342	0.190043
1	-1.209464	-4.782541	1.470130
1	-1.809276	-2.390277	1.673786
1	3.834811	-3.325098	-3.212189
1	2.443184	-2.558192	-2.379707
1	3.116375	-1.822886	-3.866537
1	1.908415	-1.568716	3.956209

1	1.807549	-2.358427	2.359328
1	2.822910	-0.907526	2.573708
1	2.862562	1.407385	-0.659345
6	4.678608	0.802328	0.315867
6	6.016293	0.436180	0.161929
6	6.908959	0.640725	1.198935
6	6.477458	1.195621	2.396916
6	5.150746	1.571745	2.553493
6	4.260195	1.395954	1.509078
1	6.369748	0.019202	-0.769226
1	7.946413	0.364734	1.071582
1	7.180101	1.343570	3.205943
1	4.810406	2.007741	3.482397
1	3.224269	1.692096	1.621094

11’

Eelec = -1870.9573917, -1870.7286505
E = -1870.449412
H = -1870.419083
G = -1870.513606
Nimag = 0

6	3.777048	-0.475733	-1.345036
6	3.125069	-1.462008	-0.624903
6	3.744653	-2.120863	0.424973
6	5.040912	-1.771230	0.767353
6	5.706778	-0.783620	0.055253
6	5.076913	-0.140233	-0.999777
7	1.799863	-1.837664	-1.001952
6	0.688593	-1.686104	-0.268334
7	-0.310290	-2.230453	-0.972633
6	0.174577	-2.715638	-2.165215
6	1.497229	-2.470308	-2.186624
6	0.629205	-0.986538	1.050945
6	-0.459308	0.045286	1.114497
6	-1.351630	-0.267606	2.066804
6	-1.037953	-1.531711	2.792379
6	0.341672	-1.924441	2.255710
6	-0.523751	1.219053	0.182011
6	0.666031	2.150246	0.354000
6	1.437805	2.533961	-0.735959
6	2.498366	3.420476	-0.585610
6	2.801011	3.932635	0.665585
6	2.033946	3.556755	1.763142
6	0.977530	2.674967	1.606546
8	-2.451403	0.397417	2.383934
6	-1.683650	-2.400562	-0.584996
6	-2.048884	-3.596155	0.012677
6	-3.382180	-3.809678	0.328252

6	-4.325295	-2.832086	0.046550
6	-3.941729	-1.643841	-0.559151
6	-2.614399	-1.423303	-0.891186
7	-1.788741	1.894586	0.404721
16	-2.545884	2.493236	-0.831384
8	-3.969910	2.612771	-0.504279
6	-1.992699	4.164760	-1.095282
8	-2.235730	1.788856	-2.095046
1	-0.470661	0.819967	-0.899346
1	2.252430	-2.690866	-2.918937
1	-0.474519	-3.187655	-2.880596
1	1.626050	-0.517738	1.162612
1	-1.036129	-1.374953	3.872140
1	-1.806011	-2.278487	2.579001
1	1.111133	-1.753299	3.012888
1	0.392263	-2.981132	1.978669
1	-2.505634	1.128144	1.695185
1	1.191813	2.149125	-1.718611
1	3.082236	3.714616	-1.448012
1	3.623656	4.624258	0.787588
1	2.259243	3.958358	2.742298
1	0.372929	2.391930	2.458790
1	3.267965	0.030772	-2.153077
1	5.592020	0.634138	-1.550448
1	6.718506	-0.514071	0.324573
1	5.531612	-2.275441	1.588029
1	3.218757	-2.897622	0.962831
1	-1.301297	-4.349478	0.221070
1	-3.680183	-4.737815	0.795689
1	-5.363223	-2.994829	0.302085
1	-4.669374	-0.872797	-0.770858
1	-2.318634	-0.497943	-1.365999
1	-2.530628	4.571540	-1.947030
1	-2.210926	4.734992	-0.197775
1	-0.923907	4.157990	-1.286060

TS(11-6)

Eelec = -1870.9527143, -1870.7231228
E = -1870.448965
H = -1870.418883
G = -1870.512888
Nimag = 1(-1043.7630)

6	3.617046	-0.741477	-1.297482
6	2.953756	-1.752314	-0.623397
6	3.584400	-2.506761	0.353110
6	4.905315	-2.230915	0.667699
6	5.582493	-1.218945	0.001676
6	4.940430	-0.478011	-0.979381

7	1.600686	-2.051750	-0.974093
6	0.508149	-1.809290	-0.235630
7	-0.529068	-2.304419	-0.922273
6	-0.086386	-2.853430	-2.103923
6	1.248660	-2.695024	-2.139690
6	0.499740	-1.072754	1.068208
6	-0.431606	0.097888	1.073033
6	-1.430273	-0.056891	1.977177
6	-1.322283	-1.355487	2.719509
6	0.023337	-1.932925	2.273178
6	-0.323385	1.264316	0.137689
6	0.912564	2.119566	0.368068
6	1.664378	2.583229	-0.705162
6	2.768615	3.403159	-0.503702
6	3.135069	3.767798	0.782243
6	2.389607	3.309843	1.862686
6	1.289410	2.493713	1.655423
8	-2.408653	0.768232	2.183068
6	-1.906555	-2.368230	-0.524686
6	-2.380419	-3.560008	-0.000307
6	-3.724375	-3.663576	0.325805
6	-4.569400	-2.580743	0.130797
6	-4.078815	-1.396014	-0.400333
6	-2.740817	-1.286566	-0.743535
7	-1.554548	2.031665	0.310992
16	-2.238888	2.761186	-0.920627
8	-3.673155	2.855965	-0.664869
6	-1.634738	4.428234	-0.948290
8	-1.828105	2.165116	-2.200096
1	-0.264550	0.885381	-0.945447
1	1.982300	-2.978135	-2.872392
1	-0.770559	-3.298070	-2.803927
1	1.553701	-0.766315	1.217250
1	-1.370981	-1.193594	3.797067
1	-2.168182	-1.993557	2.453936
1	0.765603	-1.836104	3.069755
1	-0.040895	-2.995611	2.021620
1	-2.190118	1.556234	1.246131
1	1.370458	2.312058	-1.712430
1	3.338040	3.759542	-1.352113
1	3.992872	4.406433	0.944593
1	2.666629	3.594022	2.869304
1	0.704313	2.140385	2.495059
1	3.099047	-0.161409	-2.048291
1	5.464771	0.315483	-1.492804
1	6.612906	-1.005980	0.250156
1	5.405408	-2.809604	1.431588
1	3.045526	-3.297211	0.857252
1	-1.706747	-4.393357	0.146596
1	-4.106521	-4.587738	0.736302

1	-5.614679	-2.658167	0.396151
1	-4.729482	-0.545058	-0.544636
1	-2.355365	-0.369407	-1.164532
1	-2.095954	4.937760	-1.789735
1	-1.914279	4.901336	-0.012305
1	-0.554748	4.408410	-1.056036

(III) Potential Side Reactions

PRC(1+4)

Eelec = =-1601.6063627, -1601.4117583
E = -1601.202304
H = -1601.175669
G = -1601.266006
Nimag = 0

6	-0.303685	4.005385	1.214274
6	-0.351455	2.985612	0.274029
6	0.782533	2.639652	-0.447062
6	1.971860	3.311099	-0.213572
6	2.027563	4.337357	0.719589
6	0.886763	4.684031	1.428242
7	-1.564204	2.292967	0.043573
6	-1.629139	0.955558	-0.164766
7	-2.960129	0.752740	-0.331040
6	-3.695566	1.920113	-0.225624
6	-2.807064	2.899320	0.012427
6	1.852326	-1.214846	0.131742
6	1.680820	-1.677484	1.498775
6	2.720012	-2.284119	2.207656
6	2.505767	-2.720332	3.500126
6	1.257075	-2.554721	4.093157
6	0.223021	-1.949915	3.394617
6	0.433149	-1.509780	2.097473
6	-3.523440	-0.520872	-0.573454
6	-4.744266	-0.859989	-0.006669
6	-5.294184	-2.108608	-0.255683
6	-4.624112	-3.021946	-1.055454
6	-3.399840	-2.676843	-1.611647
6	-2.848666	-1.427101	-1.380475
7	2.957246	-1.359700	-0.495082
16	3.016054	-0.753586	-2.045441
6	3.634400	-2.152381	-2.919372
8	4.024951	0.290552	-2.063215
8	1.690583	-0.432429	-2.554078
1	0.983887	-0.741676	-0.337201
1	-4.759849	1.960053	-0.369887
1	-2.944830	3.960167	0.117403
1	3.684582	-2.401587	1.733959
1	3.308363	-3.189087	4.052454
1	1.094419	-2.897855	5.106083
1	-0.744520	-1.819513	3.858787
1	-0.360986	-1.026983	1.541252
1	2.908246	-2.956286	-2.851804
1	3.766449	-1.840677	-3.952110

1	4.583775	-2.440291	-2.479957
1	-5.253961	-0.160731	0.641691
1	-6.244679	-2.369463	0.189059
1	-5.052781	-3.996168	-1.244996
1	-2.872708	-3.380375	-2.241402
1	-1.903558	-1.141226	-1.819168
1	0.725002	1.852641	-1.185228
1	2.854199	3.031052	-0.772944
1	2.956182	4.862821	0.894052
1	0.922624	5.476621	2.163012
1	-1.184615	4.253758	1.790210

TS(1-13)

Eelec = -1601.5972886, -1601.4120485
E = -1601.192245
H = -1601.167122
G = -1601.24958
Nimag = 1(-190.1108)

6	-2.999770	-1.852963	-1.240199
6	-2.101650	-0.804865	-1.388034
6	-2.537246	0.509649	-1.414250
6	-3.892362	0.772082	-1.282946
6	-4.802239	-0.265827	-1.144004
6	-4.353142	-1.579010	-1.124932
7	-0.720066	-1.092660	-1.536864
6	0.276292	-0.446516	-0.899911
7	1.392361	-1.062523	-1.343606
6	1.098591	-2.073972	-2.238093
6	-0.239164	-2.091631	-2.360708
6	0.116404	0.662819	1.018890
6	-0.296372	-0.531193	1.783726
6	-1.631579	-0.763964	2.098663
6	-1.983407	-1.873183	2.850077
6	-1.007121	-2.753239	3.298818
6	0.327052	-2.520191	2.993790
6	0.679835	-1.414068	2.237913
6	2.712467	-0.733246	-0.943533
6	3.601845	-1.752376	-0.629543
6	4.897381	-1.434825	-0.253070
6	5.296742	-0.107956	-0.174857
6	4.396498	0.901772	-0.482044
6	3.104040	0.594907	-0.878859
7	-0.710533	1.677220	0.956722
16	-0.124018	3.050072	0.317284
6	-0.822424	4.263483	1.389911
8	-0.693586	3.262237	-1.012813
8	1.333727	3.142069	0.410907
1	1.187860	0.827605	0.952306

1	1.860205	-2.648014	-2.733741
1	-0.882254	-2.685581	-2.984425
1	-2.382378	-0.068576	1.751129
1	-3.022987	-2.050131	3.090238
1	-1.284927	-3.615358	3.890038
1	1.092198	-3.196745	3.349358
1	1.719721	-1.228447	1.999839
1	-0.427282	4.114092	2.389411
1	-0.532114	5.235490	1.001108
1	-1.901617	4.152159	1.378276
1	3.277471	-2.783591	-0.663452
1	5.590905	-2.227459	-0.008262
1	6.305806	0.137464	0.125939
1	4.696086	1.938797	-0.422094
1	2.404425	1.380172	-1.127619
1	-1.826920	1.314953	-1.529865
1	-4.233875	1.797784	-1.300689
1	-5.858370	-0.053212	-1.050886
1	-5.054714	-2.393473	-1.008305
1	-2.640438	-2.871918	-1.194197

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Eelec = -1601.637447, -1601.4493469
E = -1601.228292
H = -1601.203286
G = -1601.285263
Nimag = 0

6	-2.777768	1.101742	1.420865
6	-2.068989	-0.085645	1.382995
6	-2.696998	-1.307855	1.219599
6	-4.075821	-1.333068	1.088027
6	-4.804727	-0.151571	1.120599
6	-4.157454	1.063791	1.284679
7	-0.653497	-0.052974	1.606103
6	0.321765	0.031368	0.698811
7	1.478800	0.051984	1.371875
6	1.226395	-0.031691	2.722947
6	-0.108983	-0.098932	2.866503
6	0.153859	0.075659	-0.804641
6	-0.427663	1.425040	-1.199048
6	-1.646930	1.513128	-1.852898
6	-2.155763	2.751911	-2.219071
6	-1.451668	3.912018	-1.934507
6	-0.227353	3.828223	-1.284274
6	0.280744	2.590860	-0.921303
6	2.801145	0.200214	0.845857
6	3.541694	1.298423	1.258967
6	4.841020	1.448691	0.802526

6	5.384055	0.511014	-0.064556
6	4.628276	-0.578518	-0.470294
6	3.330451	-0.749872	-0.010969
7	-0.654759	-0.998598	-1.290772
16	-0.017962	-2.428855	-1.184341
6	-1.094090	-3.377173	-2.215489
8	-0.094696	-3.024953	0.170590
8	1.345891	-2.528670	-1.748285
1	1.173187	0.046823	-1.204318
1	2.020713	-0.058626	3.442430
1	-0.725718	-0.190973	3.738831
1	-2.181369	0.601607	-2.068381
1	-3.106006	2.808343	-2.730209
1	-1.847909	4.874557	-2.223496
1	0.336399	4.724685	-1.070303
1	1.245021	2.533379	-0.433142
1	-1.028156	-2.998921	-3.228916
1	-0.754640	-4.406669	-2.165070
1	-2.106024	-3.289738	-1.836457
1	3.103220	2.027281	1.924655
1	5.423324	2.300726	1.119285
1	6.394976	0.631164	-0.424205
1	5.045086	-1.309186	-1.146517
1	2.738747	-1.594133	-0.336838
1	-2.098782	-2.205287	1.169910
1	-4.580682	-2.278069	0.955151
1	-5.879241	-0.178884	1.015924
1	-4.721827	1.983754	1.305565
1	-2.257497	2.039427	1.544748

