

Supporting Information

for

**Refined Transition State Models for Proline-Catalyzed Asymmetric Michael
Reactions Under Basic and Base-free Conditions**

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1. Additional Details on Different Transition State Models

The nomenclature used for different TS is given in Scheme S1. The prochiral faces (*re* or *si*) of enamine and nitrostyrene have been used to distinguish between different diastereomeric TSs for the stereoselective C–C bond formation. Four different TS-models have been considered in the present study as shown in Scheme S2.

The TSs (**1-2**) with two different conformations of the pyrrolidine ring in proline-enamine has been studied (Figure S1a) for first model system. The enamine (**1**) in ‘*up*’ conformation is of lower energy than the ‘*down*’ conformation. Calculations were carried out, first using the ‘*up*’ conformation. For each mode of addition (*re-re*, *si-si*, *si-re*, and *re-si*) two different types of TSs have been located that maintain H-bonding interaction between the –COOH group and –NO₂ group. These TSs differ in the interacting O-atom of NO₂ group in the H-bonding (Figure S1b). The optimized geometries of these TSs are given in Figure S2.

In the case of *syn*-face addition, since the electrophile is very close to the COOH group we have also studied the different position of OH in both *si-si* and *si-re* modes of addition. For example, (**1-2**)**I**_{*syn*} (*si-si*)₁ and (**1-2**)**I**_{*syn-Cont*}(*si-si*)₁ in Figure S2. Then we have studied the C–C bond formation with ‘*down*’ conformation of proline enamine (**1**). Only the TS for the *re-re* mode of addition is lower in energy in the ‘*down*’ conformation than the ‘*up*’ conformation. Hence, the difference between *re-re* and *si-si* mode further increases. Besides, TSs with different cyclohexane ring conformations, with its C4 pointing away from the incoming electrophile is also considered. Such TSs are found to be of higher energy (Table S2). The stereoselectivity could not be explained by TS **1-2** model (*syn*-face addition) at all levels of theory (Table S1).

The Michael reaction is quite different as compared to an aldol reaction. In Michael addition transition states for the critical C–C bond formation (1) the developing negative charge is stabilized by the NO₂ group, (2) H-transfer occurs after the C–C bond formation and, (3) there are two extra atoms between the site of attack of the nucleophile and the O-atom involved in H-bonding (Scheme S3). Hence, the addition of nitrostyrene can occur from the face *anti* to the COOH group (*anti*-face addition) while still maintaining H-bonding. The *anti*-face addition has been studied mainly with ‘*down*’ conformer, as the two TSs optimized with the ‘*up*’ conformer (*re-re* and *re-si* mode) are of higher energy. In *anti*-face addition, the *re-re* and *re-si* modes of addition are of lower energy than the *syn*-face addition (except in the *re-si* mode at the SMD/mPW1K/6-31+G** level of theory) whereas for the other two modes of addition *syn*-face addition with ‘*up*’ conformer is more preferred. All these different models are

considered toward identifying the lowest energy diastereomer. The stereoselectivity could not be explained (Table S1).

Since, in nitrostyrene the NO₂ group can stabilize the developing negative charge, the TS without H-bonding ((**1-2**)') has also been studied. It is found to be lower energy than TS (**1-2**) with H-bonding. We have studied different rotameric possibilities along the C–C bond formation named as 60, 180, 300 depending on the dihedral between enamine double bond and the double bond of nitrostyrene. We have first done conformational sampling by optimizing TS in the *re-re* mode (Figure S8, Table S3-S4). The lowest energy TS is considered for further analyses. This model has been found to be successful in rationalizing the experimental stereoselectivity (Table S5).

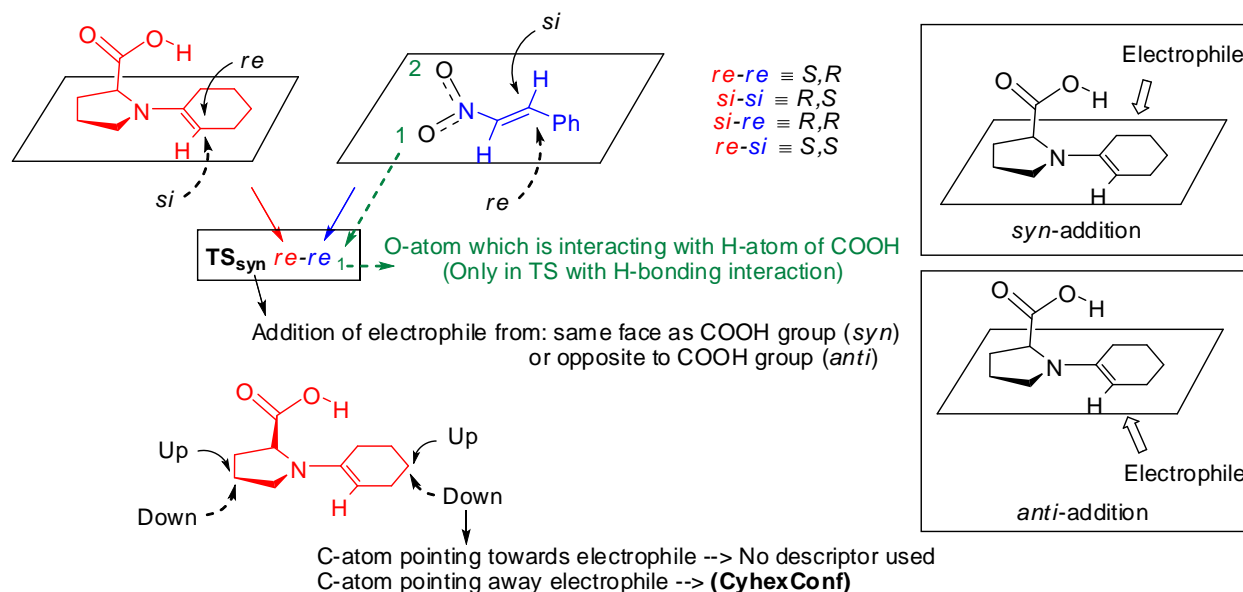
After analyzing the transition state involving enamine carboxylic acid, under base-free reaction conditions, we examined the nature of the transition states with enamine carboxylate, which is the potential intermediate under basic reaction conditions. Two model systems have been considered; one that involves enamine carboxylate and nitrostyrene (TS **3-4**), and the other consisting of enamine carboxylate (**3**) + DBUH⁺ and nitrostyrene (TS (**3-4**)_{DBU}). For the both TS models we have used the insights of conformational details derived from TS (**1-2**)'.

For TS **3-4** we have studied both *anti*- and *syn*-face addition. The TS in *syn*-face addition has been found to be of higher energy as compared to the *anti*-face addition. In *syn*-face addition due to steric interaction of COO⁻ group with nitrostyrene TSs are higher in energy. However, surprisingly in the gas phase calculation the TS for *re-re* mode ((**3-4**)*syn*(*re-re*)₁₈₀) for *syn*-addition has the lowest energy (Table S7). Whereas other TSs of *syn*-addition are of higher in energy.

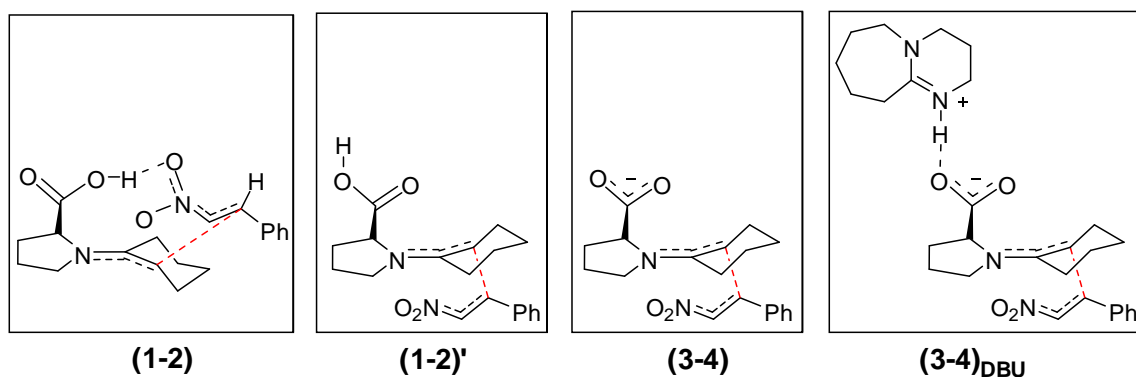
The interaction of DBU with **1** leads to the formation of **3**+DBUH⁺ (**3**_{DBU}). In TS (**3-4**)_{DBU}, DBUH⁺ can interact with COO⁻ group of enamine or NO₂ group of nitrostyrene. The interaction of DBUH⁺ with NO₂ group (instead of COO⁻) in the TS of C–C bond formation is higher in energy by ~9 kcal/mol (Figure S14). This TS is higher in energy due to steric interaction between DBU and enamine moieties. Besides this, it also reflects the fact that NO₂ stabilizes the negative charge more effectively than the COO⁻. The TS with DBUH⁺ interacting with COO⁻ of **3** (TS (**3-4**)_{DBU}) has been studied for only *anti*-addition as the *syn*-addition has been found to have higher energy in TS **3-4**.

There is difference between the gas phase and the solvent phase geometries in the case of **3**_{DBU} adduct. The proton remains with the COOH group in **3**_{DBU} adduct in the gas phase geometry. The TS in the gas phase involves simultaneous formation of C–C bond and transfer of proton from COOH to DBU.

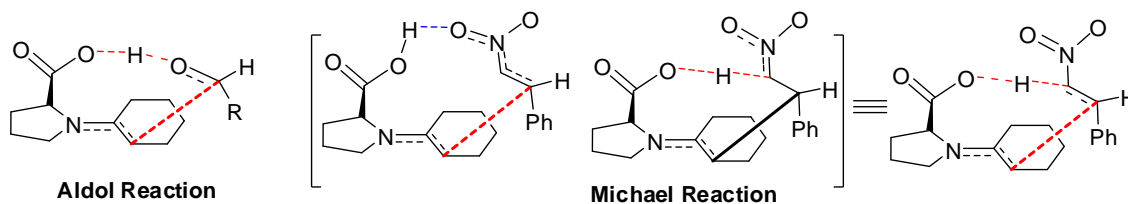
Another conformation of DBU in TS **(3-4)**_{DBU} at the SMD_{THF}/M06-2X/6-31+G** is located, in which DBU is bent toward the cyclohexane ring of enamine (Figure S17, Table S13). Also at this level of theory the TS **(3-4)**_{DBU2} has been lower in energy. Further, for *si-si* mode the TS with dihedral '300' instead of '180' is found to be lower in energy at this level of theory. It is noticed that the energy difference between TS with **3**_{DBU}, **3**_{DBU1} and **3**_{DBU2} conformations at various level of theory is very less. Also the difference between the enthalpy of TS **(3-4)**_{DBU-anti(re-re)₆₀} for different enamine-DBU adducts is very small as compared to the Gibbs free energy differences (Table S8). The %ee obtained through the SMD_{THF}/M06-2X/6-31+G** level of theory is found to be overestimated as compared to the experimental values while all other levels of theory considered in this study offers lower %ee in line with the experimental observation (Table S14). The comparison of energies of different TS-models has been provided in Table S15-S16.



Scheme S1. The TS nomenclature employed in the manuscript.



Scheme S2. Four different TS models examined for the stereoselective bond formation in Michael reaction between the enamine (derived from cyclohexanone and proline) and nitrostyrene. First two are under base-free conditions while the rest are under basic conditions.



Scheme S3. Comparison of TSs for the stereoselective C–C bond formation in aldol and Michael reaction. In Michael reaction the C–C bond formation and H-transfer occurs in two steps. The two steps are also shown together for Michael reaction.

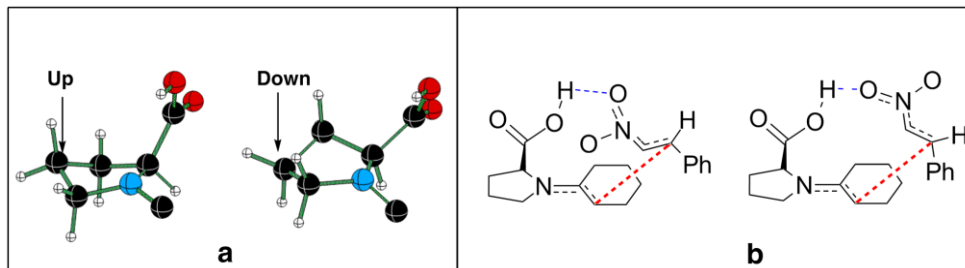
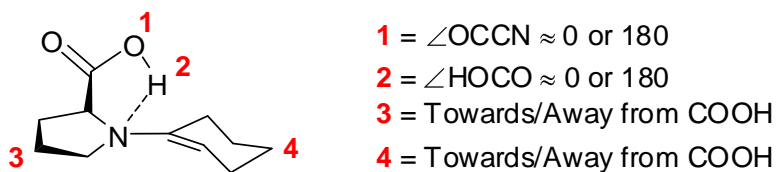
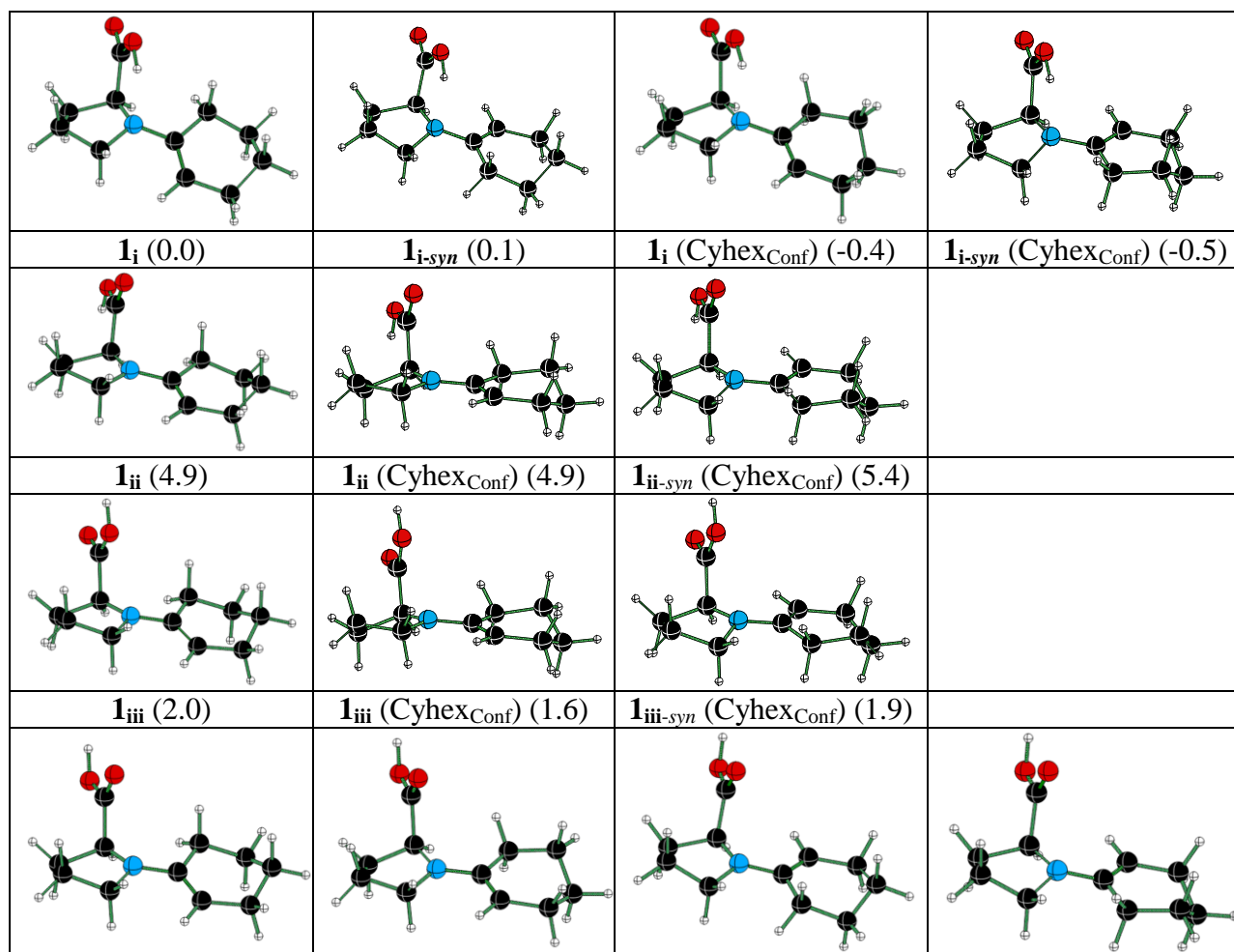


Figure S1. (a) Conformation of pyrrolidine ring in proline-enamine. (b) The TS **1-2** showing different O-atom of NO₂ group involved in H-bonding with COOH group.