9''

Eelec = -2784.4350325, -2784.1247483
E = -2783.757413
H = -2783.716314
G = -2783.830284
Nimag = 0

6	-5.207312	-1.484223	0.372878
6	-4.217771	-1.364628	-0.589594
6	-3.719967	-2.472079	-1.256239
6	-4.218966	-3.726896	-0.940311
6	-5.198936	-3.863587	0.032119
6	-5.691868	-2.743915	0.687618
7	-3.735472	-0.070064	-0.947102
6	-2.961634	0.736955	-0.206441
7	-2.782888	1.849232	-0.929979
6	-3.427757	1.730159	-2.139043
6	-4.023041	0.525908	-2.153624
6	-2.099514	3.051429	-0.556669

6	-2.849259	4.109418	-0.067807
6	-2.212204	5.301863	0.238700
6	-0.842152	5.422918	0.054026
6	-0.107149	4.359259	-0.449824
6	-0.737653	3.166195	-0.768832
6	-2.420259	0.387537	1.148055
6	-0.918258	0.272011	1.213361
6	-0.373438	1.236780	2.026831
6	-1.459131	2.128016	2.593438
6	-2.766895	1.429520	2.242305
6	-0.227629	-0.882161	0.553378
6	0.251372	-1.990889	1.480729
6	0.671157	-1.758081	2.787709
6	1.083494	-2.806878	3.598444
6	1.067566	-4.111271	3.125625
6	0.630954	-4.359921	1.832375
6	0.228423	-3.307319	1.024508
8	0.844729	1.433533	2.314533
7	0.853849	-0.520070	-0.431705
16	0.503182	-0.610762	-2.034021
8	1.258537	0.396936	-2.747681
6	2.210491	-0.188836	0.019889
7	2.404063	1.259592	-0.098496
16	3.738906	2.023266	0.514908
6	3.939516	1.521694	2.197572
6	3.291589	-1.013576	-0.642752
6	3.599045	-2.250903	-0.083789
6	4.538846	-3.081034	-0.675286
6	5.189239	-2.674504	-1.831847
6	4.898761	-1.434801	-2.383811
6	3.956836	-0.605910	-1.793265
8	3.378851	3.431012	0.506285
8	4.920819	1.605849	-0.213644
6	1.014668	-2.193343	-2.646318
8	-0.949039	-0.596242	-2.157177
1	-1.008042	-1.376405	-0.082024
1	-3.389795	2.515672	-2.871613
1	-4.619831	0.033480	-2.899063
1	-2.910832	-0.571826	1.394074
1	-1.317926	2.237645	3.669123
1	-1.373927	3.126388	2.160317
1	-3.144897	0.880575	3.109461
1	-3.556524	2.120043	1.931616
1	1.615961	1.704936	0.388677
1	0.686885	-0.743649	3.160612
1	1.415055	-2.600684	4.607401
1	1.383421	-4.927083	3.761640
1	0.597270	-5.373016	1.454378
1	-0.120384	-3.516703	0.021397
1	-3.916153	3.998077	0.069749

1	-2.786458	6.132481	0.624741
1	-0.343408	6.349321	0.303109
1	0.961155	4.448711	-0.590285
1	-0.178909	2.338373	-1.180251
1	-2.948847	-2.340621	-2.003081
1	-3.837131	-4.598938	-1.452766
1	-5.581550	-4.844258	0.278753
1	-6.459048	-2.848923	1.441942
1	-5.590412	-0.601460	0.866083
1	4.735554	2.138591	2.606008
1	2.995695	1.681695	2.710718
1	4.232131	0.475891	2.217353
1	2.193143	-0.474192	1.114637
1	3.732952	0.356258	-2.224685
1	5.412009	-1.104866	-3.276698
1	5.927138	-3.315989	-2.294609
1	4.767337	-4.039096	-0.228492
1	3.092227	-2.571492	0.817366
1	0.720134	-2.216487	-3.692541
1	2.089153	-2.293902	-2.550198
1	0.498405	-2.967582	-2.089246

TS(9-12)

Eelec = -2784.3930383, -2784.0823236
E = -2783.71825
H = -2783.676761
G = -2783.792419
Nimag = 1(-278.5526)

6	-5.155691	-1.442636	0.296537
6	-4.294837	-1.343595	-0.787339
6	-3.995589	-2.458714	-1.557484
6	-4.571209	-3.679160	-1.239901
6	-5.426130	-3.790263	-0.152593
6	-5.712155	-2.671240	0.616418
7	-3.731897	-0.089245	-1.122196
6	-3.193467	0.769324	-0.228022
7	-2.821962	1.818642	-0.985671
6	-3.110295	1.620527	-2.321799
6	-3.686153	0.410705	-2.408591
6	-2.289837	3.035874	-0.482096
6	-3.070998	3.821358	0.351840
6	-2.567778	5.025062	0.819925
6	-1.295641	5.438214	0.449361
6	-0.526074	4.650279	-0.394719
6	-1.023071	3.444859	-0.868354
6	-2.206540	-0.001964	1.540781
6	-0.820353	0.006134	1.425226
6	-0.290453	1.063766	2.223553

6	-1.429019	1.816464	2.869820
6	-2.643148	0.927784	2.639526
6	-0.069721	-1.070783	0.687971
6	0.559195	-2.132197	1.581132
6	1.087295	-1.865575	2.843370
6	1.631693	-2.882423	3.615646
6	1.646005	-4.189134	3.151071
6	1.098906	-4.474079	1.908586
6	0.558984	-3.454665	1.140140
8	0.896649	1.340305	2.423758
7	0.866331	-0.587737	-0.375816
16	0.501822	-0.912354	-1.957300
8	1.075430	0.132897	-2.777340
6	2.182798	-0.035616	-0.030806
7	2.184256	1.395241	-0.348389
16	3.408911	2.411030	0.106691
6	3.875300	2.016652	1.763218
6	3.355563	-0.785131	-0.623210
6	3.834884	-1.897142	0.064257
6	4.872555	-2.655662	-0.454835
6	5.449412	-2.301030	-1.666472
6	4.986313	-1.184485	-2.347578
6	3.945286	-0.428043	-1.830166
8	2.799574	3.730174	0.098232
8	4.569725	2.180179	-0.728979
6	1.263820	-2.439666	-2.434280
8	-0.930040	-1.149573	-2.035065
1	-0.869185	-1.614440	0.108692
1	-2.894119	2.359815	-3.071794
1	-4.075963	-0.126645	-3.253513
1	-2.774788	-0.900794	1.350664
1	-1.202695	1.999828	3.921036
1	-1.525985	2.789918	2.384004
1	-2.844305	0.318871	3.526832
1	-3.554056	1.470742	2.396896
1	1.317085	1.817346	-0.010010
1	1.083729	-0.853719	3.221103
1	2.041795	-2.649053	4.589108
1	2.066749	-4.979945	3.757034
1	1.080890	-5.491551	1.541818
1	0.107669	-3.696870	0.186725
1	-4.064121	3.488862	0.619756
1	-3.172223	5.641712	1.470880
1	-0.901391	6.374677	0.819000
1	0.471746	4.958966	-0.672054
1	-0.430630	2.820632	-1.525254
1	-3.299522	-2.370195	-2.379730
1	-4.339486	-4.548892	-1.839208
1	-5.868967	-4.745219	0.093927
1	-6.381951	-2.749385	1.461639

1	-5.388987	-0.557453	0.871823
1	4.620440	2.754909	2.048051
1	2.995183	2.069769	2.395034
1	4.317359	1.024415	1.774037
1	2.229141	-0.165268	1.090792
1	3.585996	0.438368	-2.361452
1	5.439354	-0.894275	-3.285645
1	6.262988	-2.886657	-2.072914
1	5.233357	-3.517362	0.089984
1	3.386307	-2.178043	1.008270
1	0.937114	-2.617672	-3.455873
1	2.341785	-2.347618	-2.389805
1	0.911041	-3.229549	-1.781246

12

Eelec = -2784.4134377, -2784.091563
E = -2783.740319
H = -2783.697176
G = -2783.82142
Nimag = 0

6	-6.716013	-1.053952	0.243325
6	-5.680154	-1.230737	-0.664415
6	-5.474064	-2.469981	-1.255969
6	-6.315148	-3.528456	-0.946516
6	-7.350268	-3.360011	-0.039431
6	-7.542083	-2.120739	0.556219
7	-4.834900	-0.145284	-0.984602
6	-4.464447	0.800204	-0.085747
7	-3.647828	1.593988	-0.821192
6	-3.514283	1.158710	-2.127827
6	-4.268657	0.054289	-2.232226
6	-2.985948	2.726265	-0.292395
6	-3.619396	3.506181	0.666185
6	-2.967324	4.611731	1.188425
6	-1.693667	4.950002	0.751422
6	-1.069315	4.169443	-0.210427
6	-1.709073	3.053343	-0.730248
6	-1.328574	-0.868100	2.119193
6	-0.042991	-0.596988	1.853028
6	0.300759	0.667478	2.517143
6	-0.925504	1.190191	3.219181
6	-2.002647	0.139722	2.981045
6	0.834319	-1.449531	0.975735
6	1.912232	-2.237058	1.692725
6	2.476490	-1.830855	2.895941
6	3.432900	-2.611881	3.532305
6	3.834406	-3.816822	2.978854
6	3.269305	-4.239591	1.783113

6	2.317776	-3.455972	1.152378
8	1.386793	1.217392	2.506771
7	1.336892	-0.717991	-0.216318
16	0.479930	-0.930948	-1.619672
8	0.659528	0.240745	-2.447650
6	2.606746	0.022635	-0.192732
7	2.312997	1.444360	-0.365332
16	3.409846	2.647193	-0.115699
6	4.102169	2.466093	1.499734
6	3.635982	-0.480828	-1.183908
6	4.502117	-1.494702	-0.788041
6	5.429369	-2.019404	-1.675780
6	5.505240	-1.524847	-2.969667
6	4.658039	-0.498673	-3.363383
6	3.730538	0.024472	-2.475729
8	2.613429	3.861395	-0.125442
8	4.497922	2.504884	-1.059941
6	1.176778	-2.315035	-2.474449
8	-0.864330	-1.323406	-1.236550
1	0.127861	-2.231654	0.562840
1	-2.922218	1.673240	-2.862370
1	-4.469733	-0.576098	-3.078594
1	-1.857922	-1.730194	1.731589
1	-0.693829	1.356813	4.273149
1	-1.182298	2.162165	2.788879
1	-2.359294	-0.322769	3.906219
1	-2.885302	0.536190	2.469012
1	1.439837	1.708052	0.092831
1	2.181545	-0.893118	3.342072
1	3.860457	-2.274139	4.466613
1	4.575104	-4.426818	3.477540
1	3.564038	-5.183661	1.345405
1	1.878965	-3.800959	0.225592
1	-4.613793	3.237862	0.990797
1	-3.464646	5.218162	1.933256
1	-1.189153	5.815940	1.156975
1	-0.071772	4.415295	-0.548187
1	-1.204748	2.430978	-1.457527
1	-4.647430	-2.613775	-1.937711
1	-6.149615	-4.491410	-1.409891
1	-8.002615	-4.187489	0.202485
1	-8.348203	-1.977864	1.262830
1	-6.860798	-0.083178	0.693426
1	4.780076	3.305606	1.630341
1	3.302134	2.484628	2.230759
1	4.658591	1.534453	1.545011
1	3.000647	-0.179346	0.848181
1	3.078447	0.827725	-2.780366
1	4.724074	-0.094130	-4.364082
1	6.231080	-1.927008	-3.663488

1	6.098089	-2.805463	-1.352372
1	4.452609	-1.880750	0.221404
1	0.602436	-2.420375	-3.391514
1	2.220012	-2.120059	-2.695190
1	1.060426	-3.199947	-1.857770

(IV) Conformational Sampling in Conventional Pathway

C1-TS(3-5)$_{re}$

Eelec = -1870.8782482
E = -1870.367083
H = -1870.336293
G = -1870.431134
Nimag = 1(-67.0596)

6	2.207243	2.752189	1.049569
6	3.263271	1.939265	0.885158
7	2.833829	0.881483	0.119736
6	1.532454	1.030028	-0.178160
7	1.148749	2.183652	0.377393
1	2.094553	3.675884	1.581431
1	4.270856	1.998188	1.246370
6	0.751043	0.054877	-0.987845
6	-0.735843	0.226283	-1.071721
6	-1.195053	0.022014	-2.379556
6	-0.007145	-0.410690	-3.241202
6	1.207311	0.077708	-2.472937
1	1.035798	-0.915967	-0.561301
1	-0.010739	-1.498879	-3.342766
1	-0.084149	0.008433	-4.241548
1	2.108487	-0.510470	-2.635085
1	1.425387	1.107716	-2.759778
6	2.207243	2.752189	1.049569
6	3.263271	1.939265	0.885158
7	2.833829	0.881483	0.119736
6	1.532454	1.030028	-0.178160
7	1.148749	2.183652	0.377393
1	2.094553	3.675884	1.581431
1	4.270856	1.998188	1.246370
6	0.751043	0.054877	-0.987845
6	-0.735843	0.226283	-1.071721
6	-1.195053	0.022014	-2.379556
6	-0.007145	-0.410690	-3.241202
6	1.207311	0.077708	-2.472937
1	1.035798	-0.915967	-0.561301
1	-0.010739	-1.498879	-3.342766
1	-0.084149	0.008433	-4.241548
1	2.108487	-0.510470	-2.635085
1	1.425387	1.107716	-2.759778
8	-2.343869	0.089135	-2.831631
1	-1.340766	0.664277	-0.302143
6	-4.579964	-2.207564	-1.864194
6	-3.287668	-2.172343	-1.367916
6	-3.032709	-1.639846	-0.106909