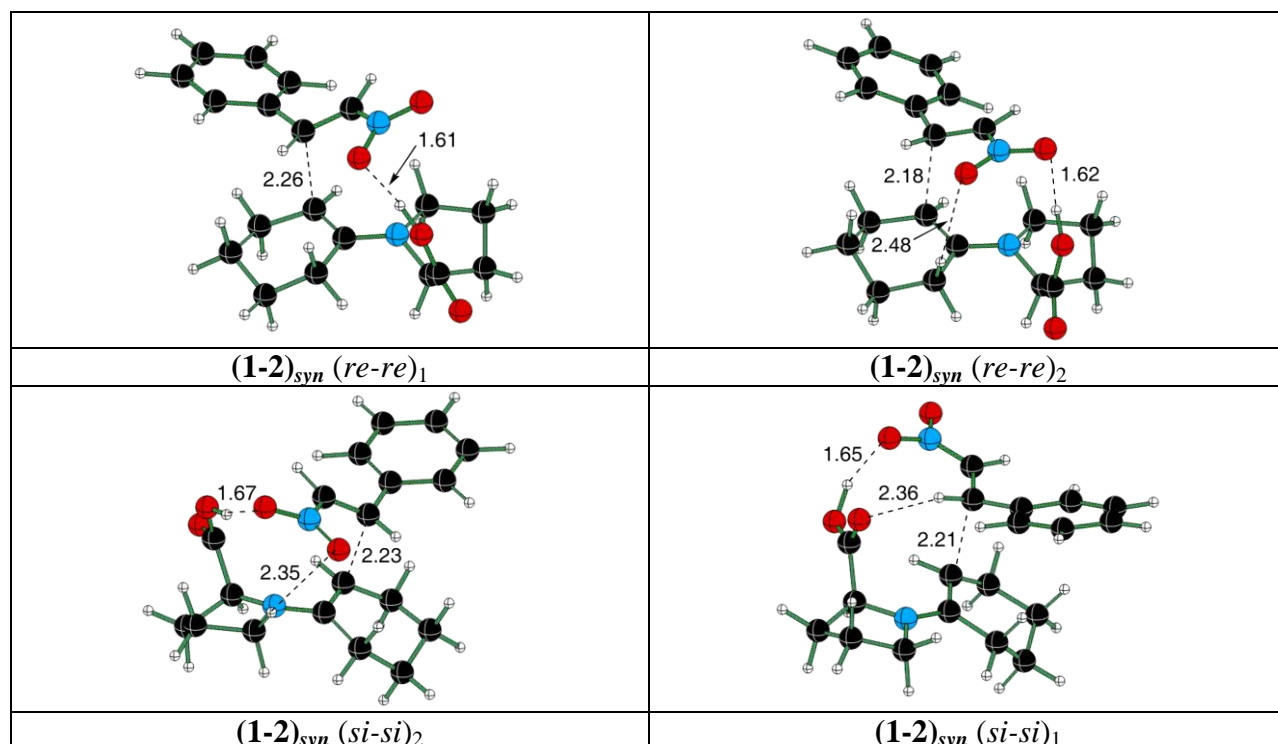


Changes in conformation/position of atoms (1, 2, 3, 4) leads to different conformations



$\mathbf{1}_{iv}$ (1.8)	$\mathbf{1}_{iv}$ (CyhexConf) (1.3)	$\mathbf{1}_{iv-syn}$ (1.6)	$\mathbf{1}_{iv-syn}$ (CyhexConf) (1.6)
$\mathbf{1}_i$ (2.5) (<i>down</i>)	$\mathbf{1}_{iii}$ (<i>down</i>) (2.5)	$\mathbf{1}_{iv}$ (<i>down</i>) (2.3)	$\mathbf{1}_{iv}$ (<i>down</i>) (CyhexConf) (1.9)
$\mathbf{1}_{iv-syn}$ (<i>down</i>) (CyhexConf) (2.0)			

Figure S2. Different conformations of proline-enamine and their relative energies with respect to the lowest energy conformer obtained at the SMD_(THF)/mPW1K/6-31+G** level of theory.



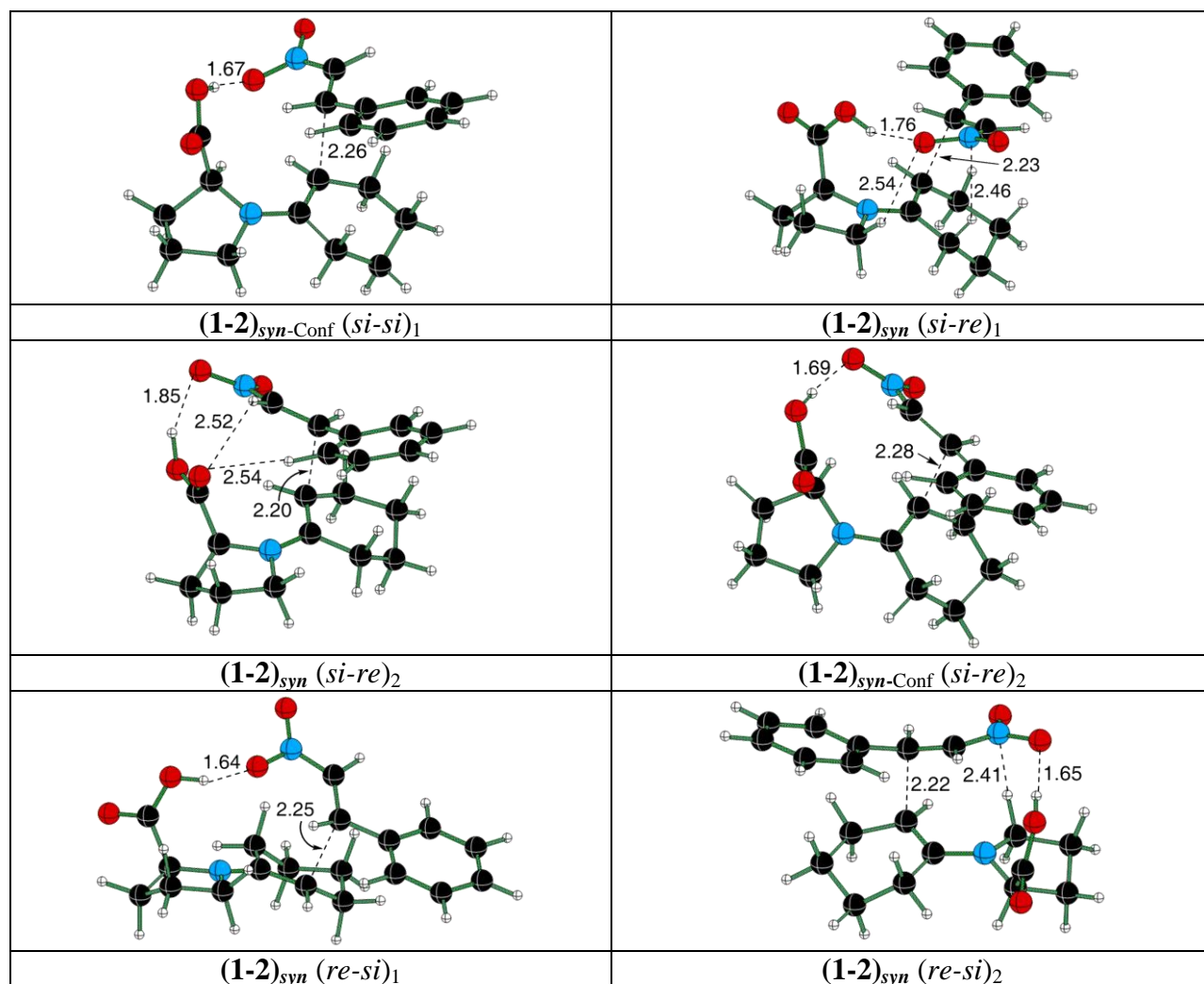


Figure S3. Optimized geometries of TS for C–C bond formation at the SMD_{THF}/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding with ‘*up*’ conformation of pyrrolidine.

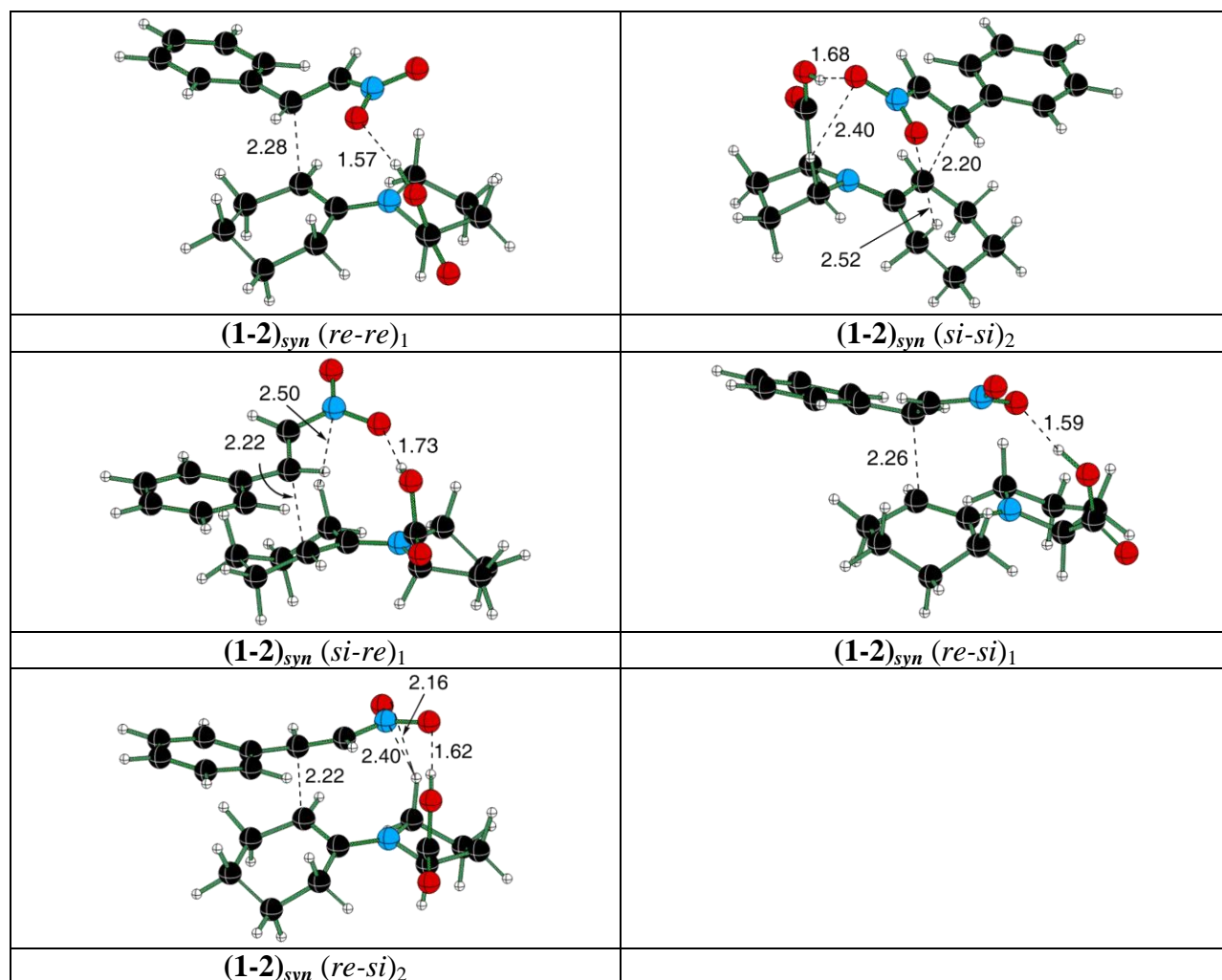


Figure S4. Optimized geometries of TSs for C–C bond formation at the SMD_{THF}/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding with ‘down’ conformation of pyrrolidine.

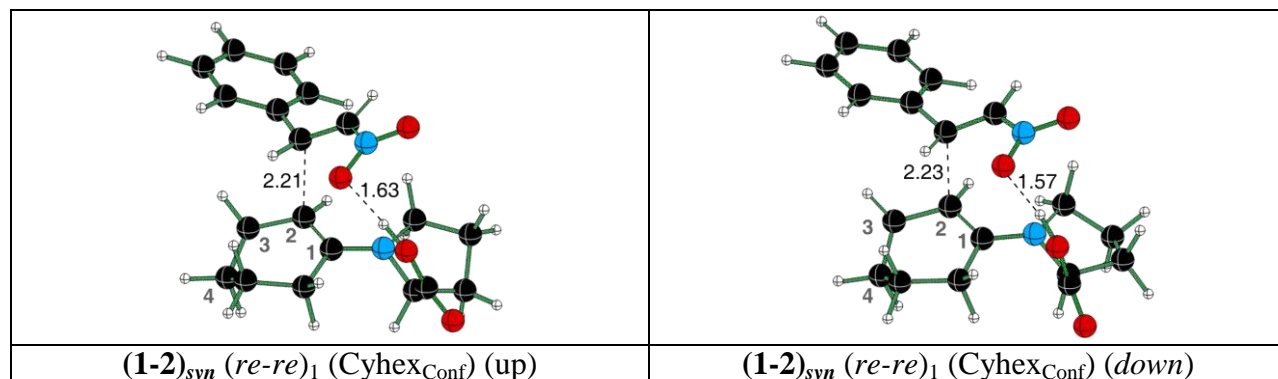


Figure S5. Optimized geometries of TS for C–C bond formation for *re-re* mode of addition having 4th-carbon in cyclohexane pointing away from the incoming electrophile at the SMD_{THF}/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding.

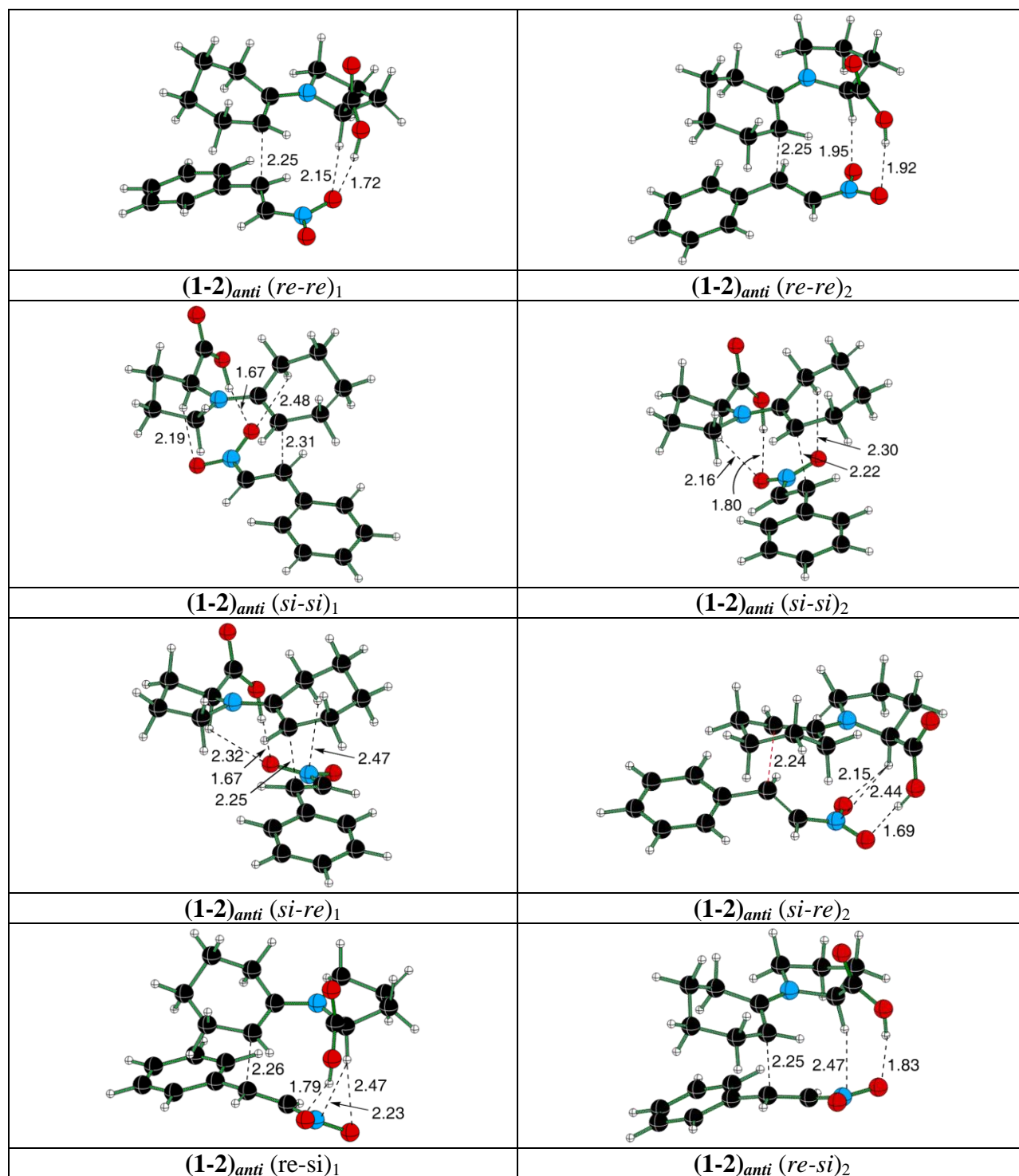


Figure S6. Optimized geometries of TS for C–C bond formation at the SMD_(THF)/mPW1K/6-31+G** level of theory for *anti*-addition having H-Bonding with ‘down’ conformation of pyrrolidine.

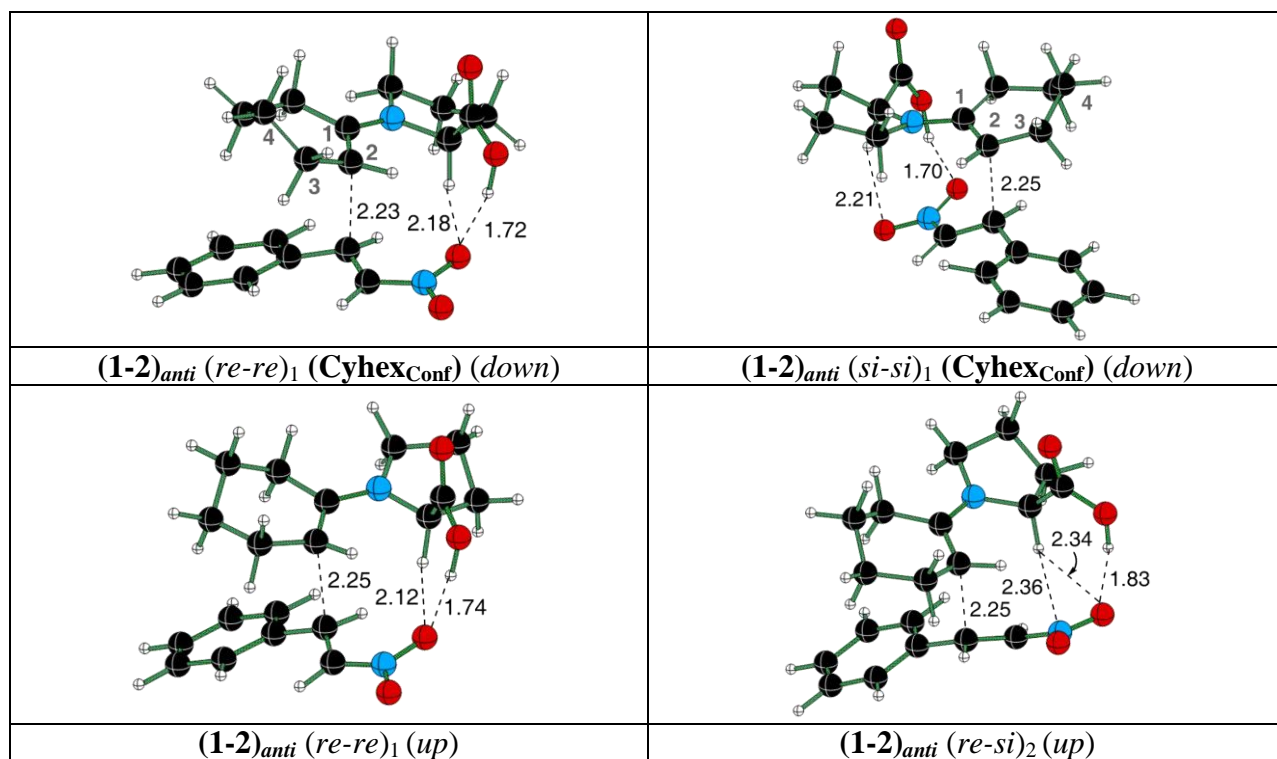
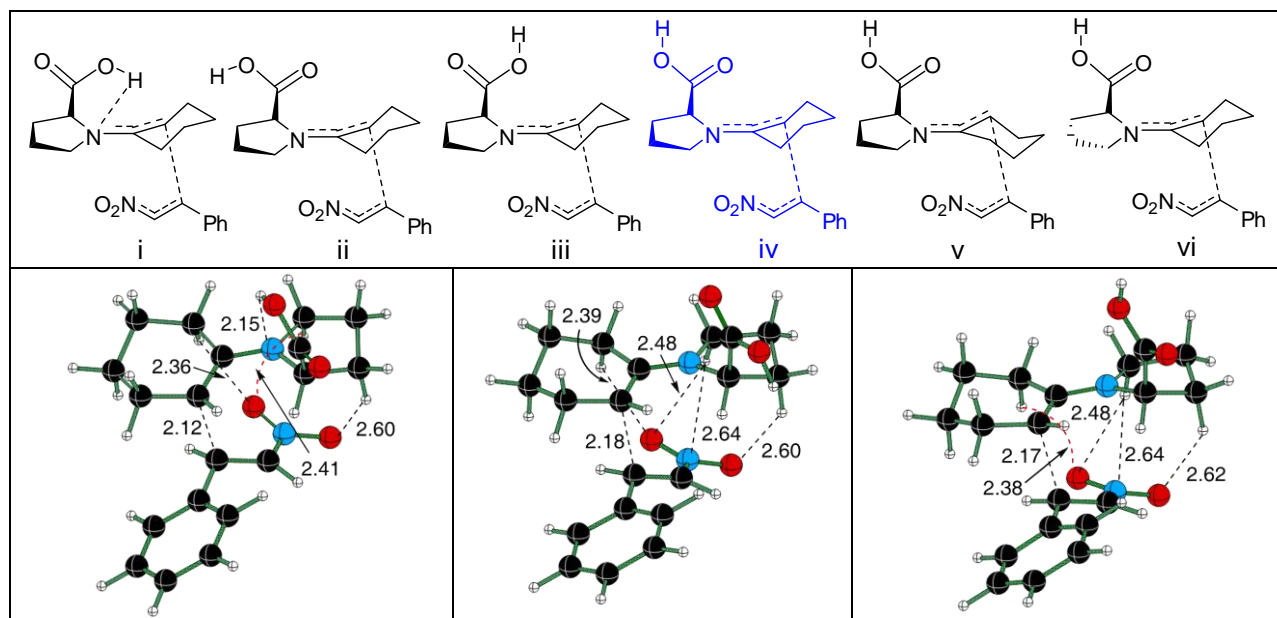


Figure S7. Optimized geometries of TS for C–C bond formation at the SMD_(THF)/mPW1K/6-31+G** level of theory for *anti*-addition having H-Bonding with ‘*up*’ conformation of pyrrolidine and ‘*down*’ conformation of pyrrolidine with different conformation of cyclohexane.



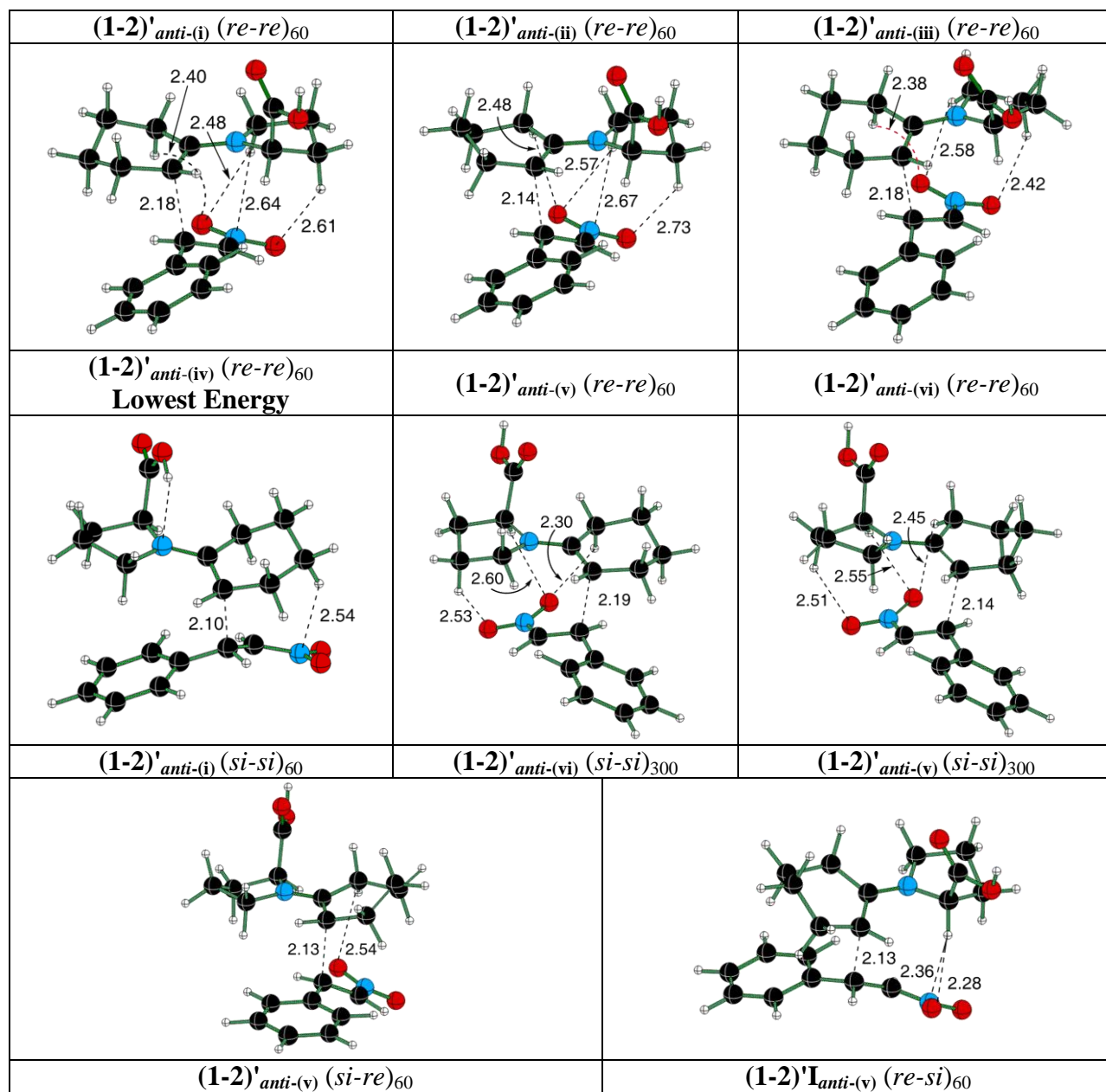


Figure S8. Optimized geometries of TS for C–C bond formation at the SMD_(THF)/mPW1K/6-31+G** level of theory for *anti*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene with different conformation of pyrrolidine and cyclohexane. Among the different TSs (re-re)₆₀ (**iv**) is most preferred and used in the main text for discussions and further calculation are done with same conformation (see Table S9).

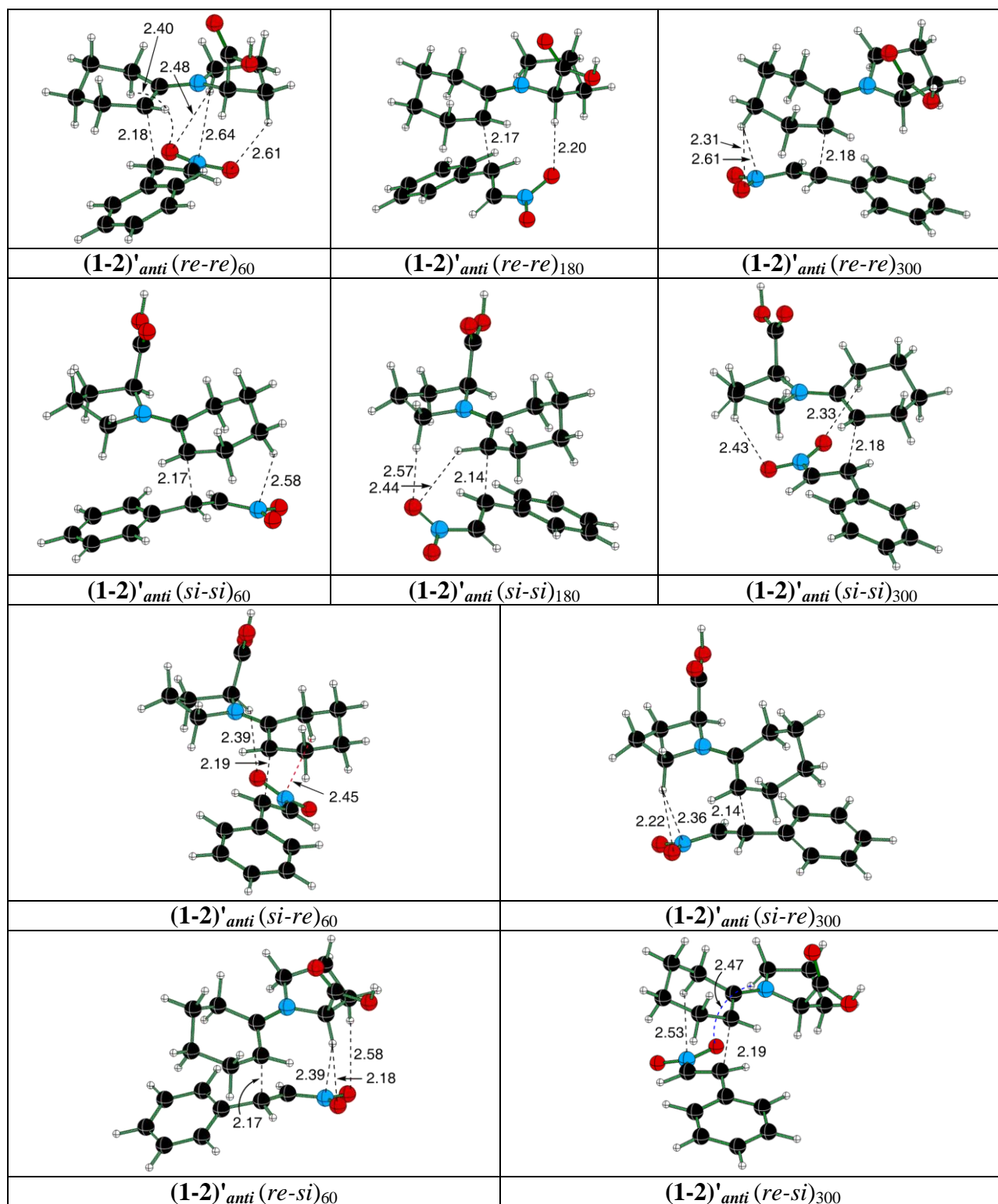


Figure S9. Optimized geometries of TS for the C–C bond formation at the SMD_(THF)/mPW1K/6-31+G** level of theory for *anti*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene.

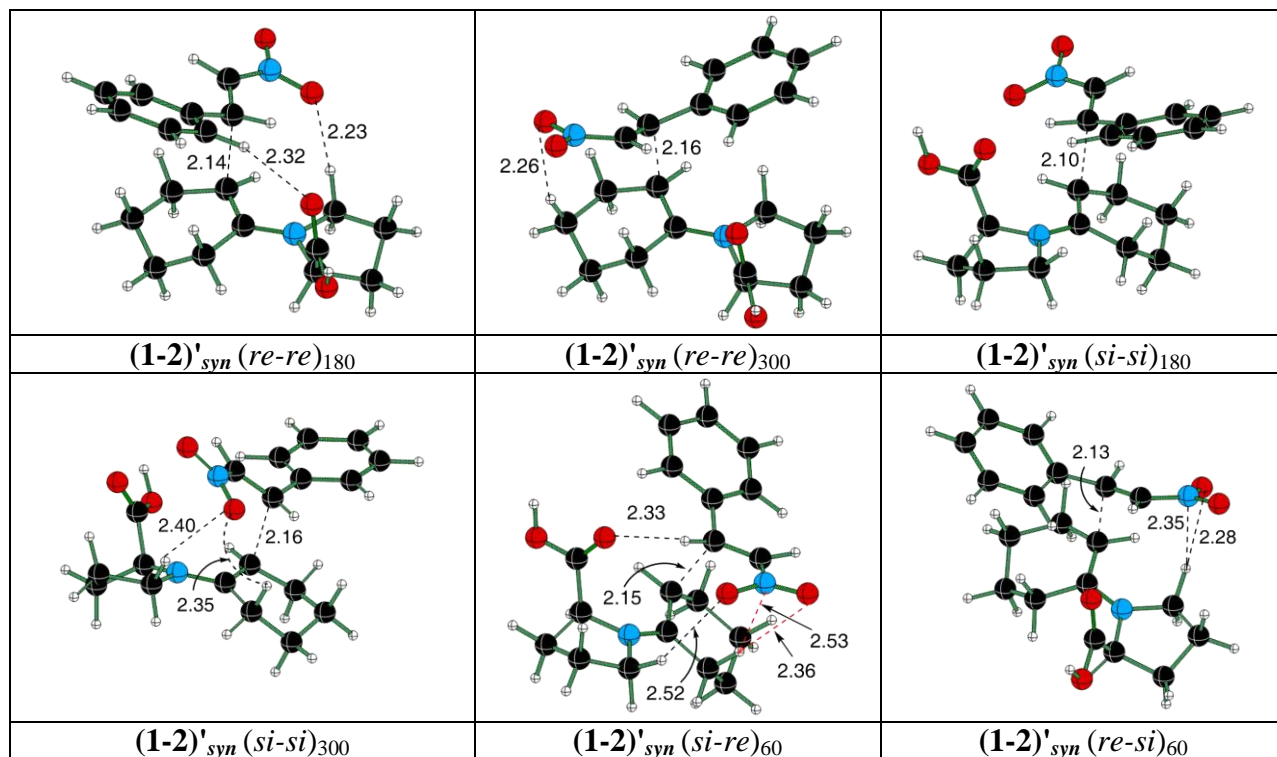


Figure S10. Optimized geometries of TS for C–C bond formation at the SMD_(THF)/mPW1K/6-31+G** level of theory for *syn*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene with ‘*up*’ conformation of pyrrolidine.

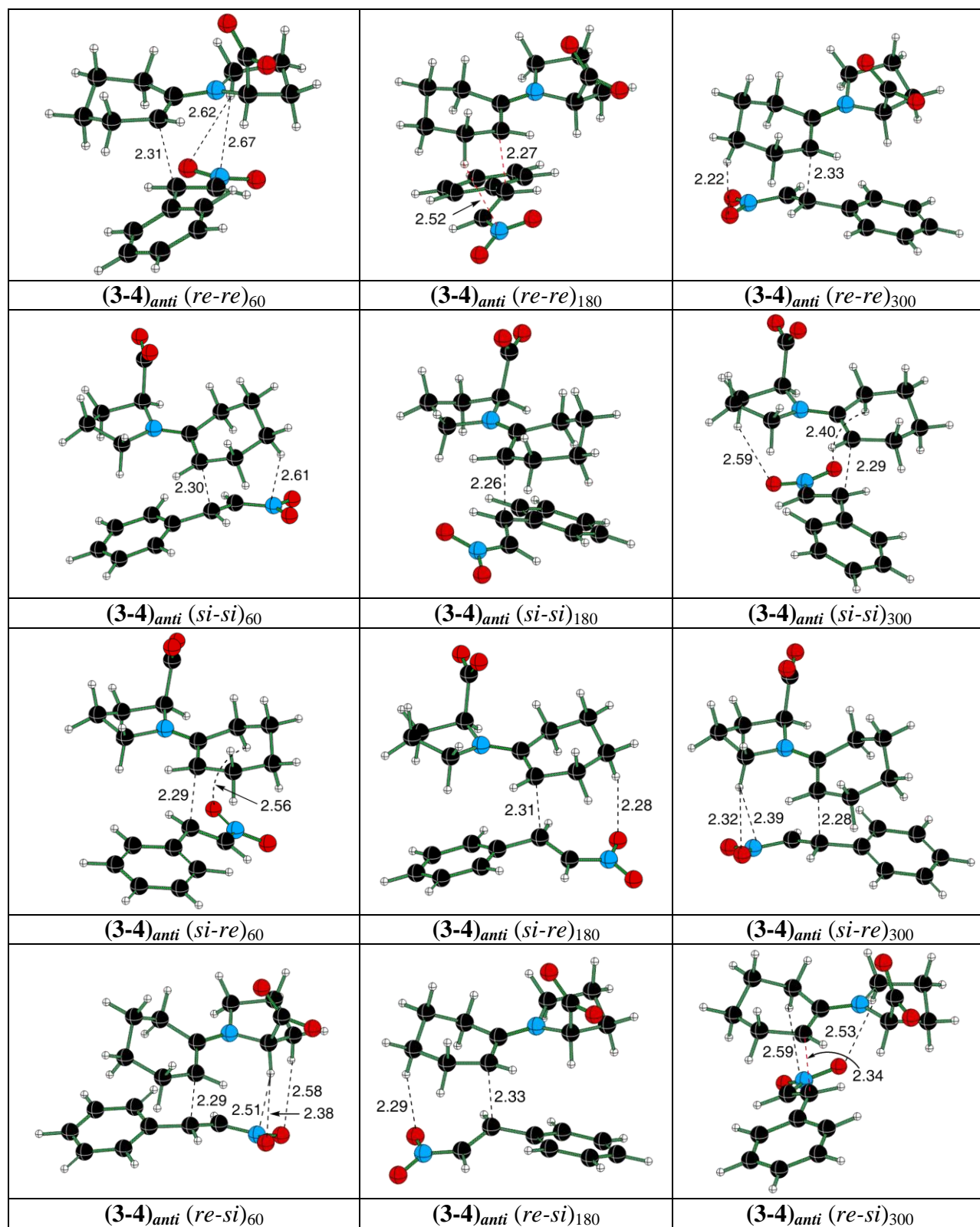


Figure S11. The optimized geometries of TSs at the SMD_(THF)/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine to nitrostyrene from the face opposite to the carboxylate group (*anti*-face addition) of enamine carboxylate (**3**).