6	-4.090697	-1.118356	0.643496
6	-5.375120	-1.145735	0.142100
6	-5.622588	-1.694907	-1.112850
1	-4.764382	-2.610811	-2.847964
1	-2.471437	-2.553375	-1.961678
1	-3.882666	-0.706137	1.618862
1	-6.190495	-0.743527	0.725401
1	-6.629386	-1.712745	-1.504077
6	-1.684756	-1.669874	0.427954
1	-0.940380	-2.240103	-0.117664
7	-1.458108	-1.262656	1.646939
16	0.029170	-1.461548	2.255259
8	0.819775	-2.465419	1.542270
8	0.668868	-0.159813	2.436697
6	-0.338401	-2.099632	3.859714
1	-0.985713	-1.395005	4.368989
1	-0.826445	-3.061266	3.746805
1	0.604965	-2.206331	4.385789
6	3.704576	-0.170530	-0.302405
6	4.739708	0.145850	-1.169191
6	5.622355	-0.846894	-1.561287
6	5.459312	-2.142375	-1.092807
6	4.418396	-2.442082	-0.227307
6	3.535154	-1.455271	0.184227
1	4.842191	1.155358	-1.539214
1	6.429056	-0.609160	-2.237978
1	6.143380	-2.917641	-1.403886
1	4.287999	-3.449031	0.138915
1	2.722126	-1.689320	0.856498
6	-0.146954	2.794522	0.391864
6	-0.562999	3.546437	-0.691514
6	-1.798921	4.167592	-0.638610
6	-2.593249	4.040318	0.491534
6	-2.155479	3.289823	1.572103
6	-0.921684	2.659731	1.529965
1	0.059242	3.619884	-1.569847
1	-2.147479	4.736731	-1.486497
1	-3.560894	4.517879	0.523934
1	-2.780619	3.179479	2.445149
1	-0.574264	2.028889	2.334334

C2-TS(3-5)*re*

Eelec = -1870.8793957
E = -1870.366998
H = -1870.33666
G = -1870.4294
Nimag = 1(-242.8905)

6	-1.337965	2.769825	-0.648660

6	-0.281109	3.182222	0.146229
6	-0.444945	4.127366	1.146652
6	-1.701717	4.670867	1.357765
6	-2.773979	4.263395	0.576421
6	-2.592343	3.315438	-0.419283
7	1.027862	2.654036	-0.093132
6	1.451349	1.413028	0.189905
7	2.714619	1.334522	-0.254801
6	3.085560	2.537495	-0.815723
6	2.029956	3.363089	-0.716944
6	0.585777	0.358423	0.781314
6	0.100548	-0.556294	-0.307054
6	0.700197	-1.836109	-0.188857
6	1.387380	-1.949862	1.163543
6	1.244940	-0.580994	1.825419
8	0.671832	-2.750298	-1.010028
6	3.574464	0.190149	-0.263902
6	3.423878	-0.759417	-1.259483
6	4.293702	-1.837812	-1.292684
6	5.303840	-1.948246	-0.349939
6	5.450107	-0.982071	0.635668
6	4.582211	0.096494	0.682387
6	-2.050382	-0.913773	-0.012265
6	-2.092057	-1.428510	1.367561
6	-2.009626	-2.796839	1.620387
6	-2.071341	-3.268918	2.918884
6	-2.228717	-2.386581	3.981837
6	-2.330709	-1.026386	3.736209
6	-2.264161	-0.550574	2.434352
7	-2.490271	-1.697793	-0.967492
16	-2.636571	-1.049474	-2.449852
8	-4.011573	-1.136337	-2.907778
8	-2.001712	0.276708	-2.535413
6	-1.661958	-2.169724	-3.407248
1	-2.116196	0.166965	-0.102326
1	4.060510	2.676340	-1.239782
1	1.884364	4.374887	-1.040188
1	-0.230931	0.909816	1.258184
1	-0.145464	-0.155242	-1.279186
1	-2.476049	-0.336481	4.554921
1	-2.377540	0.507865	2.242315
1	-1.898815	-3.468573	0.782606
1	-2.004086	-4.330833	3.105873
1	-2.285146	-2.760729	4.993633
1	-0.684180	-2.261391	-2.940729
1	-2.166337	-3.129659	-3.399347
1	-1.605443	-1.773499	-4.416470
1	0.397984	4.424004	1.753312
1	-1.842966	5.406013	2.135424
1	-3.753507	4.684439	0.746420

1	-3.421365	2.987747	-1.027900
1	-1.211915	2.024141	-1.422671
1	4.677856	0.854389	1.445798
1	6.235294	-1.069308	1.371103
1	5.975629	-2.792821	-0.378150
1	4.164656	-2.596983	-2.047926
1	2.622701	-0.674355	-1.976483
1	0.575898	-0.635311	2.679558
1	2.191835	-0.188675	2.190159
1	0.921856	-2.742897	1.745781
1	2.425249	-2.238300	1.002472

C3-TS(3-5)*re*

Eelec = -1870.8829939
E = -1870.371225
H = -1870.340564
G = -1870.434936
Nimag = 1(-39.6425)

1	4.608180	1.664198	1.136981
1	6.398995	0.054740	1.713078
1	6.456694	-2.159615	0.618913
1	4.735789	-2.757124	-1.051166
1	2.966086	-1.144708	-1.633538
6	3.731185	-0.882393	-0.921365
6	4.727881	-1.784598	-0.584938
6	5.687246	-1.448669	0.358047
6	5.655322	-0.207061	0.975874
6	4.656786	0.698435	0.655783
6	3.702923	0.346923	-0.286042
7	2.713544	1.317226	-0.648468
6	3.004657	2.390622	-1.459001
1	3.993020	2.545096	-1.844978
6	1.870187	3.094047	-1.609371
1	1.660503	4.000405	-2.141980
6	1.416290	1.347655	-0.298778
7	0.897168	2.441023	-0.882712
6	-0.456460	2.891808	-0.828474
6	-1.049762	3.190127	0.385461
1	-0.516689	3.044011	1.311381
6	-2.356536	3.649513	0.398146
1	-2.829785	3.854851	1.345265
6	-3.047342	3.829052	-0.789273
1	-4.064391	4.190867	-0.772136
6	-2.439404	3.530885	-2.000182
1	-2.979368	3.655265	-2.926518
6	-1.140792	3.052062	-2.023985
6	0.648131	0.334927	0.476341
1	-0.326251	0.793336	0.668766

6	1.308428	-0.072425	1.825685
1	0.592931	0.109756	2.620978
1	2.182655	0.537518	2.045469
6	1.652814	-1.555043	1.714685
1	2.723234	-1.749654	1.781802
1	1.168747	-2.145967	2.490365
6	1.159107	-2.012263	0.348050
8	1.300115	-3.180044	-0.048414
6	0.532993	-0.938398	-0.292040
1	0.183183	-0.965414	-1.311571
8	-1.554292	-1.321616	3.195903
8	-1.921321	1.090476	2.682067
16	-2.332388	-0.296300	2.517451
6	-4.006150	-0.419913	3.075259
1	-4.004937	-0.171485	4.132088
1	-4.351161	-1.436689	2.923408
1	-4.610954	0.284137	2.515480
7	-2.512405	-0.595649	0.911049
1	-1.348669	-2.310716	1.073505
1	-0.666353	2.787570	-2.957364
6	-1.918401	-1.643735	0.434805
6	-2.226020	-2.108441	-0.917052
6	-3.162879	-1.441791	-1.705819
6	-3.482183	-1.925593	-2.961722
6	-2.870405	-3.078013	-3.439516
6	-1.933366	-3.740575	-2.658953
6	-1.610868	-3.263234	-1.399743
1	-3.631826	-0.551287	-1.315513
1	-4.212949	-1.410343	-3.568147
1	-3.124184	-3.457735	-4.418730
1	-1.446971	-4.629306	-3.032753
1	-0.841766	-3.743078	-0.809115

C1-TS(3-5)*si*

Eelec = -1870.8666555
E = -1870.354662
H = -1870.324211
G = -1870.418027
Nimag = 1(-273.4093)

6	-0.806927	0.810667	-1.878845
6	0.155925	0.568088	-0.679128
6	-0.711088	-0.086384	0.361954
6	-2.089621	0.139375	0.056343
6	-2.220877	0.768779	-1.318345
8	-3.047589	-0.147685	0.761945
6	0.873172	1.783194	-0.199339
7	2.209720	1.930906	-0.203226
6	2.555267	3.128815	0.382365

6	1.407698	3.729460	0.738322
7	0.378545	2.892781	0.371554
6	3.173594	1.041925	-0.766428
6	3.148576	0.769993	-2.125172
6	4.112386	-0.067022	-2.662681
6	5.099920	-0.604363	-1.850249
6	5.121158	-0.312621	-0.495011
6	4.151053	0.508684	0.056570
6	-0.993188	3.280493	0.520762
6	-1.504062	4.208379	-0.373643
6	-2.810090	4.642777	-0.220916
6	-3.588208	4.143941	0.813632
6	-3.060533	3.221055	1.703080
6	-1.750468	2.790359	1.568689
6	-0.447580	-2.191262	0.102669
7	-1.554446	-2.901021	0.215147
16	-2.385287	-3.154036	-1.156145
8	-2.078661	-2.134969	-2.167455
6	0.533875	-2.354333	1.201770
6	0.102288	-2.664660	2.490079
6	1.016456	-2.829474	3.514229
6	2.379146	-2.703007	3.268008
6	2.815696	-2.412659	1.985867
6	1.897315	-2.236828	0.958951
8	-2.256638	-4.541035	-1.577971
6	-4.056838	-2.925957	-0.629752
1	-4.687195	-3.108901	-1.494724
1	-4.168087	-1.917026	-0.247989
1	-4.258899	-3.655134	0.147112
1	-0.013919	-2.012029	-0.879570
1	-0.957430	-2.781927	2.659334
1	0.668936	-3.071419	4.508270
1	3.092176	-2.847978	4.066576
1	3.873821	-2.343444	1.777079
1	2.247391	-2.038710	-0.045062
1	-0.888109	4.574887	-1.181529
1	-3.220811	5.359402	-0.915622
1	-4.611849	4.468922	0.921653
1	-3.670534	2.814999	2.494180
1	-1.338204	2.060594	2.246144
1	2.383473	1.204867	-2.750531
1	4.091996	-0.294721	-3.717270
1	5.850511	-1.254348	-2.273451
1	5.884645	-0.736343	0.139391
1	4.136589	0.714350	1.116182
1	3.578158	3.437136	0.471999
1	1.215763	4.670818	1.214561
1	0.960837	-0.097582	-1.000757
1	-0.404037	-0.087826	1.396252
1	-2.658208	1.759496	-1.191880

1	-2.888274	0.179052	-1.938674
1	-0.577181	1.732290	-2.413636
1	-0.674845	-0.018475	-2.568891

C2-TS(3-5)$_{si}$

Eelec = -1870.883573
E = -1870.371752
H = -1870.341129
G = -1870.43557
Nimag = 1(-49.1177)

6	-2.525623	-1.626417	1.855271
6	-1.854607	-2.309422	0.840946
6	-1.248435	-3.533669	1.121083
6	-1.312506	-4.063132	2.399514
6	-1.974687	-3.376203	3.407184
6	-2.579037	-2.155575	3.132523
6	-1.834117	-1.794980	-0.528806
7	-2.661880	-0.849448	-0.856102
16	-2.684567	-0.411104	-2.437327
6	0.468698	-0.781017	-0.529316
6	0.558856	0.218426	0.576407
6	1.208577	-0.568606	1.752344
6	1.737415	-1.872039	1.165877
6	1.164104	-1.961437	-0.242237
6	1.310463	1.443120	0.174463
7	0.815781	2.690305	0.176770
6	1.761975	3.573749	-0.292353
6	2.856735	2.850309	-0.583487
7	2.565235	1.537212	-0.292568
6	-0.468858	3.106962	0.650454
6	-1.607622	2.799595	-0.072271
6	-2.831183	3.248468	0.401539
6	-2.905782	3.999343	1.564387
6	-1.751936	4.303655	2.272769
6	-0.523697	3.853785	1.817759
6	3.536426	0.492942	-0.428278
6	3.475471	-0.378640	-1.501567
6	4.448698	-1.356862	-1.622210
6	5.476338	-1.440239	-0.694485
6	5.536746	-0.547031	0.364430
6	4.558902	0.425189	0.504527
8	1.304927	-2.967079	-0.949847
1	-1.298042	-2.377262	-1.273306
1	3.810151	3.132761	-0.984634
1	1.552314	4.620438	-0.391485
1	-0.421288	0.591125	0.889796
1	0.158464	-0.509895	-1.525898
1	-3.099543	-1.622512	3.914932

1	-3.006498	-0.689013	1.619448
1	-0.711575	-4.049289	0.337492
1	-0.843030	-5.012929	2.609362
1	-2.024555	-3.792332	4.402945
1	0.383084	4.070243	2.363279
1	-1.806729	4.884209	3.181139
1	-3.863462	4.347018	1.922050
1	-3.724077	3.003853	-0.152654
1	-1.563976	2.209724	-0.977729
1	4.581165	1.119598	1.331531
1	6.335124	-0.611459	1.088029
1	6.227640	-2.209192	-0.792981
1	4.386471	-2.063897	-2.434011
1	2.663617	-0.317761	-2.207228
1	0.427114	-0.766954	2.481708
1	1.976045	0.014015	2.261212
1	1.442514	-2.743299	1.747341
1	2.825213	-1.891348	1.089160
8	-2.397986	1.017697	-2.514788
8	-1.912091	-1.302061	-3.286053
6	-4.395545	-0.620190	-2.831184
1	-4.528579	-0.273711	-3.851350
1	-4.644550	-1.672466	-2.750538
1	-4.987291	-0.027457	-2.143258

C3-TS(3-5)*si*

Eelec = -1870.8769259
E = -1870.365154
H = -1870.334834
G = -1870.427657
Nimag = 1(-145.2583)

6	3.105827	-1.432608	-1.242777
6	2.610164	-2.091599	-0.134587
6	3.404744	-2.365337	0.966270
6	4.730922	-1.973479	0.948297
6	5.245619	-1.319486	-0.160924
6	4.434624	-1.041693	-1.247654
7	1.277584	-2.618216	-0.161080
6	0.112527	-1.985575	0.052925
7	-0.843642	-2.923879	-0.081766
6	-0.272423	-4.140294	-0.378133
6	1.054906	-3.949033	-0.430538
6	-0.038907	-0.522997	0.332299
6	-0.625136	0.207429	-0.837632
6	-2.005869	0.446966	-0.639859
6	-2.313800	0.302159	0.842456
6	-1.014268	-0.175226	1.486727
8	-2.851182	0.764268	-1.476304

6	-2.264120	-2.797891	0.038941
6	-3.008138	-2.360988	-1.041717
6	-4.388350	-2.310703	-0.926641
6	-5.006239	-2.713612	0.246382
6	-4.247776	-3.166283	1.317378
6	-2.867657	-3.210932	1.216647
6	0.240110	2.393442	-0.424560
6	-0.977148	3.175625	-0.184829
6	-1.841825	3.466785	-1.236993
6	-2.944736	4.279558	-1.032089
6	-3.198561	4.806200	0.224166
6	-2.343201	4.516958	1.280798
6	-1.239247	3.709729	1.078081
7	1.115424	2.287475	0.550500
16	2.651606	1.961705	0.150911
8	3.175925	0.955759	1.061962
8	2.824620	1.734475	-1.283389
6	3.471781	3.482616	0.544349
1	0.557811	2.295757	-1.456478
1	-0.874807	-5.014086	-0.530185
1	1.866144	-4.617749	-0.639992
1	0.964552	-0.170910	0.594642
1	-0.215367	0.092812	-1.831767
1	-2.534290	4.930571	2.260468
1	-0.550986	3.495430	1.881565
1	-1.660114	3.039967	-2.211096
1	-3.612176	4.490100	-1.854143
1	-4.059611	5.439331	0.381974
1	3.083202	4.267092	-0.095799
1	3.289823	3.709549	1.588657
1	4.531934	3.332569	0.364613
1	2.984731	-2.871913	1.822346
1	5.358018	-2.168871	1.804609
1	6.278943	-1.006966	-0.167924
1	4.822728	-0.500500	-2.095623
1	2.461865	-1.211958	-2.079537
1	-2.260665	-3.553280	2.041559
1	-4.728457	-3.477218	2.232442
1	-6.081436	-2.666348	0.331211
1	-4.972094	-1.933443	-1.751136
1	-2.517974	-2.025756	-1.941452
1	-0.541014	0.630408	2.041774
1	-1.155070	-1.002988	2.180124
1	-2.639558	1.267025	1.228518
1	-3.145232	-0.387938	0.973611

(V) Important Diastereomeric Transition States in Conventional Pathway

TS(5-6)'

Eelec = -1870.8571809
E = -1870.347404
H = -1870.317172
G = -1870.410189
Nimag = 1(-1772.1966)

6	-3.258329	-2.400261	0.429592
6	-2.666724	-1.476374	-0.415994
6	-3.364308	-0.385970	-0.909097
6	-4.675851	-0.203030	-0.500166
6	-5.277726	-1.104387	0.365141
6	-4.572192	-2.205944	0.824901
7	-1.335236	-1.728448	-0.891580
6	-0.164111	-1.557113	-0.263503
7	0.782465	-2.011792	-1.100761
6	0.204950	-2.428435	-2.279940
6	-1.118762	-2.247119	-2.145216
6	0.105615	-0.946936	1.075373
6	-0.601709	0.375258	1.296443
6	-1.257702	0.353708	2.581989
6	-1.395680	-1.090034	3.040248
6	-0.329256	-1.856320	2.266900
6	-0.026746	1.668654	0.734226
7	-0.553064	1.473972	-0.635340
16	-1.172034	2.728799	-1.448006
6	0.144013	3.408247	-2.431064
8	-1.662039	1.303239	3.224784
6	2.181780	-2.114500	-0.854832
6	3.061226	-1.527564	-1.749535
6	4.424106	-1.678599	-1.556154
6	4.898993	-2.398827	-0.471128
6	4.009028	-2.980310	0.418978
6	2.643871	-2.850751	0.224252
6	1.453572	1.880555	0.871951
6	2.340057	1.664089	-0.174082
6	3.704883	1.856338	-0.000098
6	4.201371	2.262146	1.227414
6	3.322174	2.478002	2.281526
6	1.962198	2.291231	2.103927
8	-2.132369	2.162351	-2.394488
8	-1.614412	3.804083	-0.572477
1	-0.554537	2.478136	1.243395
1	-1.934937	-2.442312	-2.812458
1	0.790229	-2.831104	-3.082552
1	1.189056	-0.818600	1.101365

1	-1.271524	0.678164	0.115490
1	4.380543	1.694717	-0.828114
1	1.942126	1.357635	-1.130398
1	1.276374	2.472206	2.920493
1	3.697989	2.803569	3.240768
1	5.261647	2.418672	1.362452
1	1.943457	-3.321357	0.897413
1	4.375313	-3.545306	1.262396
1	5.962010	-2.506437	-0.318277
1	5.114479	-1.220636	-2.247928
1	2.680253	-0.946900	-2.576077
1	-2.702523	-3.262492	0.766179
1	-5.041665	-2.916123	1.488691
1	-6.298542	-0.949672	0.680640
1	-5.218622	0.658404	-0.857628
1	-2.890959	0.328904	-1.571504
1	0.543063	-2.022053	2.896450
1	-0.665862	-2.838283	1.937344
1	-1.267443	-1.146539	4.117777
1	-2.404788	-1.430359	2.811562
1	-0.275979	4.235659	-2.995145
1	0.930338	3.763321	-1.773204
1	0.511994	2.639959	-3.102117

TS(5-6)''

Eelec = -1870.8657536
E = -1870.356158
H = -1870.325906
G = -1870.418542
Nimag = 1(-1742.2951)

6	-1.402337	2.648523	1.490650
6	-2.445802	1.804535	1.452952
7	-2.284635	1.005437	0.345230
6	-1.149521	1.336776	-0.289478
7	-0.618928	2.356585	0.400599
1	-1.128342	3.411637	2.191072
1	-3.280542	1.674602	2.112483
6	-0.482529	0.682715	-1.455539
6	0.038060	-0.706015	-1.124643
6	0.015610	-1.488052	-2.343295
6	-0.716199	-0.698568	-3.420485
6	-1.368125	0.468465	-2.697775
1	0.338842	1.354715	-1.722149
1	0.044611	-0.361380	-4.127281
1	-1.413848	-1.324457	-3.970719
1	-1.439548	1.373216	-3.299569
1	-2.372888	0.187782	-2.401821
8	0.486775	-2.591707	-2.537104

1	-0.580630	-1.339601	-0.001879
6	1.107586	-0.833931	-0.035380
7	0.250879	-1.534094	0.944750
1	1.357456	0.166270	0.324201
16	0.221451	-1.055528	2.473345
8	0.711662	0.320550	2.629628
8	-1.109360	-1.345024	3.001344
6	1.363047	-2.079845	3.363920
1	1.355902	-1.763577	4.402569
1	1.034503	-3.108857	3.270940
1	2.349957	-1.954172	2.930413
6	2.403120	-1.526361	-0.360149
6	3.505221	-0.769738	-0.743552
6	4.715137	-1.375668	-1.048301
6	4.838542	-2.753564	-0.962769
6	3.744660	-3.514996	-0.575706
6	2.536188	-2.907098	-0.278646
1	3.418362	0.307859	-0.797683
1	5.561206	-0.771577	-1.343209
1	5.779300	-3.231074	-1.195243
1	3.830707	-4.590280	-0.515135
1	1.678932	-3.495701	0.007016
6	0.599827	3.047700	0.115721
6	1.694856	2.829115	0.935129
6	2.863333	3.531542	0.680346
6	2.927180	4.429586	-0.374379
6	1.818524	4.638461	-1.182308
6	0.642178	3.950117	-0.935016
1	1.621003	2.104852	1.735482
1	3.727411	3.367077	1.306039
1	3.842287	4.968673	-0.568424
1	1.866502	5.339833	-2.001326
1	-0.234014	4.109209	-1.545875
6	-3.270045	0.020400	-0.004144
6	-4.293073	0.383675	-0.867246
6	-5.284479	-0.535964	-1.163644
6	-5.251422	-1.797873	-0.586582
6	-4.237492	-2.133174	0.296222
6	-3.237731	-1.221480	0.603765
1	-4.306294	1.372321	-1.301999
1	-6.080722	-0.266058	-1.840610
1	-6.023020	-2.516145	-0.819984
1	-4.217858	-3.109061	0.756556
1	-2.462208	-1.459403	1.319638

(VI) Conformational Sampling in Bimolecular Pathway

C1-TS(5-8)*re*

Eelec = -2784.3504555
E = -2783.667459
H = -2783.625761
G = -2783.744113
Nimag = 1(-220.3612)

6	1.448935	4.325910	-0.224866
6	1.224109	3.247096	0.616962
6	0.082158	3.136956	1.386643
6	-0.876714	4.133556	1.277247
6	-0.679995	5.211377	0.431265
6	0.483139	5.312266	-0.317611
7	2.275214	2.273933	0.755506
6	2.520047	1.199159	-0.000648
7	3.685528	0.685340	0.424593
6	4.165873	1.433348	1.472277
6	3.279625	2.423996	1.680619
6	1.727015	0.614775	-1.107736
6	0.246155	0.262174	-0.820490
6	-0.119920	-0.188005	-2.227162
6	0.536915	0.780843	-3.190430
6	1.634244	1.473024	-2.383025
6	-0.025650	-0.509923	0.479091
6	0.461645	-1.947700	0.594528
6	1.124654	-2.294426	1.773400
6	1.577924	-3.585885	1.993709
6	1.381552	-4.562182	1.028169
6	0.710653	-4.234223	-0.140108
6	0.245429	-2.943908	-0.353476
8	-0.716497	-1.163879	-2.580062
6	4.441596	-0.363484	-0.195683
6	5.546645	-0.000119	-0.951610
6	6.315911	-0.989386	-1.540708
6	5.973249	-2.323872	-1.375220
6	4.865245	-2.669840	-0.617903
6	4.091494	-1.689433	-0.014842
7	-1.392252	-0.284646	0.940260
16	-1.514195	-0.206812	2.542320
8	-1.824427	-1.472776	3.204690
6	-3.063628	-0.427573	-0.198664
7	-2.918686	0.334898	-1.264370
16	-3.134566	1.921359	-1.119966
8	-3.704846	2.334903	0.163201
6	-3.216331	-1.886636	-0.429808
6	-3.372808	-2.364848	-1.726081

6	-3.614572	-3.710488	-1.951899
6	-3.707584	-4.589673	-0.883683
6	-3.552107	-4.116354	0.411829
6	-3.307880	-2.773043	0.639882
6	-4.355868	2.244358	-2.360469
8	-1.918364	2.613102	-1.549036
8	-0.343365	0.502854	3.097931
6	-2.915574	0.837451	2.841767
1	0.601512	0.030243	1.195278
1	5.080803	1.179318	1.969975
1	3.254128	3.218030	2.400609
1	2.248091	-0.310847	-1.356822
1	0.911075	0.224201	-4.045986
1	-0.219696	1.479683	-3.540583
1	2.585042	1.521425	-2.909632
1	1.331859	2.483226	-2.122663
1	-0.291883	1.210612	-0.716675
1	1.253171	-1.546608	2.544607
1	2.070947	-3.829227	2.923989
1	1.726902	-5.572553	1.194784
1	0.526824	-4.991476	-0.888760
1	-0.305152	-2.715267	-1.250502
1	3.227248	-1.955503	0.576069
1	4.591445	-3.705418	-0.488334
1	6.570840	-3.094067	-1.839030
1	7.177325	-0.716856	-2.131168
1	5.795633	1.043532	-1.076132
1	2.366293	4.390830	-0.791736
1	0.637233	6.153127	-0.976536
1	-1.441556	5.971409	0.345987
1	-1.792006	4.051142	1.841105
1	-0.055529	2.287414	2.045549
1	-3.607876	-0.035531	0.650450
1	-3.296989	-1.669575	-2.546083
1	-3.732674	-4.070776	-2.963669
1	-3.898773	-5.638857	-1.058769
1	-3.610274	-4.795991	1.249276
1	-3.139058	-2.423888	1.648137
1	-4.504566	3.319055	-2.394908
1	-3.986863	1.877369	-3.311466
1	-5.274470	1.738888	-2.083707
1	-2.822804	1.131428	3.882953
1	-2.909751	1.691018	2.173983
1	-3.828389	0.265677	2.715423

C2-TS(5-8)*re*

Eelec = -2784.3673892
E = -2783.684356
H = -2783.642875

G = -2783.76078
Nimag = 1(-197.3010)

6	0.563969	3.144359	-1.132525
6	1.866046	3.033099	-0.678470
6	2.454268	4.003714	0.118531
6	1.708522	5.114201	0.477903
6	0.398635	5.241259	0.034803
6	-0.170884	4.262414	-0.764895
7	2.646386	1.898367	-1.070861
6	2.850936	0.784982	-0.362448
7	3.643684	-0.002366	-1.100929
6	3.903348	0.610923	-2.302792
6	3.275290	1.799749	-2.285142
6	2.255892	0.516977	0.973132
6	1.186447	-0.595217	0.951288
6	1.391842	-1.323923	2.270582
6	2.366977	-0.546485	3.119578
6	3.246679	0.150900	2.094101
6	-0.251381	-0.012849	0.669051
6	-0.927036	0.324336	1.981369
6	-0.903741	1.641462	2.429508
6	-1.425487	1.985430	3.667592
6	-1.996942	1.014787	4.473490
6	-2.043726	-0.299198	4.029956
6	-1.509193	-0.642011	2.799040
8	0.917419	-2.389803	2.550899
6	4.212481	-1.274934	-0.760947
6	5.520013	-1.300563	-0.296241
6	6.107905	-2.518904	-0.003159
6	5.389344	-3.693658	-0.181111
6	4.090668	-3.649557	-0.661377
6	3.489221	-2.435897	-0.966984
7	-1.054974	-0.856456	-0.203657
16	-0.295202	-1.170763	-1.586972
8	0.422604	-2.455834	-1.544026
6	-1.533257	-1.361876	-2.823695
8	0.575317	-0.045505	-1.983330
6	-3.048376	-0.506611	-0.229358
7	-3.461211	0.270950	-1.212154
16	-3.318652	1.870709	-1.045814
6	-4.937806	2.411443	-1.515754
6	-3.569885	-1.908240	-0.272563
6	-2.921155	-2.993266	0.311849
6	-3.509686	-4.247337	0.309448
6	-4.753064	-4.440849	-0.274283
6	-5.402212	-3.368758	-0.865868
6	-4.813771	-2.113671	-0.866128
8	-2.397764	2.394761	-2.052901
8	-3.086318	2.298801	0.330261