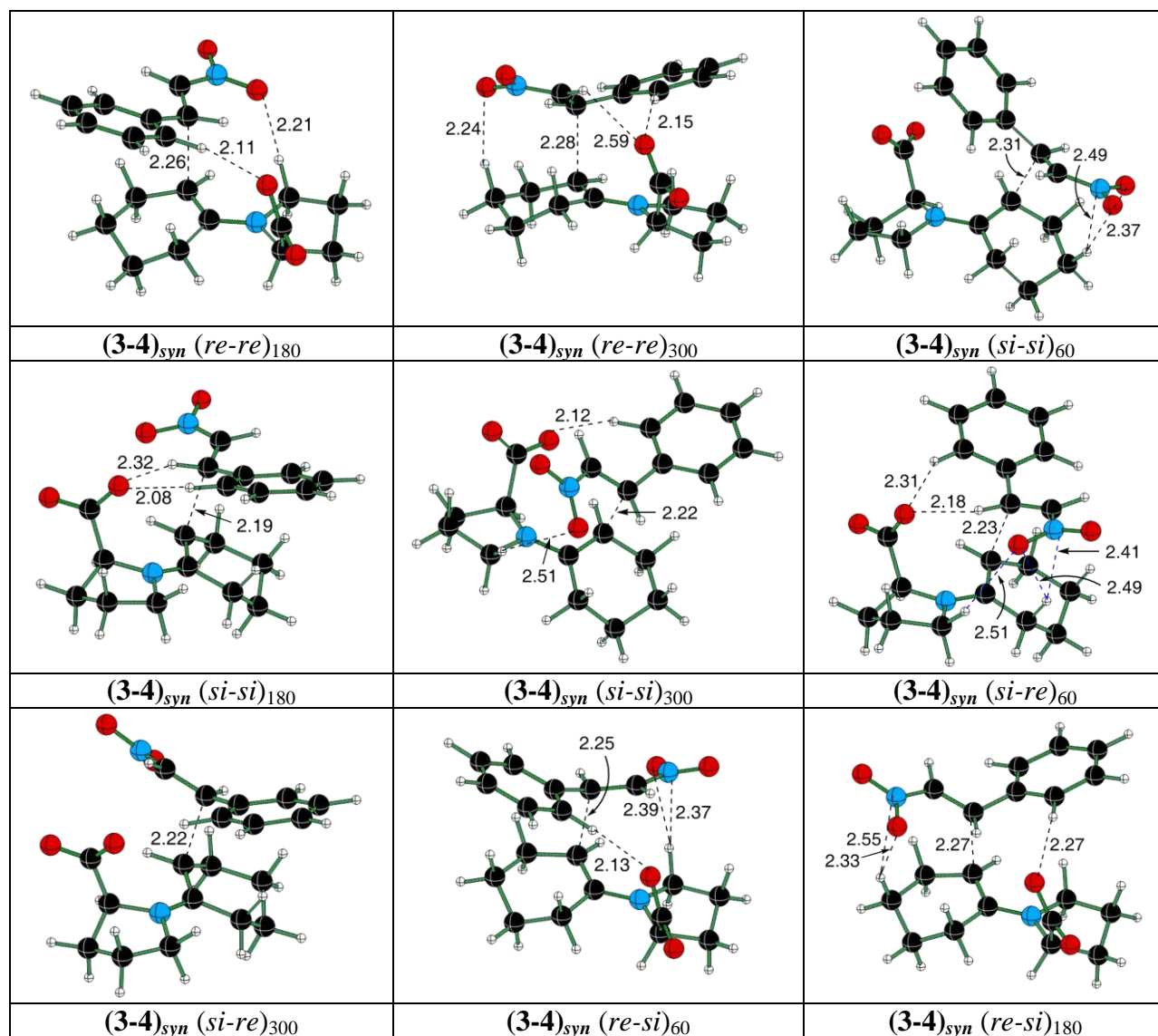


Figure S12. The optimized geometries of TSs at the SMD_(THF)/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine to nitrostyrene from the same face of the carboxylate (**3**) (*syn*-face addition).

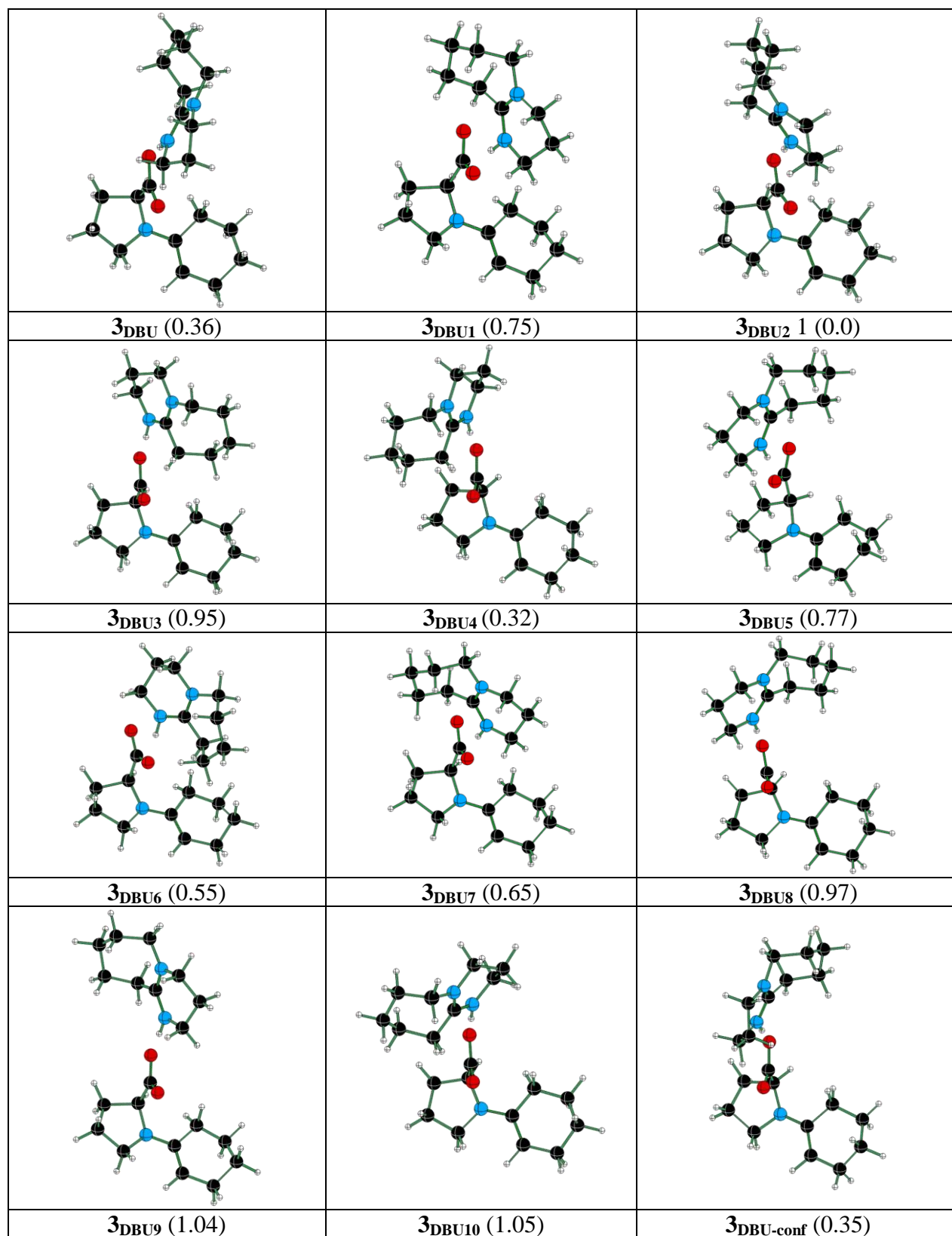


Figure S13. Different conformations of proline-enamine-DBU adduct obtained at the $\text{SMD}_{(\text{THF})}/\text{mPW1K}/6\text{-}31+\text{G}^{**}$ level of theory.

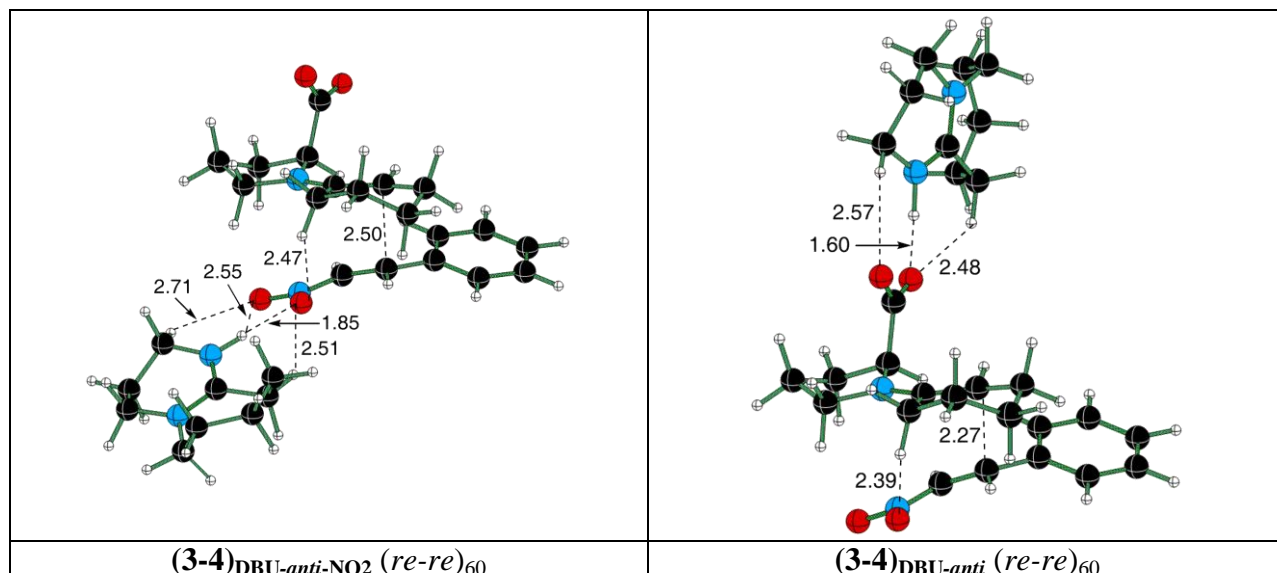
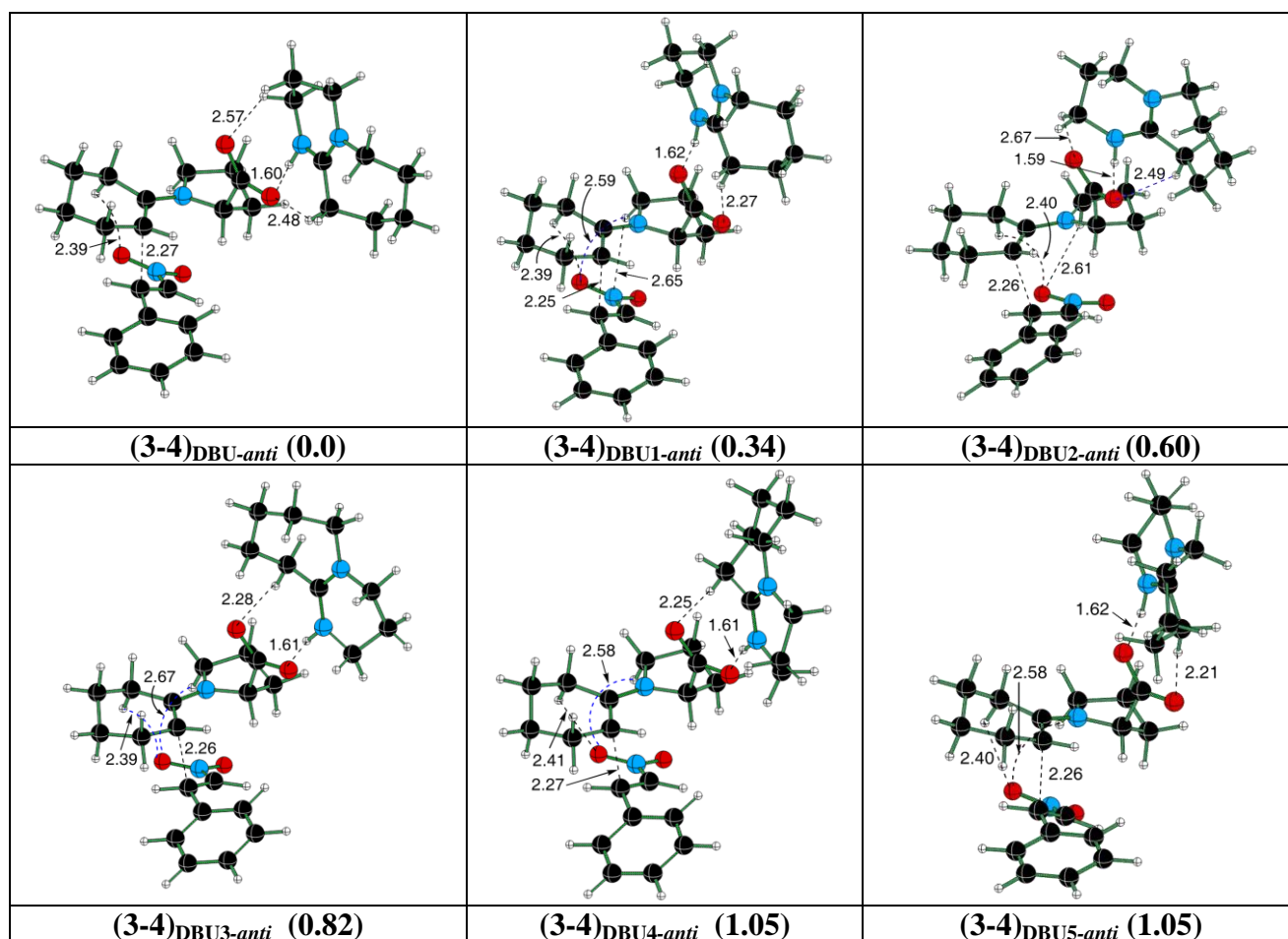


Figure S14. The two possible modes of DBU interaction in the C–C bond formation step.