1	-0.063776	0.940721	0.171005
1	3.204961	2.579522	-3.017048
1	4.500949	0.132221	-3.052855
1	1.763752	1.444161	1.265837
1	1.783619	0.180697	3.690472
1	2.893767	-1.190247	3.816603
1	3.753171	1.031808	2.482397
1	4.005512	-0.540662	1.736605
1	1.411611	-1.335695	0.190642
1	-0.514295	2.415802	1.784255
1	-1.407848	3.017104	3.987231
1	-2.414939	1.280103	5.433593
1	-2.495461	-1.063878	4.644747
1	-1.537657	-1.668575	2.473627
1	0.120178	2.364136	-1.734824
1	-1.194140	4.328871	-1.098038
1	-0.182187	6.105262	0.321569
1	2.150079	5.877290	1.101004
1	3.477184	3.888854	0.446206
1	6.062239	-0.375839	-0.162553
1	7.122544	-2.550195	0.363902
1	5.846083	-4.643656	0.052628
1	3.529943	-4.560579	-0.803933
1	2.474663	-2.403731	-1.347409
1	-2.907525	-0.081398	0.757575
1	-5.309841	-1.274229	-1.327406
1	-6.368321	-3.506737	-1.329321
1	-5.207749	-5.420850	-0.275074
1	-2.984532	-5.079075	0.755682
1	-1.931055	-2.857908	0.713679
1	-5.654620	2.037520	-0.793007
1	-4.926324	3.496844	-1.515204
1	-5.153429	2.033082	-2.508566
1	-0.977749	-1.596160	-3.726353
1	-2.178959	-2.189390	-2.552200
1	-2.100714	-0.444523	-2.919803

C3-TS(5-8)*re*

Eelec = -2784.3632445
E = -2783.680376
H = -2783.639007
G = -2783.754692
Nimag = 1(-254.2963)

6	4.039493	-1.974734	1.265567
6	3.127704	-2.043339	0.218657
6	3.575288	-1.898814	-1.088887
6	4.917727	-1.667796	-1.337938
6	5.824468	-1.594162	-0.290090

6	5.383526	-1.751967	1.015785
6	1.710608	-2.365475	0.512848
7	1.014126	-2.916971	-0.467199
16	-0.308352	-3.728484	-0.065524
8	-1.487781	-3.113525	-0.677254
8	-0.406454	-4.013987	1.369599
6	-0.061951	-5.269347	-0.898390
7	1.037868	-0.586681	0.992590
16	0.164899	-0.296386	2.306608
6	0.479732	-1.644119	3.398301
6	0.743817	0.446231	0.000410
6	1.990611	1.122658	-0.545793
6	3.099097	1.235076	0.288212
6	4.213294	1.960745	-0.095983
6	4.240388	2.608845	-1.322019
6	3.135406	2.524358	-2.152011
6	2.022915	1.791308	-1.764017
6	-0.372116	0.056289	-0.995644
6	-1.440980	1.156957	-1.238283
6	-2.238182	0.641537	-2.442460
6	-1.164835	0.050127	-3.341256
6	-0.037523	-0.369361	-2.416344
6	-2.232633	1.583344	-0.049037
7	-3.339366	1.053915	0.482116
6	-3.697480	1.760043	1.601988
6	-2.812072	2.760928	1.742848
7	-1.923386	2.651596	0.703843
6	-4.114211	-0.064894	0.032504
6	-5.321465	0.197202	-0.600904
6	-6.107107	-0.866240	-1.008048
6	-5.677773	-2.168676	-0.782953
6	-4.471618	-2.407472	-0.145815
6	-3.680825	-1.350738	0.283981
6	-0.891788	3.618939	0.472507
6	-1.061367	4.548572	-0.542477
6	-0.083978	5.508450	-0.744108
6	1.038163	5.536012	0.071465
6	1.183740	4.607957	1.090076
6	0.215027	3.638829	1.303953
8	0.952923	-0.931062	-2.784868
8	0.607285	0.929621	2.990375
8	-1.283785	-0.291498	2.032219
1	0.291939	1.270594	0.557637
1	-2.720466	3.535056	2.478266
1	-4.538395	1.464496	2.197019
1	-0.906699	2.057532	-1.546106
1	-0.758160	0.787822	-4.035343
1	-1.497830	-0.797901	-3.933303
1	-2.817772	1.428966	-2.920108
1	-2.926080	-0.139704	-2.134522

1	-0.877543	-0.821412	-0.582602
1	3.073765	0.735029	1.242832
1	5.066254	2.013633	0.565030
1	5.111969	3.169266	-1.627671
1	3.136527	3.021849	-3.111278
1	1.186712	1.747994	-2.444216
1	0.329684	2.888620	2.077931
1	2.063100	4.619677	1.715017
1	1.803298	6.279692	-0.092564
1	-0.201032	6.234115	-1.534637
1	-1.948568	4.521849	-1.158345
1	-5.629557	1.217466	-0.777189
1	-7.047216	-0.679711	-1.504919
1	-6.286991	-2.997800	-1.110833
1	-4.117165	-3.413026	0.013046
1	-2.744523	-1.517973	0.791998
1	1.550951	-2.718621	1.523766
1	2.856612	-1.955041	-1.891043
1	5.257960	-1.543588	-2.355621
1	6.871689	-1.418587	-0.490117
1	6.084982	-1.706286	1.836199
1	3.695685	-2.096939	2.283490
1	-0.954994	-5.867427	-0.746895
1	0.091534	-5.064836	-1.951898
1	0.806095	-5.759485	-0.471965
1	-0.069531	-1.392356	4.300182
1	0.097927	-2.563644	2.963021
1	1.540282	-1.694434	3.618520

C1-TS(5-8)*si*

Eelec = -2784.3566219
E = -2783.673483
H = -2783.632162
G = -2783.748259
Nimag = 1(-258.5316)

6	-2.632601	-2.064823	2.042873
6	-2.089336	-2.079739	0.765456
6	-1.178923	-3.075983	0.425861
6	-0.801690	-4.030006	1.357268
6	-1.343706	-4.005503	2.635858
6	-2.260261	-3.021953	2.973116
6	-2.589695	-1.144824	-0.284543
7	-3.680681	-0.453083	0.041370
16	-4.652416	-0.006387	-1.155753
8	-4.610188	1.438156	-1.382397
8	-4.494045	-0.839155	-2.353820
6	-6.241627	-0.360464	-0.466155
7	-1.105494	-0.024758	-0.652764

16	-0.537440	-0.208422	-2.145193
6	-1.719861	0.474049	-3.263103
6	-0.266536	0.748730	0.252488
6	-0.984065	1.862809	0.995863
6	-0.344105	2.569038	2.012888
6	-0.930606	3.676826	2.601735
6	-2.176890	4.111621	2.176290
6	-2.815107	3.426344	1.156131
6	-2.222270	2.318130	0.568089
6	0.688687	-0.137204	1.096980
6	2.180142	0.273174	1.052816
6	2.826116	-0.540489	2.182099
6	1.796791	-0.446718	3.296059
6	0.458902	-0.291608	2.595935
6	2.861521	0.222203	-0.268769
7	3.270235	-0.828390	-0.989523
6	3.840678	-0.388683	-2.159471
6	3.798511	0.954319	-2.141923
7	3.207676	1.316315	-0.959777
6	3.198316	-2.229031	-0.684693
6	4.258727	-2.816151	-0.009737
6	4.243264	-4.183069	0.206300
6	3.184808	-4.946536	-0.268143
6	2.144064	-4.344217	-0.955927
6	-2.632601	-2.064823	2.042873
6	-2.089336	-2.079739	0.765456
6	-1.178923	-3.075983	0.425861
6	-0.801690	-4.030006	1.357268
6	-1.343706	-4.005503	2.635858
6	-2.260261	-3.021953	2.973116
6	-2.589695	-1.144824	-0.284543
7	-3.680681	-0.453083	0.041370
16	-4.652416	-0.006387	-1.155753
8	-4.610188	1.438156	-1.382397
8	-4.494045	-0.839155	-2.353820
6	-6.241627	-0.360464	-0.466155
7	-1.105494	-0.024758	-0.652764
16	-0.537440	-0.208422	-2.145193
6	-1.719861	0.474049	-3.263103
6	-0.266536	0.748730	0.252488
6	-0.984065	1.862809	0.995863
6	-0.344105	2.569038	2.012888
6	-0.930606	3.676826	2.601735
6	-2.176890	4.111621	2.176290
6	-2.815107	3.426344	1.156131
6	-2.222270	2.318130	0.568089
6	0.688687	-0.137204	1.096980
6	2.180142	0.273174	1.052816
6	2.826116	-0.540489	2.182099
6	1.796791	-0.446718	3.296059

6	0.458902	-0.291608	2.595935
6	2.861521	0.222203	-0.268769
7	3.270235	-0.828390	-0.989523
6	3.840678	-0.388683	-2.159471
6	3.798511	0.954319	-2.141923
7	3.207676	1.316315	-0.959777
6	3.198316	-2.229031	-0.684693
6	4.258727	-2.816151	-0.009737
6	4.243264	-4.183069	0.206300
6	3.184808	-4.946536	-0.268143
6	2.144064	-4.344217	-0.955927
6	2.140771	-2.973050	-1.174319
6	2.954832	2.678301	-0.598578
6	3.802841	3.311932	0.295540
6	3.562042	4.636779	0.621747
6	2.490852	5.308122	0.050012
6	1.659495	4.661564	-0.851498
6	1.887963	3.336158	-1.186646
8	-0.597474	-0.283091	3.154054
8	0.703735	0.569101	-2.321935
8	-0.425069	-1.629627	-2.488295
1	0.416843	1.292349	-0.399061
1	4.117035	1.685831	-2.857451
1	4.207969	-1.080536	-2.891102
1	2.230138	1.325266	1.334576
1	1.945869	0.441342	3.912588
1	1.777322	-1.302886	3.964645
1	3.804740	-0.154573	2.460948
1	2.947868	-1.576484	1.877289
1	0.602545	-1.155110	0.708628
1	0.629199	2.266166	2.372614
1	-0.414241	4.195556	3.396913
1	-2.642635	4.970150	2.638055
1	-3.786933	3.740721	0.804990
1	-2.746163	1.804316	-0.218477
1	1.250639	2.798368	-1.874077
1	0.819752	5.181843	-1.285487
1	2.301157	6.337971	0.312013
1	4.211141	5.143003	1.319917
1	4.637453	2.775935	0.723095
1	5.081828	-2.208656	0.336658
1	5.059409	-4.651631	0.734883
1	3.177521	-6.013948	-0.105617
1	1.325659	-4.937773	-1.334405
1	1.333973	-2.495396	-1.718085
1	-2.549719	-1.592977	-1.274082
1	-0.785639	-3.093931	-0.580722
1	-0.098910	-4.803715	1.083237
1	-1.060516	-4.756194	3.359950
1	-2.685244	-2.995599	3.965722

1	-3.351246	-1.299024	2.286832
1	-6.983555	-0.030643	-1.186333
1	-6.317628	-1.427974	-0.293640
1	-6.338848	0.188839	0.463449
1	-1.295025	0.377852	-4.257731
1	-2.652280	-0.079608	-3.186938
1	-1.881878	1.514162	-3.002056

C2-TS(5-8)*si*

Eelec = -2784.3715668
E = -2783.688674
H = -2783.647298
G = -2783.762881
Nimag = 1(-240.4271)

6	-4.073332	-0.786778	0.937513
6	-3.446674	-1.555846	-0.035633
6	-4.208031	-2.110908	-1.059319
6	-5.568534	-1.865748	-1.129818
6	-6.188175	-1.084994	-0.162210
6	-5.438869	-0.555036	0.876298
6	-2.000267	-1.855656	0.106324
7	-1.267732	-0.219342	-0.745747
16	-0.491395	-0.257538	-2.152251
8	-0.592140	1.038635	-2.843733
6	-0.645985	0.788236	0.107004
6	-1.656300	1.757678	0.698668
6	-2.815037	2.032962	-0.020644
6	-3.705032	3.005620	0.404208
6	-3.453704	3.732720	1.558201
6	-2.298376	3.476479	2.278052
6	-1.409846	2.502390	1.847256
6	0.424649	0.209323	1.055771
6	1.730795	1.028515	1.178549
6	2.421610	0.433427	2.413388
6	1.270509	0.183921	3.376683
6	0.065004	-0.075072	2.499351
6	2.529423	1.103559	-0.077793
7	2.472693	2.140236	-0.928878
6	3.245290	1.877921	-2.031653
6	3.803383	0.671273	-1.834467
7	3.367299	0.213360	-0.617567
6	1.787489	3.384340	-0.744311
6	0.668877	3.659944	-1.512375
6	0.042966	4.886933	-1.348710
6	0.531814	5.811185	-0.439025
6	1.659433	5.520512	0.315569
6	2.299033	4.302312	0.160455
6	3.814456	-1.048645	-0.098329