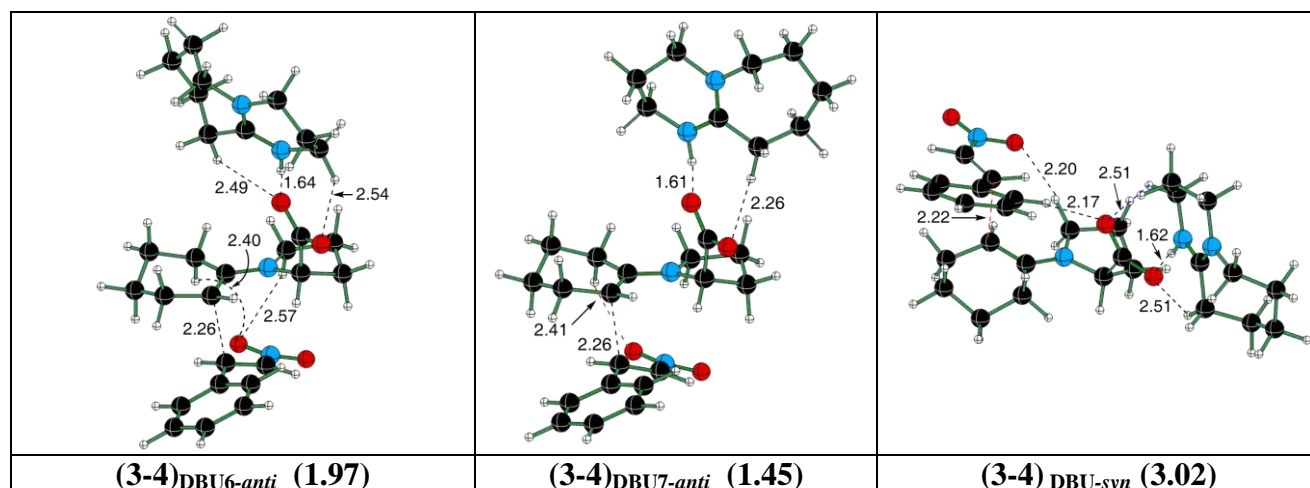
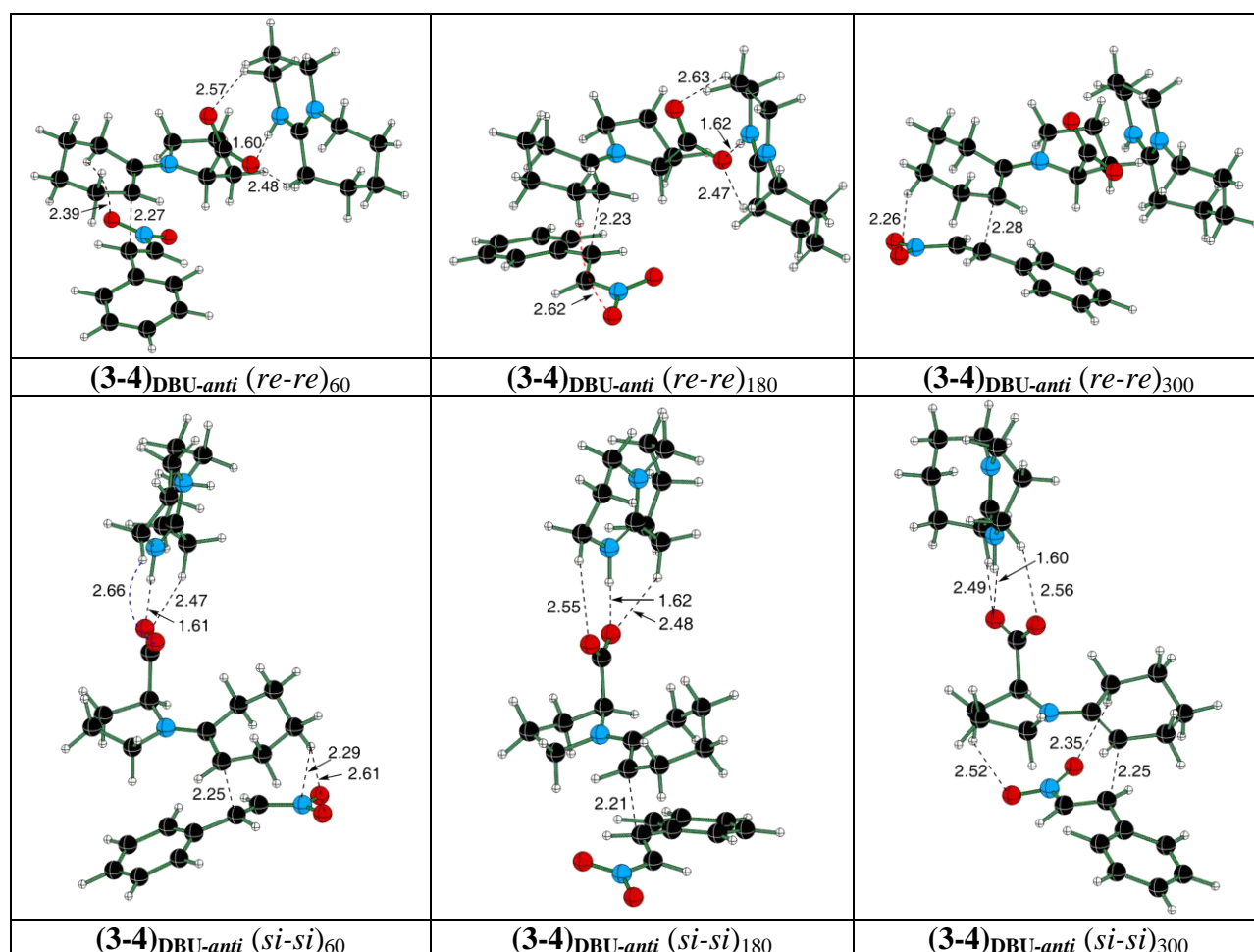


Figure S15. The optimized geometries of TS for C–C bond formation in (*re-re*)₆₀ mode having different orientation of DBU in Enamine-DBU (**3**_{DBU}) adduct at the SMD_(THF)/mPW1K/6-31+G** level of theory. The relative Gibbs free energies are provided in parenthesis.



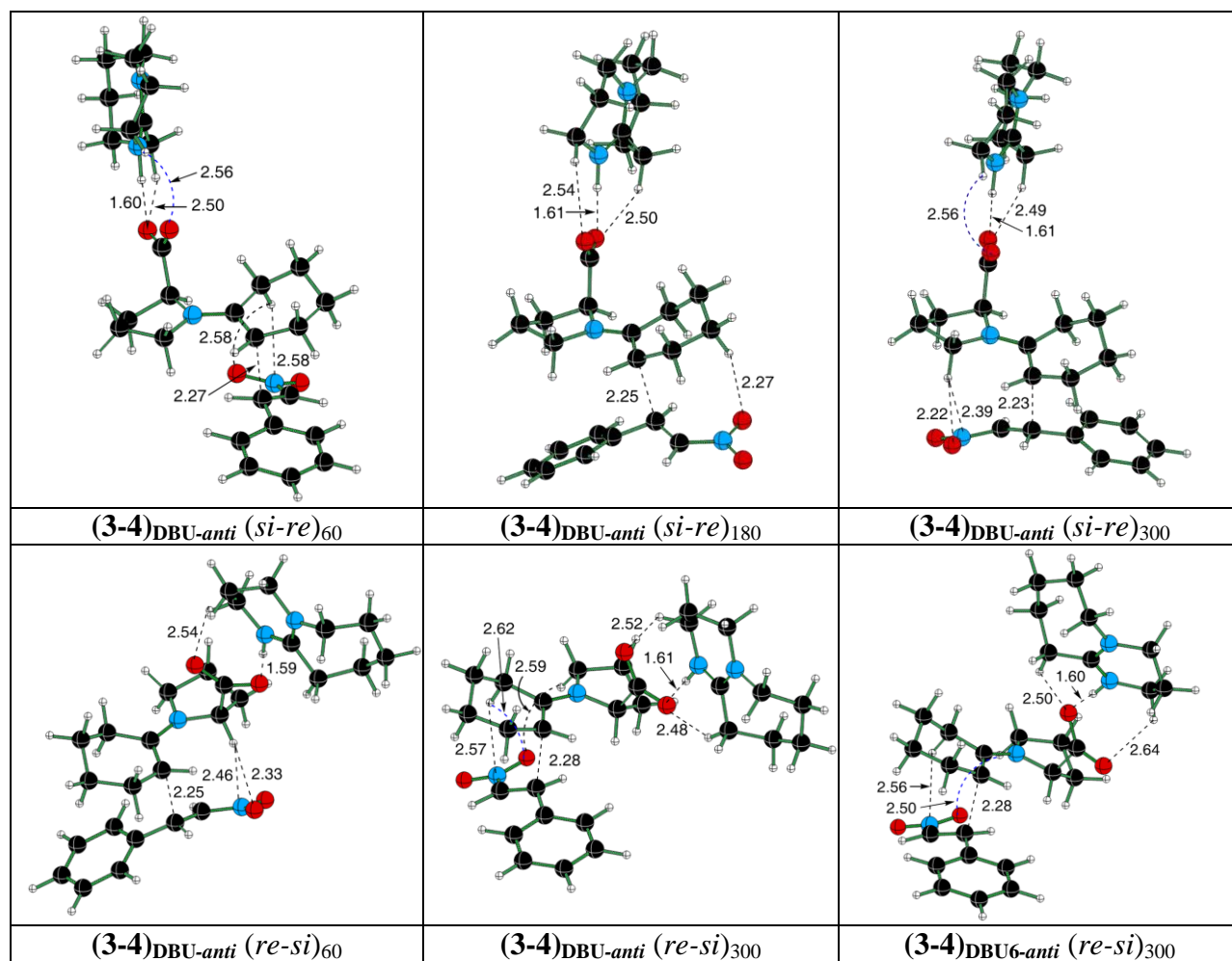


Figure S16. The optimized geometries of TSs at the SMD_(THF)/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine-DBU adduct to nitrostyrene.

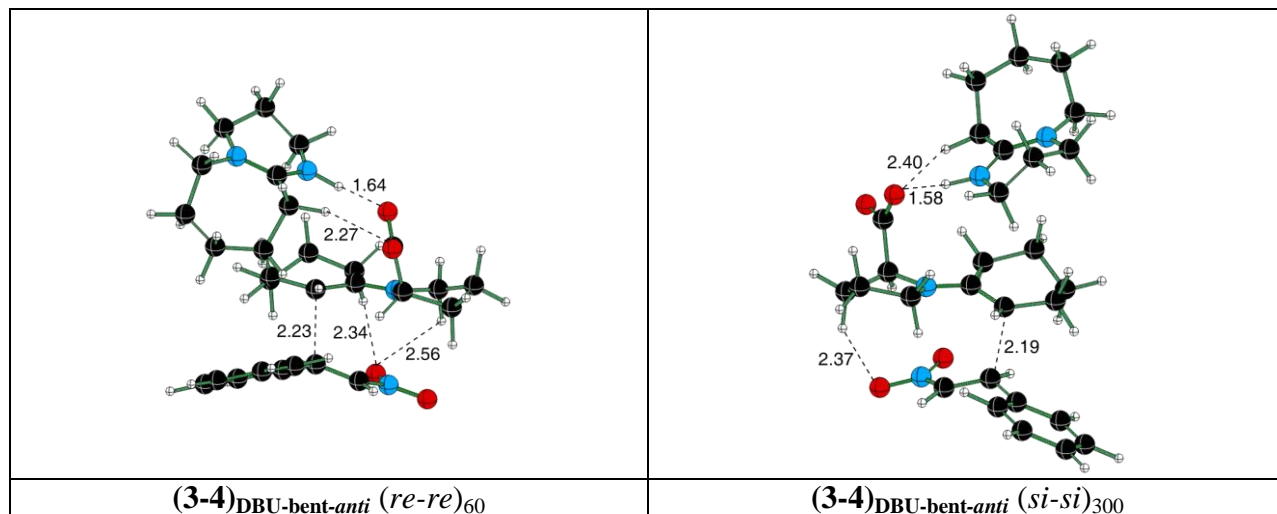


Figure S17. The optimized geometries of TS for C–C bond formation at the $\text{SMD}_{(\text{THF})}/\text{M06-2X}/6\text{-31+G}^{**}$ level of theory wherein DBU is bent towards the cyclohexane ring in Enamine-DBU adduct.

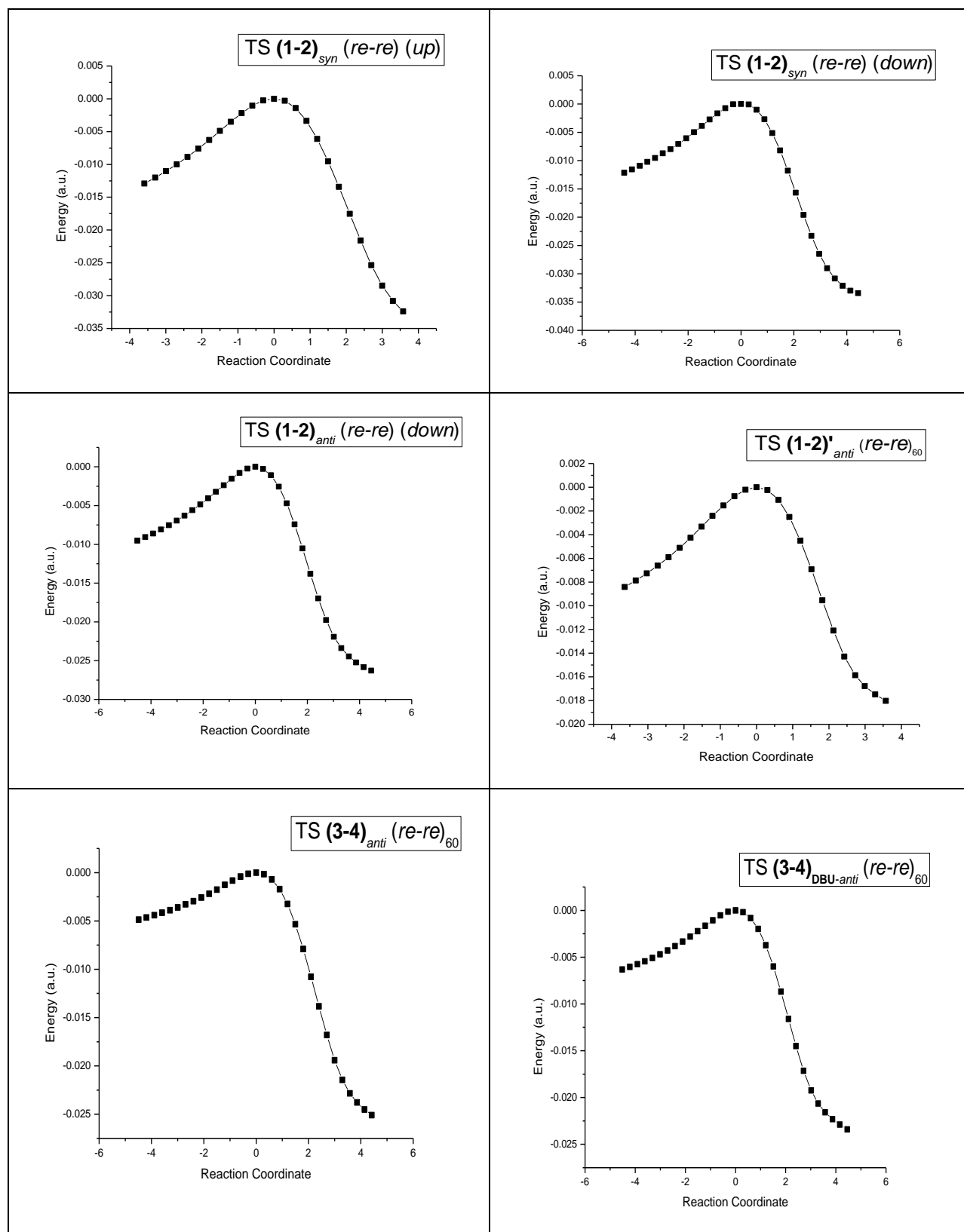


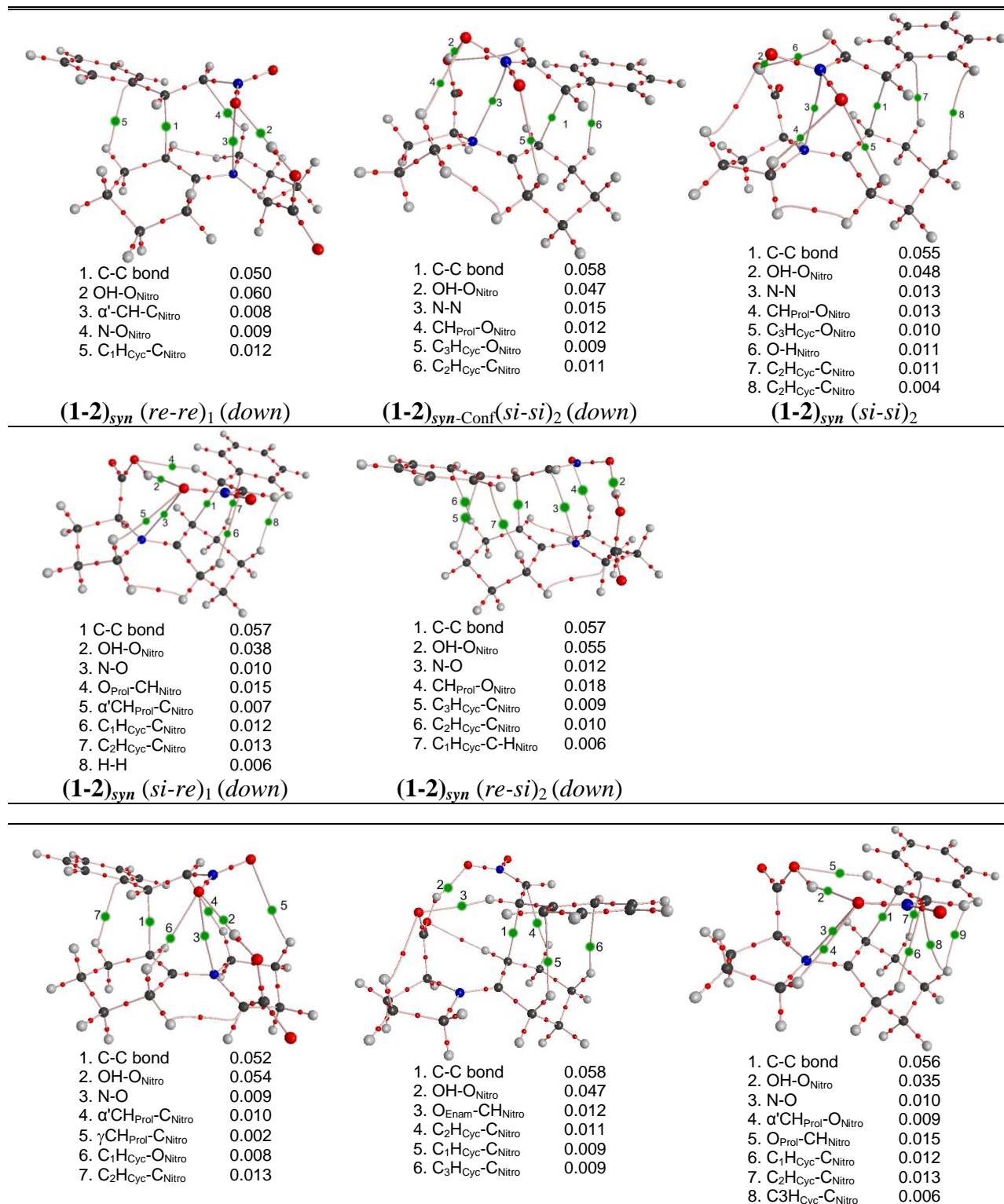
Figure S18. The energy profile along the reaction-coordinate for the different transition states calculated through intrinsic reaction coordinate (IRC) calculations.