6	5.016633	-1.079421	0.596007
6	5.495568	-2.296221	1.047110
6	4.777651	-3.459258	0.793226
6	3.587528	-3.407789	0.087477
6	3.096050	-2.194456	-0.375286
8	-1.003987	-0.450654	2.895276
8	0.902709	-0.713404	-2.019969
6	-1.372965	-1.441304	-3.105369
7	-1.586310	-2.984508	-0.459162
16	-0.278612	-3.699324	0.147094
8	0.359078	-2.919880	1.213071
6	-0.948012	-5.155062	0.904998
8	0.588103	-4.157861	-0.931669
1	-0.075056	1.444560	-0.555152
1	3.314019	2.572319	-2.844983
1	4.456531	0.080512	-2.445173
1	1.459123	2.061398	1.399624
1	1.049026	1.063129	3.985238
1	1.428855	-0.647771	4.057250
1	3.187415	1.093519	2.815436
1	2.892380	-0.511945	2.161728
1	0.688245	-0.779562	0.669941
1	-3.009079	1.460849	-0.914118
1	-4.603035	3.189556	-0.167806
1	-4.150812	4.486366	1.894351
1	-2.086403	4.030090	3.181401
1	-0.521093	2.336035	2.437255
1	0.280683	2.913488	-2.195831
1	-0.841180	5.107740	-1.926482
1	0.031420	6.759518	-0.313570
1	2.044434	6.241931	1.020212
1	3.188081	4.065596	0.726698
1	5.559682	-0.163843	0.779945
1	6.426204	-2.337431	1.592844
1	5.153003	-4.407620	1.148212
1	3.013057	-4.297681	-0.116186
1	2.177246	-2.142953	-0.939839
1	-1.576715	-1.548949	1.055724
1	-3.486059	-0.373008	1.744383
1	-5.914994	0.041299	1.640747
1	-7.251978	-0.902965	-0.212524
1	-6.151298	-2.296807	-1.931028
1	-3.727166	-2.754678	-1.779381
1	-0.115199	-5.736442	1.288301
1	-1.610154	-4.856176	1.710277
1	-1.488939	-5.713811	0.149520
1	-0.846792	-1.500947	-4.052634
1	-1.354781	-2.391413	-2.579229
1	-2.384437	-1.079343	-3.249985

C3-TS(5-8)*si*

Eelec = -2784.3474283
E = -2783.664182
H = -2783.622745
G = -2783.740489
Nimag = 1(-249.1077)

6	2.724084	2.554898	0.360377
6	2.859953	1.319513	0.987856
6	2.963868	1.271519	2.372884
6	2.896040	2.435624	3.124484
6	2.749813	3.663421	2.496379
6	2.671643	3.717939	1.110895
6	3.049994	0.078395	0.175301
7	3.314214	-1.026596	0.861696
16	4.225981	-2.150634	0.157230
8	4.706405	-1.747262	-1.168041
6	5.647442	-2.196792	1.216899
8	3.599157	-3.460810	0.262590
7	1.384161	0.032667	-0.795959
16	1.561238	0.211387	-2.386594
8	0.243507	0.396720	-3.024749
6	0.076958	-0.452562	-0.372881
6	-0.087023	-1.961474	-0.365500
6	-0.870625	-2.526936	-1.373431
6	-1.029951	-3.901815	-1.477234
6	-0.396873	-4.735967	-0.568114
6	0.411204	-4.185793	0.415304
6	0.574153	-2.812472	0.515262
6	-0.449896	0.321185	0.849745
6	-1.987515	0.348582	1.004323
6	-2.209428	1.142075	2.302607
6	-1.119788	0.594162	3.213636
6	-0.091438	-0.035271	2.288199
6	-2.817355	0.789091	-0.143076
7	-3.909975	0.125264	-0.555677
6	-4.461132	0.769914	-1.636710
6	-3.695549	1.849194	-1.877774
7	-2.693202	1.856646	-0.937475
6	-4.555682	-0.969436	0.109133
6	-4.017286	-2.242946	0.067469
6	-4.685159	-3.270992	0.715452
6	-5.877785	-3.025929	1.377869
6	-6.410517	-1.745038	1.402434
6	-5.747152	-0.707014	0.769605
6	-1.776642	2.961377	-0.839028
6	-2.090748	3.998958	0.026563
6	-1.278511	5.119732	0.046179
6	-0.181701	5.194214	-0.801349

6	0.110259	4.149256	-1.662555
6	-0.692595	3.018316	-1.693987
8	0.801414	-0.727419	2.674352
8	2.545051	1.263721	-2.618022
6	2.225480	-1.267396	-3.091873
1	-0.601679	-0.120471	-1.161319
1	-5.333144	0.390334	-2.131773
1	-3.754982	2.612516	-2.628372
1	-2.304175	-0.678738	1.189642
1	-1.484128	-0.180643	3.885893
1	-0.637841	1.353762	3.825049
1	-3.212697	1.006174	2.700561
1	-2.057574	2.202512	2.113565
1	-0.098296	1.351612	0.723485
1	-1.323047	-1.879554	-2.115083
1	-1.625017	-4.317544	-2.278505
1	-0.500480	-5.808404	-0.649986
1	0.959783	-4.826921	1.088209
1	1.254749	-2.400530	1.241972
1	-3.087048	-2.432919	-0.447592
1	-4.263869	-4.264294	0.695382
1	-6.392776	-3.832654	1.877104
1	-7.338172	-1.550629	1.918690
1	-6.144434	0.297256	0.789394
1	-2.965836	3.937466	0.656757
1	-1.507113	5.935008	0.715531
1	0.447250	6.071660	-0.786480
1	0.969624	4.194606	-2.313871
1	-0.464032	2.189102	-2.353188
1	3.595036	0.262086	-0.745889
1	2.670870	2.582564	-0.718488
1	2.582499	4.673031	0.613699
1	2.716558	4.573020	3.079402
1	2.979368	2.383650	4.200934
1	3.102211	0.309322	2.839477
1	6.297633	-2.983995	0.848003
1	6.147521	-1.235386	1.175757
1	5.316039	-2.416789	2.225574
1	2.320649	-1.091437	-4.159157
1	3.192250	-1.468089	-2.637211
1	1.534909	-2.081418	-2.896528

(VII) Important Diastereomeric Transition States in Bimolecular Pathway

TS(5-8)'

Eelec = -2784.3975568
E = -2783.721287
H = -2783.679939
G = -2783.795543
Nimag = 1(-256.1062)

6	1.416485	4.304902	-0.473321
6	1.259600	3.314387	0.482998
6	0.194858	3.311106	1.366261
6	-0.745805	4.325501	1.271670
6	-0.613581	5.317055	0.312310
6	0.463651	5.306287	-0.561411
7	2.313593	2.352686	0.654717
6	2.581940	1.244418	-0.045676
7	3.740370	0.763937	0.432472
6	4.189477	1.557682	1.459956
6	3.293477	2.550752	1.599063
6	1.823108	0.585436	-1.141094
6	0.322084	0.279095	-0.919293
6	-0.056938	-0.151048	-2.328105
6	0.852529	0.543765	-3.318604
6	1.846311	1.332798	-2.482618
6	0.023942	-0.553352	0.341831
6	0.398922	-2.029531	0.313224
6	1.239571	-2.497934	1.321904
6	1.603878	-3.833428	1.404509
6	1.132895	-4.737506	0.465710
6	0.288448	-4.289782	-0.539536
6	-0.078999	-2.954228	-0.613480
8	-0.905288	-0.932675	-2.659703
6	4.485838	-0.343113	-0.079631
6	5.104637	-0.225672	-1.314672
6	5.856319	-1.285963	-1.794059
6	5.994362	-2.439361	-1.034611
6	5.382472	-2.535418	0.206180
6	4.621027	-1.483742	0.692074
7	-1.293904	-0.252482	0.910980
16	-1.278621	-0.176854	2.518094
8	-1.551256	-1.441773	3.210437
6	-3.054461	-0.402644	-0.001456
7	-3.055898	0.344319	-1.094470
16	-3.336401	1.915399	-0.975090
8	-3.760984	2.346091	0.363035
6	-3.266574	-1.862288	-0.202773
6	-3.487476	-2.361476	-1.482356

6	-3.786218	-3.701847	-1.671372
6	-3.878372	-4.556347	-0.581960
6	-3.667950	-4.061486	0.697712
6	-3.365223	-2.723097	0.886921
6	-4.719024	2.142035	-2.055639
8	-2.225033	2.665349	-1.565419
8	-0.049797	0.494830	2.990254
6	-2.614792	0.901345	2.953177
1	0.761637	-0.110008	1.074728
1	5.105344	1.343590	1.980168
1	3.253569	3.386120	2.274419
1	2.328164	-0.381817	-1.280084
1	1.335123	-0.232529	-3.915853
1	0.257556	1.156056	-3.995401
1	2.845988	1.370064	-2.923010
1	1.488482	2.356357	-2.344322
1	-0.218658	1.249654	-0.796150
1	1.582568	-1.807574	2.082571
1	2.243233	-4.167762	2.210894
1	1.407932	-5.782070	0.524896
1	-0.103359	-4.986378	-1.268684
1	-0.753604	-2.632893	-1.387481
1	4.127017	-1.550805	1.650498
1	5.485697	-3.435336	0.795667
1	6.581402	-3.265365	-1.411351
1	6.339536	-1.207145	-2.757803
1	5.005424	0.686959	-1.885395
1	2.278157	4.299448	-1.126507
1	0.566959	6.079740	-1.309350
1	-1.359282	6.096095	0.238359
1	-1.594770	4.328749	1.939972
1	0.106654	2.519775	2.098815
1	-3.524661	-0.004938	0.889264
1	-3.417220	-1.685958	-2.320906
1	-3.953086	-4.077384	-2.672130
1	-4.114866	-5.601928	-0.728358
1	-3.731181	-4.720118	1.553178
1	-3.165128	-2.357329	1.883321
1	-4.930700	3.207003	-2.092185
1	-4.450859	1.770110	-3.039037
1	-5.566473	1.594812	-1.655335
1	-2.422560	1.169115	3.988727
1	-2.628521	1.770548	2.305728
1	-3.557957	0.368811	2.892360

TS(8-9)'

Eelec = -2784.3826752
E = -2783.712063
H = -2783.671082

G = -2783.785596
Nimag = 1(-1240.6462)

6	3.605319	1.714219	-1.423031
6	3.758123	0.709839	-0.475470
6	5.033242	0.245323	-0.178058
6	6.143255	0.763108	-0.828250
6	5.987202	1.761813	-1.779046
6	4.715450	2.237252	-2.069130
6	2.561758	0.038265	0.171440
7	1.921547	-0.906069	-0.705904
16	2.668954	-2.096527	-1.432767
6	3.543642	-1.490146	-2.851836
7	1.532595	1.062309	0.586348
16	2.020289	1.832486	1.989871
8	1.380167	3.125307	2.086199
6	0.061868	0.776561	0.547483
6	-0.803433	1.991167	0.818218
6	-1.766989	1.931225	1.816438
6	-2.641691	2.990310	2.035140
6	-2.563208	4.121672	1.241737
6	-1.608562	4.184292	0.231446
6	-0.738211	3.130858	0.018600
6	-0.399069	0.103144	-0.740976
6	-1.849207	-0.370614	-0.826498
6	-1.892267	-1.006858	-2.229001
6	-1.111522	0.007975	-3.043581
6	-0.181684	0.677929	-2.051667
6	-2.587157	-1.186005	0.180991
7	-3.935122	-1.133614	0.216934
6	-4.419278	-1.988242	1.174967
6	-3.354273	-2.572236	1.744657
7	-2.228598	-2.069256	1.124143
6	-4.813532	-0.359208	-0.610026
6	-5.547040	-1.014344	-1.586685
6	-6.448765	-0.291445	-2.351932
6	-6.608321	1.069894	-2.137296
6	-5.872788	1.711004	-1.150995
6	-4.975087	0.996335	-0.373343
6	-0.941375	-2.524184	1.555162
6	-0.654034	-2.412312	2.910738
6	0.514613	-2.967355	3.401576
6	1.381240	-3.627839	2.540571
6	1.081530	-3.725638	1.191655
6	-0.089023	-3.176972	0.687495
8	0.637975	1.518358	-2.394932
6	1.431094	0.846736	3.341468
8	3.465789	1.777429	2.042552
8	1.609643	-2.956302	-1.972885
8	3.665517	-2.744268	-0.576324

1	-0.167723	0.026995	1.371202
1	-5.473610	-2.093977	1.355785
1	-3.278068	-3.311454	2.520663
1	-2.478539	0.531644	-0.877655
1	-1.765927	0.780025	-3.457283
1	-0.545181	-0.420820	-3.869198
1	-2.911452	-1.157966	-2.593444
1	-1.372646	-1.970612	-2.210538
1	0.692326	-0.728675	-0.855770
1	-1.829083	1.053721	2.450049
1	-3.371922	2.931792	2.831707
1	-3.231337	4.955084	1.412097
1	-1.535276	5.068586	-0.387218
1	0.012742	3.187927	-0.755287
1	-4.399571	1.486799	0.399030
1	-5.996805	2.771105	-0.980182
1	-7.308498	1.632348	-2.739231
1	-7.022724	-0.793502	-3.118099
1	-5.407952	-2.075082	-1.746531
1	-0.312828	-3.258463	-0.365442
1	1.762155	-4.220852	0.516152
1	2.295721	-4.062495	2.919748
1	0.745962	-2.884403	4.454561
1	-1.341442	-1.899979	3.570840
1	2.939985	-0.507683	1.103214
1	2.613269	2.067190	-1.657994
1	4.584585	3.019820	-2.804664
1	6.851158	2.171429	-2.285067
1	7.129505	0.389800	-0.587433
1	5.158170	-0.532143	0.563240
1	3.925719	-2.362453	-3.375451
1	2.841873	-0.942533	-3.472636
1	4.356544	-0.847586	-2.534169
1	1.898068	1.264435	4.229682
1	0.353097	0.928721	3.416741
1	1.745200	-0.183028	3.199616

TS(9-10)'

Eelec = -2784.4409701
E = -2783.768574
H = -2783.727798
G = -2783.842343
Nimag = 1(-626.8477)

6	-3.986214	-1.613295	1.083918
6	-3.333694	-0.773512	0.185902
6	-3.691795	-0.814754	-1.155114
6	-4.668888	-1.697457	-1.593434
6	-5.311525	-2.535556	-0.694494

6	-4.969098	-2.488269	0.649569
6	-2.307028	0.208502	0.727084
7	-2.180129	1.417200	-0.038075
16	-2.996023	2.706862	0.407982
6	-4.666726	2.559462	-0.167907
7	-0.977230	-0.399577	0.941064
16	-0.454271	-0.340371	2.500919
8	0.855365	-0.975866	2.574591
6	-0.086143	-0.913918	-0.125954
6	0.569989	0.047968	-1.087308
6	2.068840	-0.079821	-1.274179
6	2.388129	0.685813	-2.581842
6	1.098407	1.399662	-2.975941
6	0.051497	0.852680	-2.048867
6	2.863937	0.380722	-0.096487
7	3.601943	-0.418509	0.686105
6	4.162819	0.312145	1.707526
6	3.771193	1.586405	1.531791
7	2.971046	1.616856	0.410998
8	-1.183947	1.195028	-2.248365
6	3.869580	-1.811187	0.485234
6	3.297959	-2.742338	1.335192
6	3.598489	-4.084421	1.153994
6	4.457191	-4.479137	0.139284
6	5.027263	-3.532121	-0.700531
6	4.739106	-2.188305	-0.527044
6	2.511045	2.856530	-0.148883
6	1.172824	3.205575	-0.128711
6	0.794076	4.444219	-0.626967
6	1.747450	5.318218	-1.126153
6	3.088303	4.958283	-1.136060
6	3.475804	3.722227	-0.645648
6	-0.675652	-2.160559	-0.787401
6	-0.663511	-2.352614	-2.161381
6	-1.104895	-3.547327	-2.718052
6	-1.561814	-4.570529	-1.905498
6	-1.574411	-4.389304	-0.527785
6	-1.133544	-3.198820	0.021897
6	-0.237207	1.360349	2.927119
8	-1.498370	-0.858636	3.370114
8	-2.426035	3.858480	-0.283286
8	-3.083030	2.782020	1.871511
1	0.773125	-1.338980	0.464538
1	4.780910	-0.147620	2.456932
1	3.977228	2.478477	2.095264
1	2.343729	-1.146035	-1.391302
1	0.807331	1.203709	-4.009011
1	1.156525	2.484472	-2.867128
1	2.680092	-0.041701	-3.343647
1	3.225558	1.378203	-2.464993

1	-1.721118	1.325977	-1.217727
1	-1.159143	-3.064021	1.095313
1	-1.933230	-5.177408	0.120534
1	-1.909233	-5.499329	-2.337259
1	-1.095815	-3.669956	-3.792954
1	-0.316140	-1.558541	-2.805449
1	2.617221	-2.419162	2.109766
1	3.150505	-4.821215	1.805818
1	4.683022	-5.527350	0.000848
1	5.699704	-3.837795	-1.489784
1	5.182699	-1.437371	-1.166605
1	0.422365	2.521833	0.237161
1	-0.255157	4.701456	-0.620631
1	1.444246	6.282050	-1.511296
1	3.834064	5.636883	-1.526159
1	4.516757	3.427472	-0.647379
1	-2.683862	0.480307	1.766745
1	-3.200587	-0.163076	-1.862979
1	-4.928903	-1.727087	-2.643058
1	-6.077659	-3.217573	-1.037968
1	-5.470265	-3.130173	1.361690
1	-3.715664	-1.581023	2.131586
1	-5.203690	3.450599	0.144845
1	-4.648455	2.482131	-1.250592
1	-5.112681	1.671466	0.270294
1	-1.149971	1.911665	2.712667
1	-0.019412	1.380345	3.991866
1	0.598796	1.751438	2.359248

TS(10-11)'

Eelec = -2784.4056582
E = -2783.730209
H = -2783.689474
G = -2783.803441
Nimag = 1(-250.1580)

6	-3.094779	-1.365770	2.323809
6	-3.173856	-1.603011	0.956839
6	-3.487452	-2.886619	0.516011
6	-3.678391	-3.915358	1.422705
6	-3.582444	-3.673010	2.787453
6	-3.299568	-2.392607	3.235022
6	-3.016424	-0.467492	0.000424
7	-3.775179	-0.567580	-1.099568
16	-4.325467	0.772334	-1.798144
8	-4.319421	0.607216	-3.247688
7	-1.143797	-0.616061	-0.355628
16	-0.787610	-0.749791	-1.947587
6	-1.664321	-2.171374	-2.503037

6	-0.150055	0.330762	0.240164
6	-0.735068	1.310371	1.252043
6	-1.280092	2.513532	0.810946
6	-1.782943	3.440955	1.709801
6	-1.732025	3.190733	3.073738
6	-1.179346	2.002275	3.527591
6	-0.684932	1.072840	2.622632
6	1.008317	-0.403713	0.850800
6	2.327508	0.276923	1.125341
6	3.010377	-0.653524	2.154464
6	2.275120	-1.995109	2.081688
6	1.030698	-1.649599	1.335911
6	3.111184	0.532741	-0.127679
7	3.779660	-0.337234	-0.895586
6	4.300278	0.311724	-1.990270
6	3.954259	1.605785	-1.885260
7	3.227439	1.728847	-0.723665
6	4.018935	-1.735909	-0.682946
6	5.230292	-2.115542	-0.124987
6	5.512035	-3.464638	0.017625
6	4.591444	-4.413074	-0.408267
6	3.391199	-4.013787	-0.976960
6	3.093932	-2.666003	-1.121922
6	2.729819	2.993909	-0.274607
6	3.329391	3.624735	0.805310
6	2.879061	4.878705	1.184829
6	1.857032	5.495464	0.476661
6	1.278653	4.858919	-0.610835
6	1.712972	3.599148	-0.993545
8	0.069655	-2.567657	1.247429
8	-1.231917	0.408804	-2.713460
8	0.644970	-1.048368	-2.104748
8	-3.739573	2.001625	-1.255210
6	-6.038164	0.790198	-1.328214
1	0.256905	1.008181	-0.584620
1	4.151911	2.452067	-2.517532
1	4.860831	-0.217966	-2.738838
1	2.163518	1.277597	1.567438
1	2.026434	-2.381763	3.071560
1	2.842965	-2.774638	1.572092
1	2.864623	-0.205867	3.141349
1	4.087477	-0.748419	2.000627
1	-0.627746	-2.187493	0.675350
1	-1.350374	2.703747	-0.251611
1	-2.219478	4.358780	1.340066
1	-2.120569	3.915407	3.776550
1	-1.133612	1.794587	4.588557
1	-0.257182	0.148137	2.984906
1	1.263590	3.088539	-1.835697
1	0.479559	5.335042	-1.161516

1	1.510500	6.475291	0.774558
1	3.333839	5.376944	2.029479
1	4.138954	3.140843	1.334543
1	5.941061	-1.363598	0.190424
1	6.450731	-3.773326	0.456023
1	4.813005	-5.465735	-0.298100
1	2.674854	-4.752168	-1.308936
1	2.161335	-2.329991	-1.552314
1	-2.940606	0.537832	0.496512
1	-3.607286	-3.066879	-0.541791
1	-3.917546	-4.907803	1.064907
1	-3.739148	-4.475916	3.494934
1	-3.242103	-2.188179	4.295718
1	-2.881640	-0.367525	2.678037
1	-6.501911	1.640704	-1.820428
1	-6.494839	-0.136920	-1.658913
1	-6.107044	0.888088	-0.249280
1	-1.379535	-2.288717	-3.545283
1	-1.348057	-3.029762	-1.919317
1	-2.726662	-1.970055	-2.406888

TS(11-6)'

Eelec = -2784.4317755
E = -2783.762221
H = -2783.719166
G = -2783.845557
Nimag = 1(-1054.9469)

6	4.135076	3.419413	-0.262228
6	4.473711	2.312843	0.498038
6	4.829315	2.435366	1.832513
6	4.827719	3.691496	2.416923
6	4.489360	4.808892	1.666741
6	4.147358	4.672734	0.329648
7	4.510978	1.030541	-0.130400
6	3.748913	-0.035414	0.157483
7	4.171995	-1.027652	-0.635075
6	5.197509	-0.580227	-1.435451
6	5.411142	0.710046	-1.122708
6	2.625275	-0.046545	1.146669
6	1.325394	-0.514037	0.572281
6	0.898574	-1.658311	1.160149
6	1.851851	-2.142475	2.210817
6	2.863825	-1.002464	2.350056
6	0.586770	0.181626	-0.531983
6	0.108061	1.568769	-0.137813
6	0.393654	2.677157	-0.924574
6	-0.060965	3.942978	-0.571178
6	-0.807617	4.112374	0.583219

6	-1.099325	3.008989	1.378943
6	-0.645679	1.750751	1.020061
8	-0.182120	-2.311164	0.863325
6	3.749838	-2.399809	-0.638331
6	4.522342	-3.317586	0.055700
6	4.173264	-4.658797	0.013417
6	3.061654	-5.061045	-0.712890
6	2.304657	-4.128138	-1.407455
6	2.650969	-2.786020	-1.384491
7	-0.536436	-0.685602	-0.900456
16	-0.796813	-1.002483	-2.440518
8	-1.641127	-2.192336	-2.505351
6	-1.740709	0.340228	-3.104188
8	0.447627	-1.028662	-3.225498
6	-3.820889	-2.349912	1.137704
6	-4.764194	-1.339212	1.311944
6	-5.507678	-1.271735	2.493175
6	-5.301665	-2.207773	3.486467
6	-4.350500	-3.210296	3.311913
6	-3.609265	-3.280195	2.142767
6	-4.938336	-0.370181	0.244990
7	-5.683427	0.660051	0.379993
16	-5.817346	1.661822	-0.943849
6	-5.172530	3.168147	-0.294860
8	-7.234395	1.834055	-1.202576
8	-4.966556	1.228669	-2.043140
1	1.280560	0.315742	-1.439057
1	6.117770	1.427881	-1.497641
1	5.671616	-1.228556	-2.150118
1	2.562404	1.001015	1.501329
1	1.327236	-2.350691	3.144179
1	2.308478	-3.079314	1.883985
1	2.678846	-0.438376	3.268068
1	3.896058	-1.361957	2.395298
1	-0.545372	-1.629424	-0.109563
1	0.972595	2.548877	-1.831629
1	0.167857	4.793728	-1.199389
1	-1.160559	5.095420	0.864808
1	-1.682146	3.132921	2.282402
1	-0.874143	0.890867	1.637141
1	3.855785	3.297705	-1.299607
1	3.879092	5.541621	-0.254617
1	4.492040	5.787599	2.125947
1	5.098169	3.796389	3.458222
1	5.106031	1.558496	2.401545
1	5.385273	-2.985342	0.616874
1	4.767141	-5.384754	0.550952
1	2.783149	-6.105536	-0.737909
1	1.434646	-4.435580	-1.970528
1	2.067478	-2.061836	-1.934993

1	-4.395222	-0.558723	-0.684700
1	-6.242561	-0.487559	2.610371
1	-5.879227	-2.163132	4.399455
1	-4.189285	-3.938668	4.095376
1	-2.860466	-4.048065	2.010967
1	-3.240674	-2.395281	0.224622
1	-5.289422	3.916293	-1.074545
1	-5.747447	3.437805	0.585063
1	-4.123056	3.025193	-0.055799
1	-1.904805	0.133383	-4.158105
1	-2.686770	0.407779	-2.578415
1	-1.174983	1.258980	-2.983438

TS(6-7)'

Eelec = -2784.4043893
E = -2783.731842
H = -2783.688199
G = -2783.815717
Nimag = 1(-326.8264)

6	4.738466	3.017309	1.917204
6	4.210506	1.850534	1.386171
6	5.033993	0.980126	0.673117
6	6.384638	1.284375	0.488548
6	6.903344	2.449247	1.018419
6	6.080506	3.314954	1.734092
6	4.443312	-0.236968	0.142453
7	5.142762	-1.113295	-0.472280
16	4.323855	-2.439640	-1.058537
8	2.933069	-2.452671	-0.624348
6	5.178165	-3.747728	-0.243164
8	4.597522	-2.517759	-2.480090
6	-0.150993	-3.602574	-1.643002
16	-0.822048	-2.006133	-1.996667
8	-2.265482	-2.148652	-2.118900
7	-0.545739	-1.025670	-0.728261
6	-1.413149	-1.012062	0.450077
6	-1.251388	-2.211932	1.363198
6	-2.367230	-2.969301	1.704587
6	-2.254557	-4.064242	2.551370
6	-1.016356	-4.420059	3.062779
6	0.104460	-3.673032	2.722227
6	-0.010329	-2.578316	1.880391
6	-1.226264	0.299900	1.152425
6	-2.251303	1.172431	1.489851
6	-1.711424	2.290094	2.343086
6	-0.197816	2.198700	2.174533
6	0.032916	0.869780	1.490548
6	-2.949711	1.982845	-0.312466

7	-3.920487	1.270206	-0.931990
6	-3.692714	1.163244	-2.291609
6	-2.554101	1.831663	-2.535249
7	-2.126140	2.331046	-1.321656
6	-5.038560	0.709327	-0.271689
6	-5.478962	-0.559634	-0.623496
6	-6.582282	-1.098976	0.019381
6	-7.231965	-0.385706	1.016628
6	-6.777852	0.877819	1.367058
6	-5.686265	1.434156	0.719021
6	-0.959107	3.120240	-1.171422
6	-1.053444	4.372395	-0.582590
6	0.085921	5.151136	-0.456462
6	1.305700	4.683393	-0.926169
6	1.385964	3.433132	-1.522972
6	0.253121	2.643694	-1.647256
8	1.155826	0.388323	1.293065
8	-0.067561	-1.463605	-3.112618
1	-2.471755	-1.037072	0.048126
1	-4.358179	0.641642	-2.954517
1	-2.024238	2.012875	-3.452973
1	-3.259862	0.824261	1.662243
1	0.346263	2.225246	3.120669
1	0.205459	2.994218	1.544408
1	-2.002626	2.094110	3.379082
1	-2.125247	3.258009	2.065557
1	0.448200	-0.847072	-0.557934
1	-3.335323	-2.703275	1.299002
1	-3.133903	-4.641610	2.803709
1	-0.922960	-5.274314	3.719557
1	1.074826	-3.943974	3.116387
1	0.864370	-1.996256	1.626533
1	-4.949863	-1.127359	-1.377862
1	-6.925293	-2.087278	-0.254114
1	-8.089021	-0.812630	1.518565
1	-7.282239	1.441322	2.139872
1	-5.336052	2.426770	0.965587
1	-2.015082	4.728277	-0.240572
1	0.017585	6.129624	-0.001240
1	2.192969	5.294100	-0.831102
1	2.335104	3.063255	-1.885167
1	0.307157	1.658723	-2.091889
1	3.370723	-0.371685	0.302813
1	7.008072	0.602867	-0.073266
1	7.947850	2.689704	0.876457
1	6.491838	4.225876	2.148106
1	4.102928	3.692764	2.472908
1	3.164297	1.600843	1.515537
1	4.755425	-4.676525	-0.617224
1	6.231743	-3.677865	-0.493599