2. Atoms-in-Molecules (AIM) Analysis

AIM analysis has been done to analyze the interactions in the TS between proline-enamine and nitrostyrene. The bond critical points for the key interactions between nitrostyrene and proline-enamine are shown in green color balloons along with the electron densities below each topological map (Figure S19-S22). The major stabilizing factor in the TS is H-bonding between COOH of enamine and NO₂ of nitrostyrene, except in those TSs that do not have this kind of interaction. The other interactions include C–H···X (N, O), and C–H···π. Other weak interactions are between the N of enamine with N, O, or C of nitrostyrene, which are the interactions in the TS having no H-bonding.

The interaction between N of enamine with C of nitrostyrene is noticed in all lower energy TSs for C–C bond formation having no H-bonding, except for *si-re* mode where N–O interaction is present (Figure S19). In *si-re* and *re-si* mode this interaction is weaker, as evident from the electron density at the bond critical point, than that in *re-re* and *si-si* modes. Also the *si-re* mode has weaker interaction than the other modes of approaches due to which it is higher in energy. In the *re-si* mode, although the interactions are more due to C–H···π interaction, the deformation is noticed to be higher due to the positioning of the phenyl group of nitrostyrene below the cyclohexyl ring, which makes the energy of the TS higher as compared to *re-re* and *si-si* modes. Among the *re-re* and *si-si* modes, a slight variation in energy arises due to small differences in interaction/strain energy or corresponding difference in the entropies. Similar interactions can be noticed for the TS-model involving enamine carboxylate (**3-4**) (Figure S21) and TS-model with explicitly bound DBU in the system ((**3-4**)_{DBU}) (Figure S22).

Figure S19. The Summary of AIM Analysis for TS(1-2) at the SMD_{THF}/mPW1K/6-31+G** level of theory



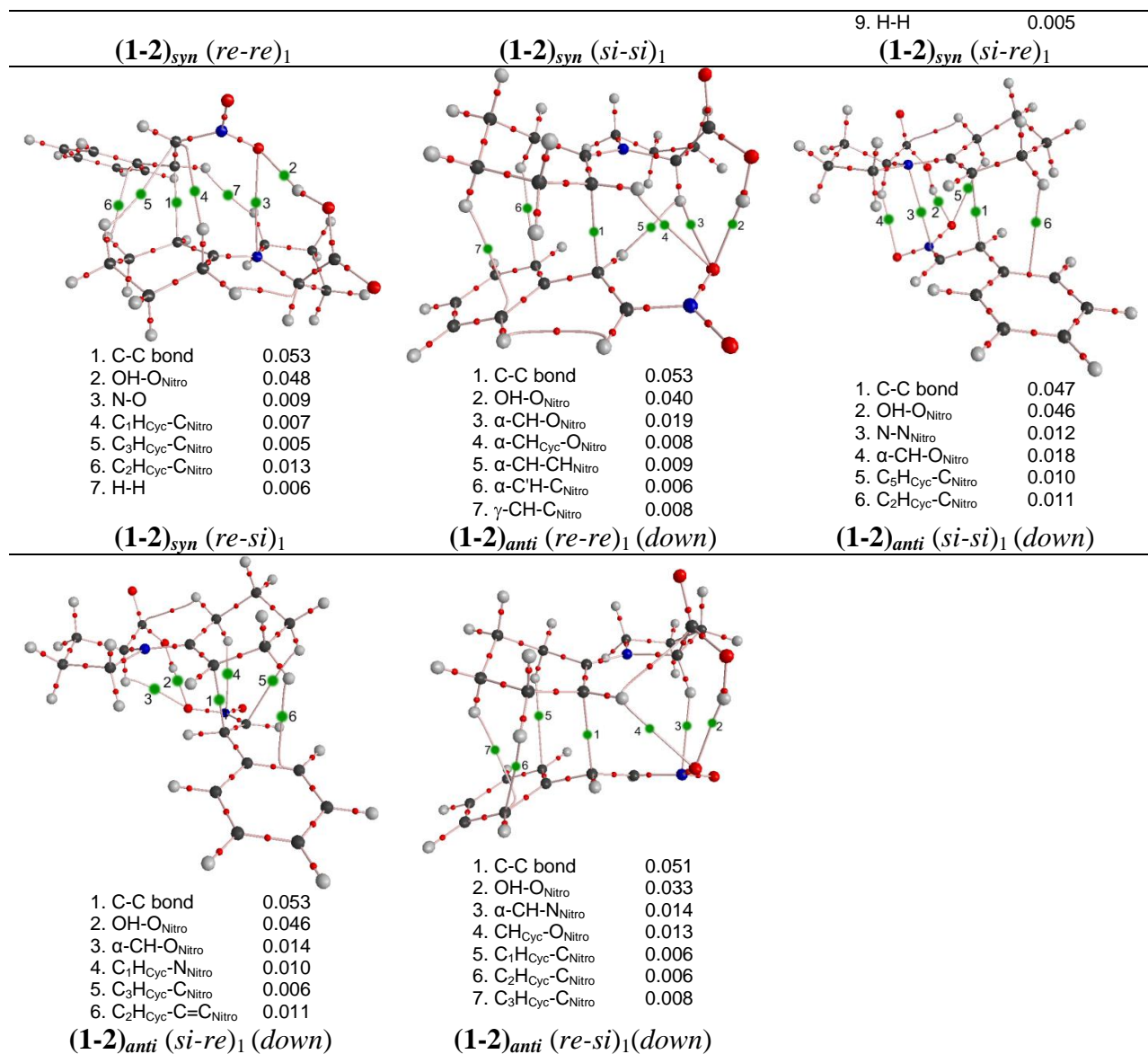


Figure S20. The Summary of AIM analysis for (TS (1-2)') at the SMD_{THF}/6-31+G** level of theory

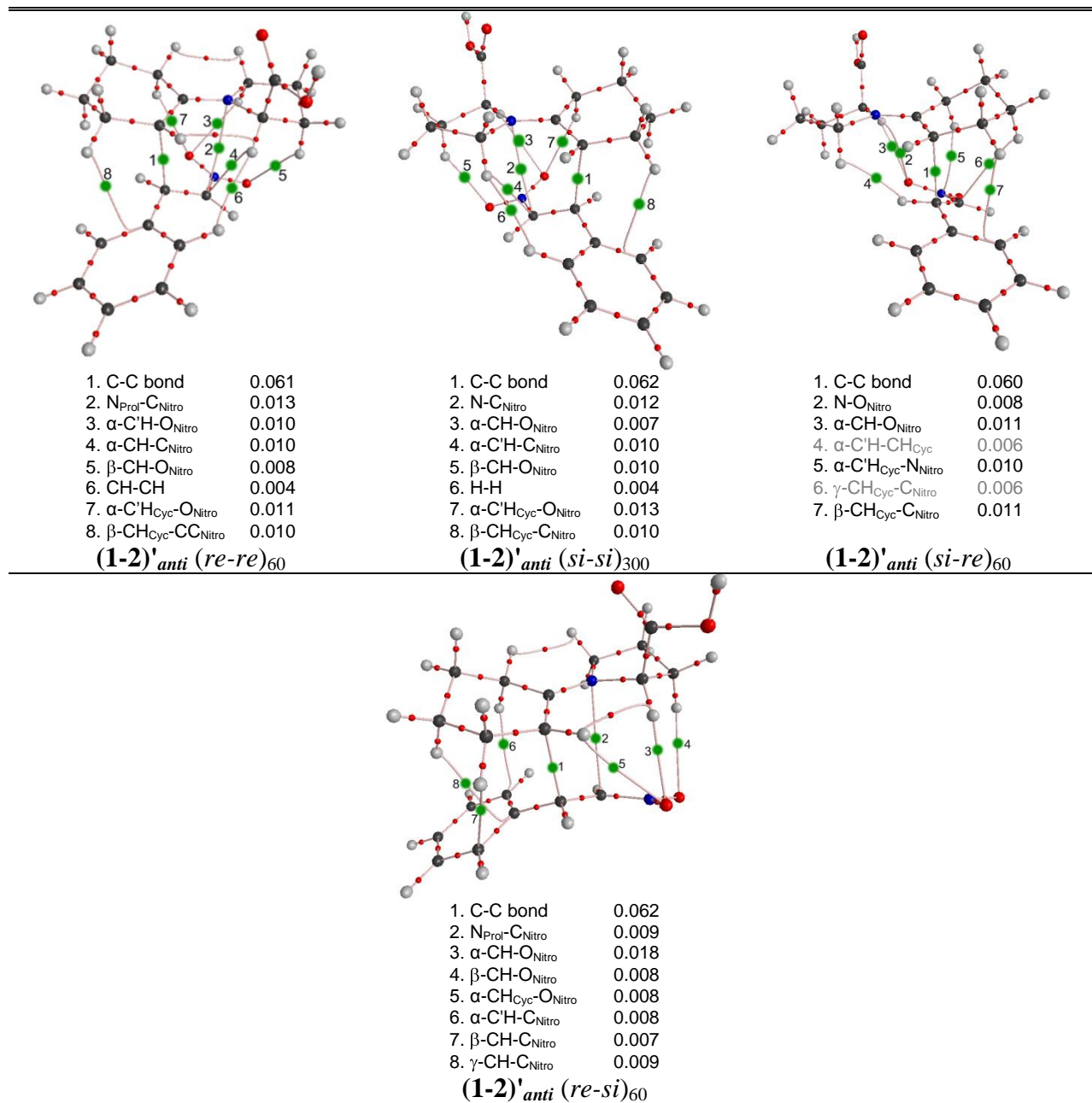


Figure S21. The Summary of AIM analysis for (TS 3-4) at the $\text{SMD}_{\text{THF}}/6-31+G^{**}$ level of theory

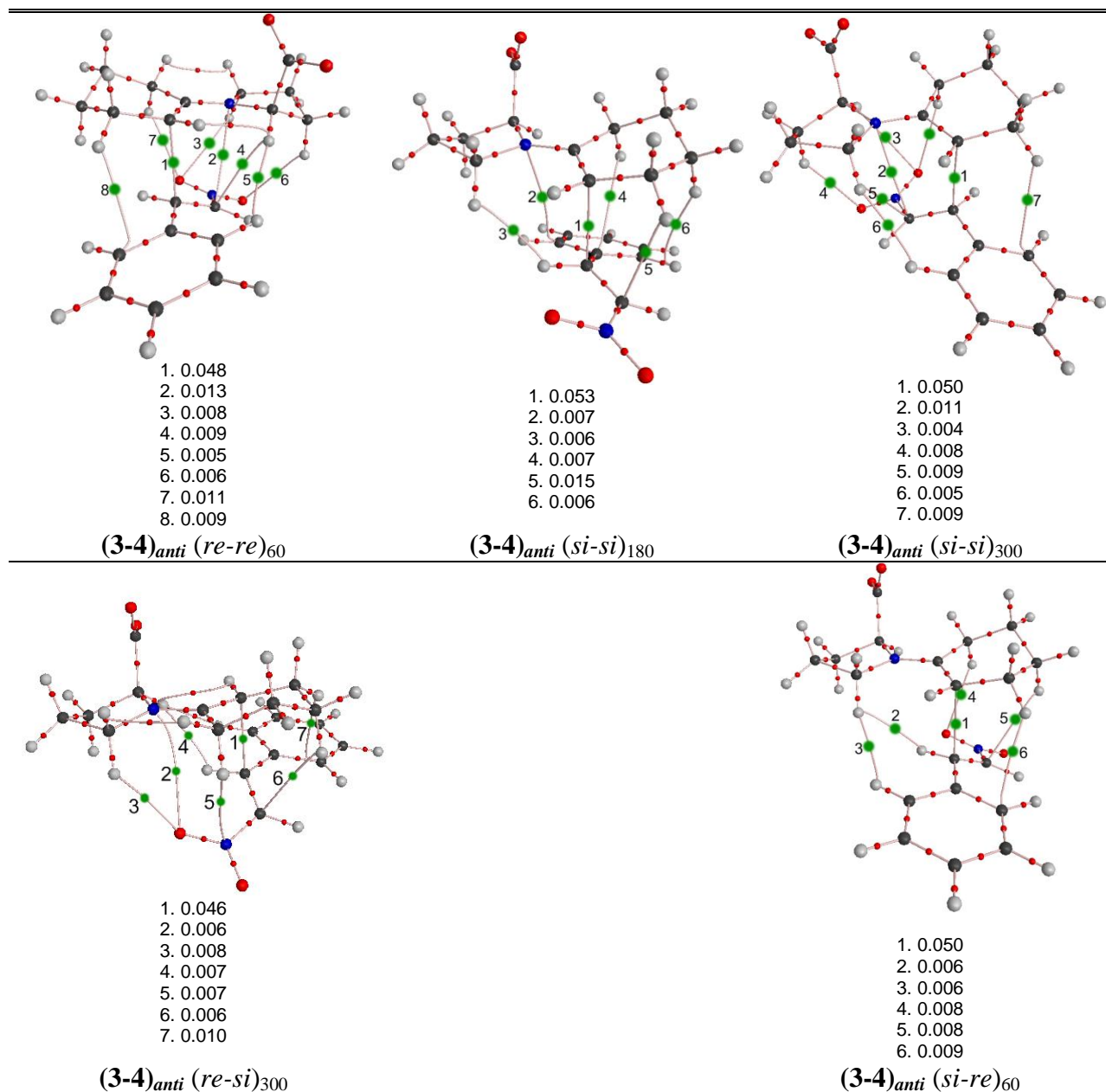
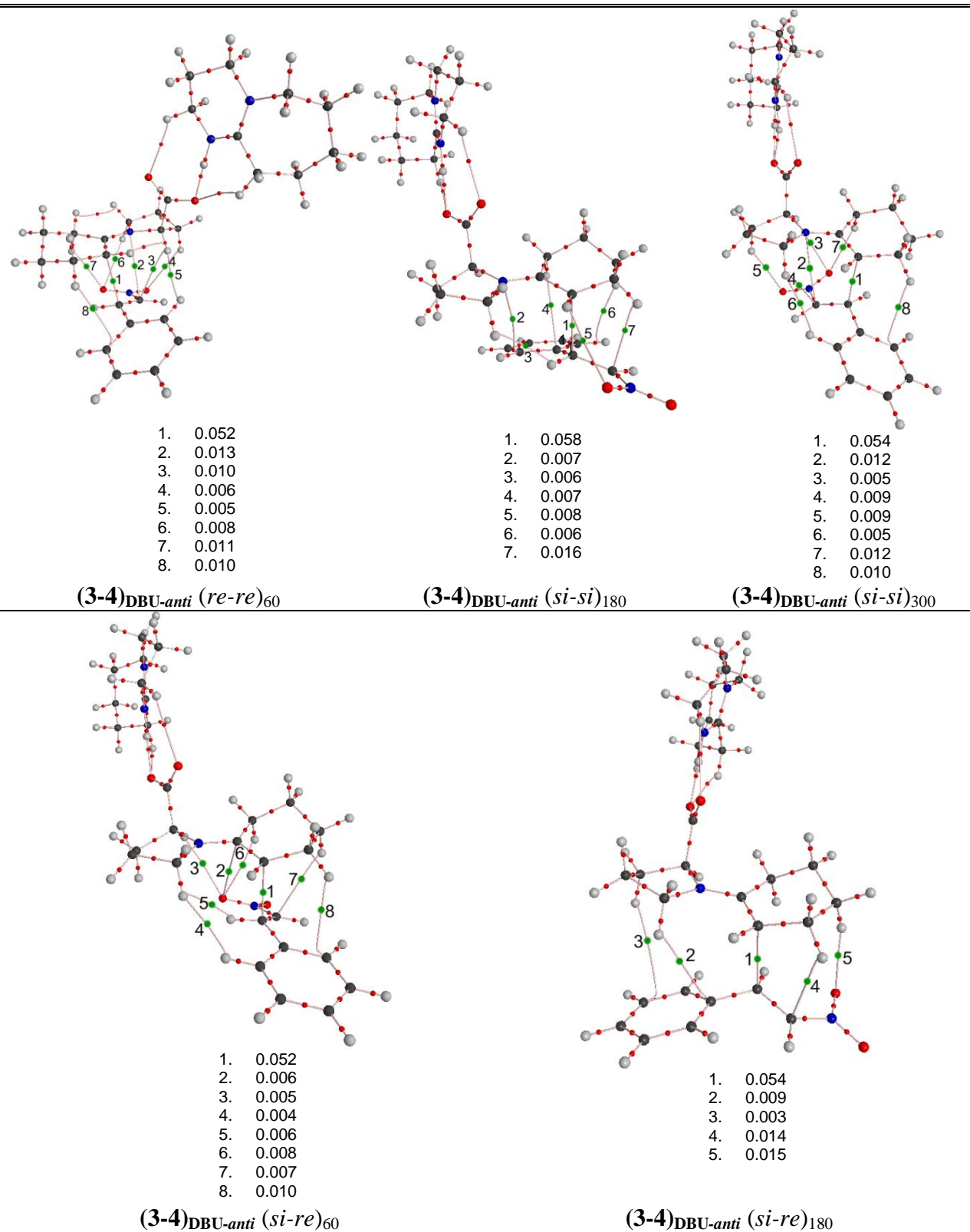
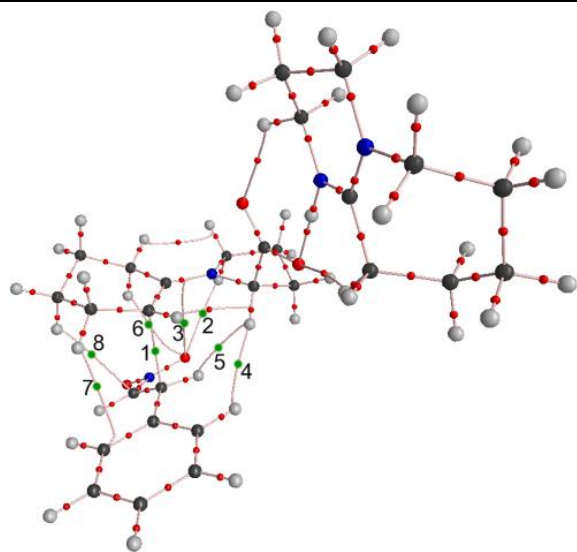


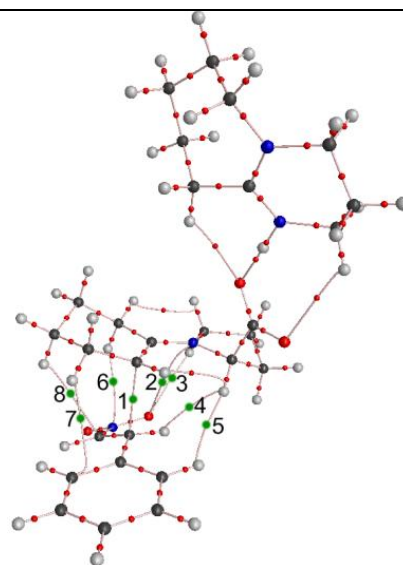
Figure S22. The summary of AIM analysis for (TS (3-4)_{DBU}) at the SMD_{THF}/6-31+G** level of theory





1. 0.051
2. 0.007
3. 0.006
4. 0.005
5. 0.007
6. 0.008
7. 0.010
8. 0.006

(3-4)DBU-anti (*re-si*)₃₀₀



1. 0.051
2. 0.006
3. 0.009
4. 0.007
5. 0.004
6. 0.008
7. 0.019
8. 0.006

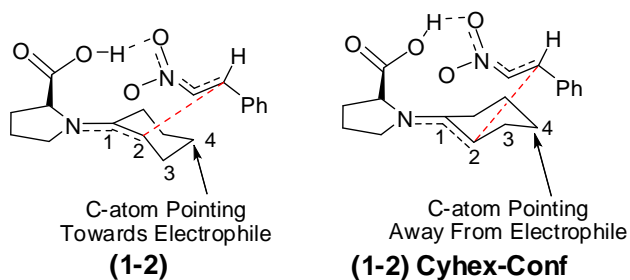
(3-4)DBU₆-anti (*re-si*)₃₀₀

Table S1. The Relative Energies^a (in kcal/mol) of **TS(1-2)** involving Reaction through Enamine Carboxylic Acid having H-bonding Interaction between –COOH and –NO₂ groups

TS ^b	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)_{syn} <i>syn</i> -addition with ‘ <i>up</i> ’ conformation of Pyrrolidine								
<i>re-re</i> ₁	43.07	25.96	28.40	11.46	41.39	23.99	44.64	27.55
<i>re-re</i> ₂	45.70	27.57	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>si-si</i> ₁	46.65	29.53	- ^c	- ^c	45.30	26.88	49.28	31.06
<i>si-si</i> ₂	45.39	27.08	28.95	10.28	40.96	21.77	45.46	26.86
<i>si-si</i> ₁ -Conf	46.69	29.62	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>si-re</i> ₁	43.18	25.64	28.92	11.10	41.09	22.71	45.86	27.72
<i>si-re</i> ₂	46.06	28.12	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>si-re</i> ₂ -Conf	50.01	32.80	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>re-si</i> ₁	42.96	26.63	30.13	13.22	44.84	27.55	47.95	29.14
<i>re-si</i> ₂	45.82	27.30	- ^c	- ^c	43.55	24.53	- ^c	- ^c
(1-2)_{syn} <i>syn</i> -addition with ‘ <i>down</i> ’ conformation of Pyrrolidine								
<i>re-re</i> ₁	42.76	25.63	28.44	11.19	40.85	23.30	43.97	26.76
<i>si-si</i> ₁	- ^c	- ^c	- ^c	- ^c	46.41	28.48	- ^c	- ^c
<i>si-si</i> ₂	46.12	28.13	30.51	12.10	42.53	23.40	47.23	28.59
<i>si-re</i> ₁	45.57	28.28	- ^c	- ^c	43.59	25.48	47.79	30.14
<i>re-si</i> ₁	43.96	27.00	31.28	14.13	43.13	25.78	46.47	29.14
<i>re-si</i> ₂	44.69	26.29	- ^c	- ^c	42.33	22.82	46.82	27.57
<i>re-si</i> ₁ -conf	-	-	- ^c	- ^c	44.66	27.95	- ^c	- ^c
(1-2)_{anti} <i>anti</i> -addition with ‘ <i>down</i> ’ conformation of Pyrrolidine								
<i>re-re</i> ₁	41.45	24.10	28.24	10.67	40.09	22.06	44.27	26.40
<i>re-re</i> ₂	48.99	31.81	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>si-si</i> ₁	46.40	28.49	31.57	13.09	42.03	23.32	46.07	27.88
<i>si-si</i> ₂	49.96	32.52	- ^c	- ^c	- ^c	- ^c	- ^c	- ^c
<i>si-re</i> ₁	49.24	31.70	34.94	17.31	46.63	28.37	50.46	32.64
<i>si-re</i> ₂	52.49	34.31	- ^c	- ^c	48.41	30.25	52.61	34.82
<i>re-si</i> ₁	43.86	26.47	28.86	11.54	41.27	22.93	45.35	27.17
<i>re-si</i> ₂	46.15	28.63	- ^c	- ^c	44.80	26.94	- ^c	- ^c
%de (<i>S,R</i>)	85	85	47	59 (<i>R,S</i>)	69	47	83	59
%ee (<i>S,R</i>)	> 99	99	53	33 (<i>R,S</i>)	64	-25	85	40

^a Computed with reference to **Proline+Cyclohexanone+Nitrostyrene**, with 6-31+G** basis set. ^b 1 and 2 represents the O-atom of NO₂ group which is interacting with –COOH (See Scheme 1). The lowest energy TS for different modes are in bold font type. ^c Not optimized because corresponding TS at other level of theory are of high energy.

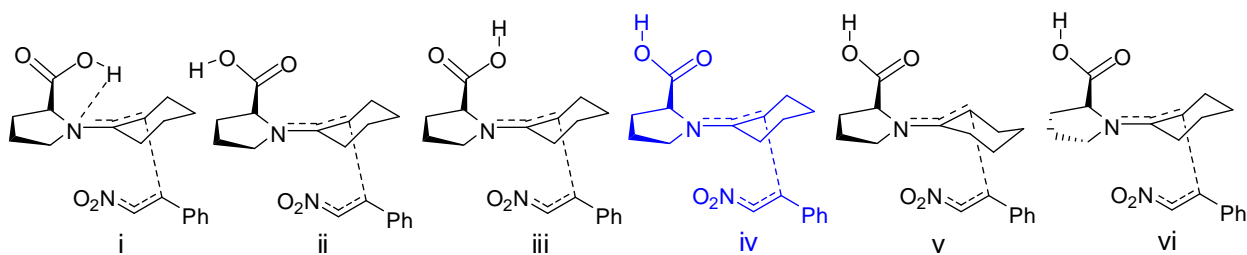
Table S2. Comparison of Energies^a of Lowest Energy **TS(1-2)** (*re-re* mode) which differs by 4th-Carbon of Cyclohexyl Group in Proline Enamine at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



	ΔG (1-2)	ΔG (1-2)Cyhex-Conf	ΔH (1-2)	ΔH (1-2)Cyhex-Conf
I _{syn} <i>re-re</i> ₁	43.07	44.24	25.96	26.69
II _{syn} <i>re-re</i> ₁	42.76	43.35	25.63	26.37
II _{anti} <i>re-re</i> ₁	41.45	42.00	24.10	24.60
II _{anti} <i>si-si</i> ₁	46.40	47.88	28.49	29.87

^a Computed with reference to **Proline**+ **Cyclohexanone** +**Nitrostyrene**.

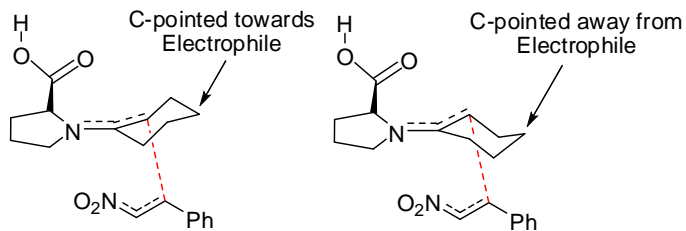
Table S3. The Relative Energies^a of **TS(1-2)'***re-re* Mode in different Conformations Obtained at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



TS (1-2)'	ΔG	ΔH
(i)	44.4	26.9
(ii)	44.0	27.6
(iii)	41.2	24.7
(iv)	40.5	24.0
(v)	40.6	24.0
(vi)	41.3	24.6

^a Computed with reference to **Proline**+ **Cyclohexanone** +**Nitrostyrene**.

Table S4. The Relative Energies^a of **TS(1-2)'** for Different Modes of Addition in Two Different Cyclohexyl Conformations (4th-carbon away or towards the Electrophile) at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



Conf. Cyclohex	TS (1-2)'	
(iv) vs (v)	ΔG	ΔH
<i>re-re</i>	40.5 / 40.6	24.0 / 24.0
<i>si-si</i>	41.0 / 41.5	24.4 / 24.8
<i>si-re</i>	42.1 / 43.1	26.3 / 27.6
<i>re-si</i>	42.7 / 43.1	26.9 / 26.4

^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene.**

Table S5. The Relative Energies^a (in kcal/mol) of 'TS(1-2)' involving Reaction Through Enamine Carboxylic Acid having no H-bonding Interaction between –COOH and –NO₂ Group

TS	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)'_{anti} <i>anti</i>-addition								
<i>(re-re)</i> ₆₀	40.47	23.98	26.03	8.71	36.63	19.64	42.06	25.52
<i>(re-re)</i> ₁₈₀	40.77	26.31	- ^c	- ^c	41.57	24.87	47.31	30.57
<i>(re-re)</i> ₃₀₀	45.56	29.57	- ^c	- ^c	46.20	29.29	51.52	35.25
<i>(si-si)</i> ₆₀	45.67	29.38	- ^c	- ^c	46.21	29.12	51.89	35.35
<i>(si-si)</i> ₁₈₀	41.99	26.62	29.66	12.59	42.99	26.37	49.37	32.90
<i>(si-si)</i> ₃₀₀	40.99	24.38	26.15	9.37	36.92	19.81	42.51	25.74
<i>(si-re)</i> ₆₀	42.07	26.28	28.84	12.87	39.96	23.55	45.51	29.29
<i>(si-re)</i> ₁₈₀	- ^b	- ^b	- ^c	- ^c	- ^b	- ^b	- ^b	- ^b
<i>(si-re)</i> ₃₀₀	43.33	27.39	- ^c	- ^c	42.26	25.30	53.94	35.51
<i>(re-si)</i> ₆₀	42.73	26.86	29.36	12.38	41.24	23.99	46.92	29.96
<i>(re-si)</i> ₁₈₀	-	-	- ^c	- ^c	- ^b	- ^b	- ^b	- ^b
<i>(re-si)</i> ₃₀₀	43.32	27.05	- ^c	- ^c	41.09	24.87	46.06	30.09
(1-2)'_{syn} <i>syn</i>-addition								
<i>(re-re)</i> ₁₈₀	43.6	27.31	- ^c	- ^c	43.66	26.53	- ^b	- ^b
<i>(re-re)</i> ₃₀₀	47.1	30.81	- ^c	- ^c	47.59	30.45	52.59	36.45
<i>(si-si)</i> ₁₈₀	44.4	28.27	- ^c	- ^c	- ^b	- ^b	- ^b	- ^b
<i>(si-si)</i> ₃₀₀	48.0	31.40	- ^c	- ^c	45.95	28.18	50.70	33.72
<i>(si-re)</i> ₆₀	46.6	29.84	- ^c	- ^c	45.83	28.46	51.45	34.56
<i>(re-si)</i> ₆₀	45.7	28.79	- ^c	- ^c	44.63	26.58	- ^b	- ^b
%de (<i>S,R</i>)	87	96	98	>99	>99	>99	>99	>99
%ee (<i>S,R</i>)	40	33	8	53	25	17	40	17

^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. ^b Could not optimize the TS. ^c Only the lowest energy TS are attempted at this level of theory.

Table S6. The Energetics^a of *Activation-Strain Analysis* for the Lowest Energy TS for **TS(3-4)** calculated at the SMD_{THF}/mPWPW91/6-31+G** Level of Theory

3-4	$\Delta E^\ddagger_{\text{strain-Enamine}}$	$\Delta E^\ddagger_{\text{strain-Nitrostyrene}}$	$\Delta E^\ddagger_{\text{strain}}$	$\Delta E^\ddagger_{\text{int}}$	ΔE^\ddagger
TS (3-4)' <i>anti</i> (up)					
<i>re-re</i> ₆₀	6.4	9.0	15.4	-8.6	6.8
<i>si-si</i> ₁₈₀	5.0	9.9	14.9	-7.9	7.0
<i>si-si</i> ₃₀₀	4.5	9.7	14.3	-7.3	7.0
<i>si-re</i> ₆₀	4.7	9.3	14.0	-4.7	9.3
<i>re-si</i> ₃₀₀	6.5	9.1	15.6	-6.1	9.5

^a The energies given in table are total electronic energy and calculated with respect to the separated lowest energy enamine+nitrostyrene

Table S7. The Relative Energies^a (in kcal/mol) of **TS(3-4)** involving C–C Bond Formation Through Enamine Carboxylate Intermediate (**3**)

TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K ^b		B3LYP ^b	
3-4	<i>anti</i> -addition							
(<i>re-re</i>) ₆₀	42.16	25.78	29.93	12.12	111.34	94.66	112.17	96.43
(<i>re-re</i>) ₁₈₀	44.86	28.46	- ^d	- ^d	- ^c	- ^c	- ^c	- ^c
(<i>re-re</i>) ₃₀₀	46.87	30.95	- ^d	- ^d	115.34	99.87	116.63	100.98
(<i>si-si</i>) ₆₀	45.89	29.38	- ^d	- ^d	113.52	96.76	115.07	98.72
(<i>si-si</i>) ₁₈₀	42.35	25.88	30.42	13.33	109.60	93.43	110.89	95.45
(<i>si-si</i>) ₃₀₀	42.72	26.10	30.60	13.11	111.96	95.15	113.26	97.24
(<i>si-re</i>) ₆₀	44.11	28.21	32.52	16.64	- ^c	- ^c	- ^c	- ^c
(<i>si-re</i>) ₁₈₀	44.47	27.85	- ^d	- ^d	111.93	94.98	112.77	96.85
(<i>si-re</i>) ₃₀₀	44.25	27.61	31.76	14.40	112.28	95.76	113.31	97.46
(<i>re-si</i>) ₆₀	46.71	30.02	- ^d	- ^d	117.27	100.68	119.09	102.54
(<i>re-si</i>) ₁₈₀	45.78	30.03	- ^d	- ^d	114.86	98.92	- ^c	- ^c
(<i>re-si</i>) ₃₀₀	44.23	28.43	34.17	17.41	114.08	97.63	113.80	98.44
	<i>syn</i> -addition							
(<i>re-re</i>) ₆₀	- ^c	- ^c	- ^d	- ^d	- ^c	- ^c	- ^c	- ^c
(<i>re-re</i>) ₁₈₀	43.73	26.69	- ^d	- ^d	108.38	91.45	110.88	94.23
(<i>re-re</i>) ₃₀₀	47.94	31.21	- ^d	- ^d	114.38	96.61	115.53	99.37
(<i>si-si</i>) ₆₀	58.63	40.72	- ^d	- ^d	- ^c	- ^c	- ^c	- ^c
(<i>si-si</i>) ₁₈₀	47.31	29.53	- ^d	- ^d	116.40	99.38	119.15	102.65
(<i>si-si</i>) ₃₀₀	50.16	32.33	- ^d	- ^d	117.00	98.47	119.90	102.04
(<i>si-re</i>) ₆₀	47.38	29.93	- ^d	- ^d	114.37	96.83	117.41	100.57
(<i>si-re</i>) ₁₈₀	- ^c	- ^c	- ^d	- ^d	- ^c	- ^c	- ^c	- ^c
(<i>si-re</i>) ₃₀₀	51.01	33.10	- ^d	- ^d	120.46	103.71	123.09	106.33
(<i>re-si</i>) ₆₀	46.31	29.09	- ^d	- ^d	112.49	94.57	114.60	97.57
(<i>re-si</i>) ₁₈₀	45.38	29.57	- ^d	- ^d	111.99	94.39	114.36	97.26
(<i>re-si</i>) ₃₀₀	- ^c	- ^c	- ^d	- ^d	- ^c	- ^c	- ^c	- ^c
%de(<i>S,R</i>)	93	91	91	96	>99	99	92	98
%ee(<i>S,R</i>)	17	8	40	69	77	93	0	77

^a Computed with reference to **Proline**+ **Cyclohexanone** +**Nitrostyrene**, with 6-31+G** basis set. ^b The computed energies are very high as the gas phase calculations fails in acid-base reaction; **1**+DBU \rightarrow **3**+DBUH⁺. ^c Could not

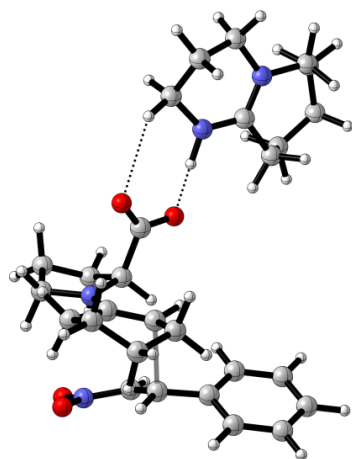
optimize the TS or the TS is less probable due to positioning of COO⁻ group in *syn*-face addition. ^d Only the lowest energy TS are attempted at this level of theory.