1	5.019527	-3.657415	0.826811
1	-0.321422	-4.218462	-2.522194
1	0.911840	-3.487157	-1.451733
1	-0.663233	-4.013043	-0.778545

TS(9-12)'

Eelec = -2784.3901135
E = -2783.715474
H = -2783.674273
G = -2783.790565
Nimag = 1(-236.6068)

6	4.244212	-1.228840	-1.316085
6	3.423253	-0.588465	-0.393067
6	3.778971	-0.609863	0.951405
6	4.918333	-1.282657	1.362823
6	5.724785	-1.932152	0.437985
6	5.386554	-1.901629	-0.906320
6	2.224874	0.178475	-0.918501
7	2.059029	1.495018	-0.327473
16	2.996410	2.739608	-0.805423
8	2.386085	3.944006	-0.271937
7	0.964637	-0.563426	-0.909582
16	0.121256	-0.638754	-2.332989
6	0.206621	-2.330076	-2.848516
6	0.248073	-1.133109	0.263192
6	1.058301	-2.220330	0.970765
6	1.025639	-2.375822	2.350698
6	1.678312	-3.434833	2.969448
6	2.369465	-4.368248	2.216726
6	2.405099	-4.228106	0.835770
6	1.758369	-3.167462	0.226552
6	-0.467547	-0.198471	1.209948
6	-1.796795	-0.400149	1.550565
6	-2.127129	0.268587	2.853220
6	-0.995064	1.266807	3.033119
6	0.089482	0.752438	2.121005
6	-3.264952	0.567327	0.177342
7	-3.985539	-0.161992	-0.703794
6	-4.343802	0.578776	-1.813610
6	-3.845860	1.811250	-1.617664
7	-3.198225	1.779197	-0.399080
6	-4.341075	-1.515538	-0.505514
6	-4.234929	-2.419990	-1.553111
6	-4.600411	-3.742474	-1.353364
6	-5.055041	-4.165379	-0.112437
6	-5.153629	-3.255514	0.930553
6	-4.808011	-1.927591	0.735245
6	-2.611304	2.928644	0.204109

6	-1.330982	3.319615	-0.148307
6	-0.787088	4.456532	0.432636
6	-1.524386	5.190736	1.350481
6	-2.808563	4.791320	1.695573
6	-3.356992	3.655440	1.120679
8	1.270542	1.104849	2.232928
8	-1.278448	-0.355436	-2.080273
8	0.820537	0.138762	-3.337929
8	3.207601	2.619941	-2.236719
6	4.580293	2.597745	-0.026980
1	-0.612729	-1.710380	-0.213129
1	-3.895886	2.701208	-2.218698
1	-4.928734	0.173571	-2.618918
1	-2.311667	-1.305408	1.266035
1	-0.620157	1.352901	4.053437
1	-1.277333	2.269888	2.700760
1	-2.088002	-0.496489	3.636594
1	-3.120929	0.709727	2.867651
1	1.847942	1.507950	0.679334
1	0.489865	-1.663155	2.958484
1	1.643610	-3.523317	4.047036
1	2.878704	-5.192618	2.696864
1	2.947679	-4.941765	0.230622
1	1.825880	-3.059997	-0.844320
1	-4.356808	3.329098	1.372605
1	-3.384298	5.363400	2.410166
1	-1.094667	6.075238	1.800484
1	0.219589	4.747578	0.173004
1	-0.762823	2.732630	-0.856644
1	-3.850175	-2.090843	-2.508477
1	-4.518090	-4.446878	-2.169677
1	-5.333624	-5.198695	0.040552
1	-5.514506	-3.575417	1.898405
1	-4.904041	-1.203422	1.532220
1	2.437767	0.385619	-2.012601
1	3.158236	-0.105542	1.678762
1	5.177485	-1.298915	2.412772
1	6.616619	-2.450606	0.763126
1	6.017443	-2.387313	-1.638553
1	3.996625	-1.186043	-2.369825
1	5.151275	3.471131	-0.331269
1	4.439677	2.590586	1.049578
1	5.064603	1.686900	-0.362729
1	-0.379864	-2.396054	-3.761344
1	1.242880	-2.583056	-3.049146
1	-0.216495	-2.975721	-2.085821

(VIII) Direct and Water Assisted Proton Transfers

Water

Eelec = -76.4120525, -76.4031898
E = -76.390531
H = -76.386752
G = -76.408162
Nimag = 0

1	0.000000	0.764366	-0.463066
8	0.000000	0.000000	0.115767
1	0.000000	-0.764366	-0.463066

TS(5-11)

Eelec = -1870.8402849, -1870.6138
E = -1870.3320899
H = -1870.3017759
G = -1870.3950459
Nimag = (-2388.1642)

6	3.554151	-1.017407	-0.272803
6	2.527452	-1.428369	0.568560
6	2.839402	-2.239092	1.654067
6	4.149033	-2.620829	1.905329
6	5.168668	-2.196493	1.065477
6	4.865629	-1.394786	-0.026201
6	1.087666	-1.017920	0.319456
7	0.753477	-0.778639	-1.063266
16	0.243029	-1.984390	-1.918759
8	-0.551770	-2.966111	-1.144300
6	0.681698	0.248657	1.080941
6	1.240318	0.777918	2.255678
6	0.244602	1.181511	3.282835
6	-0.959679	1.477695	2.378865
6	-0.810034	0.507537	1.180496
8	2.467221	1.134687	2.160363
6	-1.493955	0.990054	-0.046889
7	-2.678402	0.535321	-0.470043
6	-3.060742	1.218412	-1.599675
6	-2.093964	2.117691	-1.854949
7	-1.138627	1.974669	-0.875811
6	-3.507627	-0.433368	0.182740
6	-3.249971	-1.784918	0.033301
6	-4.094775	-2.690508	0.660279
6	-5.175572	-2.247884	1.408225
6	-5.421891	-0.888065	1.540836
6	-4.583617	0.028346	0.926600

6	0.024572	2.808396	-0.814077
6	1.223914	2.345810	-1.328785
6	2.321181	3.193220	-1.306766
6	2.210771	4.475937	-0.786366
6	0.998240	4.924095	-0.284284
6	-0.108016	4.086853	-0.299294
8	-0.424538	-1.454307	-3.115994
6	1.616753	-2.932711	-2.541837
1	0.463933	-1.821591	0.734845
1	-1.977489	2.829076	-2.648543
1	-3.967152	0.980379	-2.120110
1	-1.303445	-0.436440	1.425672
1	1.934109	1.015578	0.975776
1	4.372317	-3.255091	2.751178
1	2.046376	-2.582329	2.305845
1	3.309143	-0.412120	-1.133344
1	5.652737	-1.067001	-0.690309
1	6.189519	-2.494513	1.255463
1	2.239082	-2.280082	-3.145140
1	2.183209	-3.327305	-1.704454
1	1.218809	-3.742573	-3.145604
1	-4.759816	1.090168	1.017842
1	-6.263233	-0.540044	2.120871
1	-5.828554	-2.962089	1.887380
1	-3.901683	-3.747224	0.554451
1	-2.400003	-2.127140	-0.543791
1	-1.062320	4.421725	0.080348
1	0.909909	5.921860	0.118134
1	3.072124	5.126895	-0.771951
1	3.267185	2.847754	-1.695610
1	1.272686	1.328315	-1.696194
1	-1.911878	1.351150	2.886780
1	-0.893697	2.506893	2.031093
1	0.042335	0.328694	3.933599
1	0.559665	2.025014	3.888666

$\underline{\text{TS(5-11)}_{w}}$

Eelec = -1947.3079769, -1947.0819786
E = -1946.779758
H = -1946.748289
G = -1946.841541
Nimag = 1(-1307.0622)

6	-3.435880	-1.441496	0.364061
6	-2.263149	-1.780012	-0.299240
6	-2.283552	-2.874774	-1.159528
6	-3.443286	-3.604885	-1.363114
6	-4.612292	-3.250959	-0.702356
6	-4.602256	-2.166919	0.162738

6	-0.965391	-1.025001	-0.067413
7	-0.918594	-0.276855	1.164983
16	-0.328304	-0.929226	2.446717
8	0.010499	0.147563	3.394815
6	-0.567090	-0.070121	-1.201645
6	0.924821	0.197071	-1.297115
6	1.130002	0.856073	-2.674817
6	0.010194	0.266352	-3.517929
6	-1.072757	-0.039042	-2.518725
6	1.572332	0.942777	-0.184314
7	1.194368	2.055029	0.457566
6	2.135235	2.379975	1.408410
6	3.118330	1.468341	1.325016
7	2.759280	0.593517	0.328020
6	-0.000717	2.827919	0.318695
6	-0.927251	2.789889	1.349045
6	-2.032707	3.623973	1.281360
6	-2.207327	4.475552	0.198473
6	-1.266076	4.504672	-0.822794
6	-0.146756	3.687046	-0.758049
6	3.585108	-0.499680	-0.089688
6	3.434790	-1.734595	0.518423
6	4.272640	-2.769653	0.129095
6	5.240866	-2.563339	-0.843168
6	5.380310	-1.316381	-1.437205
6	4.549290	-0.273182	-1.059456
8	-2.287009	-0.096515	-2.857710
6	-1.561636	-1.896220	3.298644
8	0.766200	-1.897101	2.193859
1	4.026111	1.343818	1.885961
1	1.999256	3.221763	2.062056
1	1.446077	-0.772506	-1.304102
1	0.312536	-0.683767	-3.970276
1	-0.341139	0.914498	-4.319274
1	2.128786	0.659749	-3.074619
1	1.003246	1.938425	-2.603004
1	-0.134861	-1.848278	-0.071613
1	-1.113109	-2.296046	4.203778
1	-2.396408	-1.246796	3.543249
1	-1.889827	-2.702315	2.649098
1	-1.374232	-3.162171	-1.673557
1	-3.434735	-4.453928	-2.033651
1	-5.519134	-3.820435	-0.855304
1	-5.505491	-1.886588	0.688841
1	-3.417669	-0.602910	1.045150
1	2.660464	-1.871391	1.263091
1	4.164133	-3.740669	0.591959
1	5.891028	-3.375518	-1.138241
1	6.137081	-1.153503	-2.191871
1	4.648402	0.707281	-1.505274

1	0.613169	3.734597	-1.524079
1	-1.388101	5.179803	-1.658570
1	-3.071531	5.124531	0.153860
1	-2.764947	3.598012	2.076126
1	-0.786291	2.091844	2.162168
1	-1.673075	0.968596	-0.863742
8	-2.773451	1.255464	-0.923432
1	-2.856583	2.185277	-1.160283
1	-2.880356	0.658832	-1.784010

$\underline{TS(5\text{-}6)_w}$

Eelec = -1947.3404327, -1947.107329
E = -1946.810143
H = -1946.778026
G = -1946.873071
Nimag = 1(-1112.8581)

6	3.006507	-1.968866	-1.053541
6	3.206417	-0.850778	-0.262691
6	4.190479	-0.819071	0.711995
6	4.960649	-1.950598	0.929018
6	4.760853	-3.085334	0.155399
6	3.792578	-3.090460	-0.838106
7	2.481979	0.345024	-0.571454
6	2.778594	1.040030	-1.721693
6	2.022476	2.149196	-1.724100
7	1.272811	2.116640	-0.574238
6	1.532714	0.993749	0.119102
6	0.806997	0.662509	1.378406
6	-0.245374	-0.464233	1.359739
6	-0.598584	-0.591094	2.775324
6	0.548992	-0.052701	3.614915
6	1.635417	0.321376	2.620116
6	0.429351	3.210710	-0.196005
6	-0.766944	3.407073	-0.864069
6	-1.542480	4.508900	-0.532284
6	-1.120306	5.394319	0.448184
6	0.087899	5.188728	1.100349
6	0.875184	4.096806	0.773152
6	-1.302151	-0.348076	0.267268
6	-2.614386	-1.058114	0.517678
6	-3.793183	-0.324522	0.556806
6	-5.020007	-0.955045	0.724892
6	-5.076090	-2.333582	0.849524
6	-3.899983	-3.073861	0.809256
6	-2.678483	-2.444040	0.645091
8	-1.601353	-1.063516	3.276730
7	-0.617124	-0.838144	-0.944786
16	-1.174357	-0.615330	-2.443234

6	-2.534967	-1.701132	-2.760025
8	-1.685577	0.747620	-2.535501
8	-0.102670	-1.019229	-3.343150
1	1.946294	2.960093	-2.424973
1	3.506389	0.672749	-2.421820
1	0.275190	1.599652	1.602391
1	0.172232	0.824662	4.148101
1	0.852687	-0.783160	4.363061
1	2.266606	1.151476	2.951992
1	2.267745	-0.547078	2.425953
1	-0.140171	-1.746105	-0.772695
1	-1.545763	0.745205	0.083113
1	-2.832851	-1.534537	-3.791923
1	-2.197808	-2.723347	-2.618264
1	-3.345236	-1.465159	-2.078588
1	-3.755342	0.752234	0.449044
1	-5.928033	-0.367769	0.754145
1	-6.028107	-2.830409	0.979807
1	-3.935569	-4.149932	0.915841
1	-1.760539	-3.017378	0.629150
1	-1.085461	2.697987	-1.616088
1	-2.481652	4.669327	-1.043225
1	-1.731608	6.248899	0.703335
1	0.422336	5.882221	1.859170
1	1.825938	3.930905	1.261224
1	4.355938	0.081548	1.286080
1	5.724683	-1.939358	1.693620
1	5.366285	-3.965347	0.323021
1	3.636693	-3.972295	-1.443423
1	2.239517	-1.960043	-1.815526
8	0.447826	-2.810554	0.503948
1	1.351974	-3.109815	0.587906
1	0.264873	-1.630495	1.096261