Table S8. The Relative Energies^a (in kcal/mol) of TS **(3-4)**_{DBU}(*re-re*)₆₀ having Different Orientation of DBU in **3**_{DBU} Adduct at the SMD_{THF}/mPW1K/6-31+G** Level of Theory

	(3-4) _{DBU} <i>n-anti</i> (<i>re-re</i>) ^b		Enamine _{anti} -DBU adduct ^c	
	ΔG	ΔH	ΔG	ΔH
3 _{DBU}	33.98 (0.00)	7.13 (0.0)	0.36	-0.06
3 _{DBU1}	34.32 (0.34)	7.73 (0.60)	0.75	-0.14
3 _{DBU2}	34.58 (0.60)	7.26 (0.13)	0.0	0.0
3 _{DBU3}	34.80 (0.82)	7.43 (0.30)	0.95	0.0
3 _{DBU4}	35.03 (1.05)	7.26 (0.13)	0.32	0.03
3 _{DBU5}	35.04 (1.06)	7.40 (0.27)	0.77	-0.01
3 _{DBU6}	35.96 (1.98)	7.54 (0.41)	0.55	-0.11
3 _{DBU7}	35.45 (1.47)	7.29 (0.16)	0.65	0.02

^a Computed with reference to **Proline**+ **Cyclohexanone** +**Nitrostyrene**. ^b The energies in parenthesis are energies with respect to lowest energy **3**_{DBU} adduct. The *syn*-enamine is involved in this TS. ^cEnamine-DBU adducts involves *anti*-enamine as it is more stable than *syn*-enamine.

Table S9. The Relative Energies^a (in kcal/mol) for the Lowest Energy TS **(3-4)**_{DBU} involving C–C Bond Formation in Presence of DBU



TS	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(3-4) _{DBU}	<i>anti</i> -addition							
(<i>re-re</i>) ₆₀	33.98	7.13	19.48	-8.74	31.43	3.60	37.23	9.80
(<i>re-re</i>) ₁₈₀	36.52	9.02	- ^c	- ^c	- ^b	- ^b	- ^b	- ^b
(<i>re-re</i>) ₃₀₀	41.09	12.13	- ^c	- ^c	39.82	11.88	44.82	17.62
(<i>si-si</i>) ₆₀	38.80	11.39	- ^c	- ^c	39.53	9.83	42.99	16.56

$(si-si)_{180}$	34.51	8.33	22.77	-6.14	$-^b$	$-^b$	40.92	13.85
$(si-si)_{300}$	35.53	7.48	20.86	-7.82	31.68	3.82	37.22	10.18
$(si-re)_{60}$	36.32	9.46	22.78	-4.52	34.12	7.21	39.63	13.10
$(si-re)_{180}$	36.49	10.11	$-^c$	$-^c$	37.07	9.96	$-^b$	$-^b$
$(si-re)_{300}$	37.95	9.76	$-^c$	$-^c$	$-^b$	$-^b$	42.20	14.44
$(re-si)_{60}$	38.4	10.7	22.79	-4.51	34.60	7.82	40.98	13.90
$(re-si)_{180}$	$-^b$	$-^b$	$-^c$	$-^c$	$-^b$	$-^b$	$-^b$	$-^b$
$(re-si)_{300}$	36.99	10.21	23.18	-3.28	35.64	8.30	40.70	13.50
<i>syn-addition</i>								
$(re-re)_{180}$	37.00	9.19	25.01	-4.30	$-^d$	$-^d$	$-^d$	$-^d$
%de (<i>S,R</i>)	For % <i>ee</i> and % <i>de</i> see Table S14 which is calculated according to all TS in different							
% <i>ee</i> (<i>S,R</i>)	conformation							

^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. ^b Could not optimize TS. ^c Only the lowest energy TS are attempted at this level of theory. ^d not attempted.

Table S10. The Relative Energies^a (in kcal/mol) for TS (**3-4**)_{DBU} involving C–C Bond Formation in Presence of DBU for **3**_{DBU6} Conformation

TS	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(3-4) _{DBU6}	<i>anti-addition</i>							
$(re-re)_{60}$	35.96	7.54	$-^c$	$-^c$	32.34	4.31	38.05	10.60
$(re-re)_{180}$	36.91	10.04	$-^c$	$-^c$	35.09	6.35	$-^b$	$-^b$
$(re-re)_{300}$	39.80	12.88	$-^c$	$-^c$	39.72	12.39	44.97	18.21
$(si-si)_{60}$	38.83	11.74	$-^c$	$-^c$	39.11	11.13	44.52	17.24
$(si-si)_{180}$	35.76	8.27	$-^c$	$-^c$	$-^b$	$-^b$	$-^b$	$-^b$
$(si-si)_{300}$	35.50	7.83	$-^c$	$-^c$	33.47	5.51	$-^b$	$-^b$
$(si-re)_{60}$	36.82	9.97	$-^c$	$-^c$	38.15	8.26	$-^b$	$-^b$
$(si-re)_{180}$	37.88	10.33	$-^c$	$-^c$	37.46	10.37	$-^b$	$-^b$
$(si-re)_{300}$	37.63	9.95	$-^c$	$-^c$	36.22	8.67	42.79	15.02
$(re-si)_{60}$	38.50	11.29	$-^c$	$-^c$	$-^b$	$-^b$	$-^b$	$-^b$
$(re-si)_{180}$	37.96	11.69	$-^c$	$-^c$	36.18	8.85	$-^b$	$-^b$
$(re-si)_{300}$	36.49	10.17	$-^c$	$-^c$	$-^b$	$-^b$	40.26	14.15

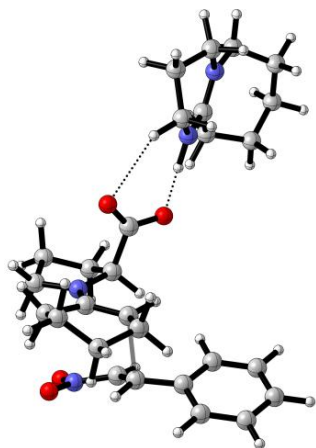
^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. ^b Could not optimize the TS. ^c TSs are not attempted as it is higher in energy at other level of theory.

Table S11. The Relative Energies^a (in kcal/mol) for TS (3-4)_{DBU1} involving C–C Bond Formation in presence of DBU for 3_{DBU1} Conformation at the SMD_{THF}/mPW1K/6-31+G** Level of Theory

TS (3-4) _{DBU1}	ΔG	ΔH
(<i>re-re</i>) ₆₀	34.32	7.73
(<i>si-si</i>) ₃₀₀	36.01	8.27
(<i>si-si</i>) ₁₈₀	36.07	8.54

^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**.

Table S12. The Relative Energies^a (in kcal/mol) for TS (3-4)_{DBU2} involving C–C Bond Formation in Presence of DBU for 3_{DBU2} Conformation



(3-4) _{DBU2}	<i>anti</i> -addition							
	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(<i>re-re</i>) ₆₀	34.58	7.26	19.09	-8.98	31.44	3.52	37.19	9.75
(<i>si-si</i>) ₁₈₀	- ^c	- ^c	- ^c	- ^c	31.99	4.03	38.45	10.32
(<i>si-si</i>) ₃₀₀	35.29	7.54	20.06	-7.71	35.47	7.96	- ^b	- ^b
(<i>si-re</i>) ₆₀	- ^b	- ^b	- ^b	- ^b	34.49	7.49	39.80	13.36
(<i>re-si</i>) ₃₀₀	36.85	10.25	24.36	-3.34	35.79	8.31	40.73	13.57

^a Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. ^b Could not optimize the TS. ^c TSs are not attempted as it is higher in energy at other levels of theory.

Table S13. The Relative Energies^a (in kcal/mol) for TS **(3-4)**_{DBU-bent} involving C–C Bond Formation in Presence of DBU^b at the SMD_{THF}/M06-2X/6-31+G** Level of Theory

(3-4) _{DBU-bent}	ΔG	ΔH
<i>re-re</i>	20.17	-9.59
<i>si-si</i>	21.69	-7.97

^a Computed with reference to **Proline**+ **Cyclohexanone** +**Nitrostyrene**. ^b The 3-DBU adduct involves DBU bent towards cyclohexane carbon of enamine. These are higher in energy in free energy than TS **(3-4)**_{DBU} and but lower in enthalpy.

Table S14. The Relative Energies^a (in kcal/mol) of the Lowest Energy TS for Each Mode from Different **3**_{DBU}-adducts and Computed Stereoselectivity

(3-4) _{DBU} TS	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
<i>re-re</i> ₆₀	33.98	7.13	19.09	-8.98	31.43	3.52	37.19	9.75
<i>si-si</i> ₃₀₀	34.51 ₁₈₀	7.48 ₁₈₀	20.06	-7.82	31.68	3.82	37.22	10.18
<i>si-re</i> ₆₀	36.32	9.46	22.78	-4.52	34.12	7.21	39.63	13.10
<i>re-si</i> ₆₀	36.49 ₃₀₀	10.17 ₃₀₀	22.79	-4.51	34.60	7.82	40.26 ₃₀₀	13.50 ₃₀₀
Relative energies of TS with reference to lowest energy TS								
	$\Delta\Delta G$	$\Delta\Delta H$	$\Delta\Delta G$	$\Delta\Delta H$	$\Delta\Delta G$	$\Delta\Delta H$	$\Delta\Delta G$	$\Delta\Delta H$
<i>re-re</i> ₆₀	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>si-si</i> ₃₀₀	0.5	0.4	1.0	1.2	0.2	0.3	0.0	0.4
<i>si-re</i> ₆₀	2.3	2.3	3.7	4.5	2.7	3.7	2.4	3.3
<i>re-si</i> ₆₀	2.5	3.0	3.7	4.5	3.2	4.3	3.1	3.8
%de (<i>S,R</i>)	96	96	> 99	> 99	98	> 99	97	> 99
%ee (<i>S,R</i>)	40	33	69	77	17	25	0	33

^a Lowest TS for different modes has been taken from Table S9-S12.

Table S15. Comparison of Relative Energies (in kcal/mol) of the Lowest Energy TS (*re-re* mode) for Different TS-Models with Respect to Proline, Enamine, and Nitrostyrene

(3-4) _{DBU} TS	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2) _{anti} (<i>Down</i>)	41.45	24.10	28.24	10.67	40.09	22.06	43.97 ^a	26.76 ^a
(1-2) '	40.47	23.98	26.03	8.71	36.63	19.64	42.06	25.52
(3-4) _{anti} (<i>re-re</i>) ₆₀	42.16	25.78	29.93	12.12	108.38 ^b	91.45 ^b	110.88 ^b	94.23 ^b
(3-4) _{DBU-anti} (<i>re-re</i>) ₆₀	33.98	7.13	19.09 ^c	-8.98 ^c	31.43	3.60	37.19 ^c	9.75 ^c

^a TS **(1-2)**_{syn} (*down*) ^b TS **(3-4)**_{syn}, computed energies are very high as gas phase calculations failed in acid-base reaction; **1**+DBU \rightarrow **3**+DBUH⁺. ^c TS **(3-4)**_{DBU2-anti} (*re-re*)₆₀. The lowest energy TS chosen on the basis of Gibbs free energy.

Table S16. Comparison of Relative Energy of Lowest Energy TS (*re-re* mode) for Different TS-Models with Respect to Enamine and Nitrostyrene

(3-4)_{DBU}	SMD _{THF} /mPW1K		SMD _{THF} /M06-2X		mPW1K		B3LYP		
	TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)		29.21	14.33	20.65	5.14	29.48	13.79	31.22 ^a	16.30 ^a
(1-2)'		28.24	14.22	18.43	3.18	26.02	11.37	29.30	15.05
(3-4)_{anti} (re-re)₆₀		22.17	7.51	12.03	-3.14	11.67 ^b	-3.87 ^b	14.14 ^b	-1.34 ^b
(3-4)_{DBU-anti} (re-re)₆₀		21.75	-2.64	11.50	-14.51	20.82 ^c	-4.67 ^c	24.43 ^c	-0.72 ^c

^a TS **(1-2)_{syn}** (*down*). ^b TS **(3-4)_{syn}**. ^c TS **(3-4)_{DBU2-anti} (re-re)₆₀**. TS chosen on basis of lower free energy.

3. The Cartesian coordinates of the optimized geometries of stationary points. Total Electronic Energy (E_0), Zero Point Energy Correction to E_0 (E_{0+ZPE}), Internal Energy (E_{298}), Enthalpy (H_{298}), Free Energy (G_{298}) and Number of Imaginary Frequency (NImag) Obtained at the SMD_{THF}/mPW1K/6-31+G Level of Theory**

Note: To distinguish the pyrrolidine ‘up’ and ‘down’ conformer, the up conformation has not been mentioned, whereas for the *down* conformation ‘down’ is included after the TS name.

H₂O

$E_0 = -76.4111824$
 $E_{0+ZPE} = -76.389235$
 $E_{298} = -76.386399$
 $H_{298} = -76.385455$
 $G_{298} = -76.406856$
NImag = 0
O 0.000000 0.000000 0.115667
H 0.000000 0.760811 -0.462668
H 0.000000 -0.760811 -0.462668

Proline

$E_0 = -401.0919396$
 $E_{0+ZPE} = -400.942287$
 $E_{298} = -400.935270$
 $H_{298} = -400.934326$
 $G_{298} = -400.974413$
NImag = 0
N 0.693357 -1.014477 0.563273
C 1.962759 -0.639339 -0.067326
C 1.634605 0.654288 -0.789702
C 0.687299 1.343208 0.182428
C -0.132666 0.179683 0.747069
C -1.446946 -0.014550 -0.001675
O -2.327198 0.808004 -0.028796
O -1.531138 -1.178861 -0.609607
H -0.395395 0.342182 1.791011
H 0.062349 2.105894 -0.273352
H 1.251392 1.807764 0.989439
H 2.521601 1.243417 -1.1008502
H 1.130091 0.444158 -1.733291
H 2.737534 -0.468018 0.682848
H 2.304318 -1.427681 -0.734549
H -0.657610 -1.599190 -0.397505
H 0.828594 -1.520076 1.423443

Nitrostyrene

$E_0 = -514.0229494$
 $E_{0+ZPE} = -513.881602$
 $E_{298} = -513.872763$
 $H_{298} = -513.871819$
 $G_{298} = -513.916749$
NImag = 0
C 0.612965 0.452157 -0.000529
H 0.901332 1.494663 -0.000672
C -0.812436 0.175146 -0.000321
C -1.338335 -1.121432 -0.000385
C -2.705619 -1.318846 -0.000147
C -3.570694 -0.229478 0.000283
C -3.061630 1.060454 0.000360
C -1.691094 1.261162 0.000022
H -0.678645 -1.976037 -0.000680
H -3.101948 -2.323431 -0.000193
H -4.638873 -0.390075 0.000608
H -3.730124 1.908584 0.000746
H -1.291978 2.265593 -0.000066
C 1.592067 -0.453227 0.000203
H 1.493612 -1.523782 0.000612
N 2.957363 -0.034304 0.000202
O 3.232527 1.149421 -0.000189
O 3.791689 -0.920797 0.000353

Cyclohexane

$E_0 = -309.8478851$
 $E_{0+ZPE} = -309.692903$
 $E_{298} = -309.686546$
 $H_{298} = -309.685602$
 $G_{298} = -309.723202$
NImag = 0
C 1.009713 1.251588 -0.280960
C -0.389639 1.272543 0.332188
C -1.142582 -0.000011 0.061795
C -0.389604 -1.272554 0.332153
C 1.009777 -1.251576 -0.280926
C 1.774096 0.000031 0.117317
H -0.301040 1.361617 1.418845
H -0.979109 2.114750 -0.022766
H 0.925277 1.292242 -1.369108
H 1.549212 2.147492 0.024697
H -0.301060 -1.361663 1.418814
H -0.979050 -2.114757 -0.022849
H 1.549290 -2.147439 0.024824
H 0.925405 -1.292300 -1.369074
H 1.938506 0.000048 1.198075
H 2.758628 0.000050 -0.350928
O -2.289577 -0.000021 -0.329991

DBU

$E_0 = -462.0355954$
 $E_{0+ZPE} = -461.782798$
 $E_{298} = -461.773217$
 $H_{298} = -461.772273$
 $G_{298} = -461.817695$
NImag = 0
N -1.339223 -1.468677 0.063935
C -2.567253 -0.838264 0.495952
H -3.398294 -1.493946 0.235936
H -2.570001 -0.763175 1.588082
C -2.769890 0.535202 -0.107813
H -2.933079 0.442370 -1.182474
H -3.643237 1.026764 0.317937
C -1.535365 1.368848 0.143328
H -1.582809 2.298751 -0.421020
H -1.467027 1.634874 1.202419
C -0.350688 -0.716904 -0.272774

DBUH⁺

$E_0 = -462.5203667$
 $E_{0+ZPE} = -462.252316$
 $E_{298} = -462.242664$
 $H_{298} = -462.241720$
 $G_{298} = -462.286982$
NImag = 0
N -1.366257 -1.350899 0.059941
C -2.625125 -0.777063 0.492584
H -3.422384 -1.438972 0.169006
H -2.644567 -0.725245 1.580750
C -2.759387 0.594933 -0.119985
H -2.918049 0.505052 -1.193795
H -3.617144 1.110561 0.302719
C -1.510191 1.400312 0.147733
H -1.527325 2.322503 -0.424983
H -1.428484 1.661507 1.202949
C -0.302186 -0.651155 -0.278978

N	-0.349979	0.644475	-0.274810
C	0.841837	1.425922	-0.547243
H	1.223204	1.197796	-1.544971
H	0.520368	2.463585	-0.574345
C	1.960465	1.276229	0.475283
C	0.921862	-1.407907	-0.681112
H	0.658057	-2.455040	-0.796898
H	1.254893	-1.048006	-1.656821
C	2.061240	-1.278767	0.330333
H	1.669116	-1.441772	1.336165
H	2.767152	-2.088790	0.145002
C	2.817019	0.038279	0.269832
H	1.527722	1.282233	1.477860
H	2.600862	2.157013	0.405644
H	3.307125	0.115803	-0.704732
H	3.615002	0.025133	1.013625

N	-0.310735	0.662757	-0.249040
C	0.889288	1.450178	-0.537461
H	1.232237	1.226848	-1.547340
H	0.564665	2.484800	-0.537333
C	2.012753	1.266953	0.468306
C	0.925015	-1.407067	-0.672855
H	0.646022	-2.451183	-0.789128
H	1.254610	-1.057605	-1.651722
C	2.066015	-1.289864	0.340145
H	1.675592	-1.438118	1.347886
H	2.747727	-2.117165	0.150257
C	2.842582	0.012538	0.255870
H	1.595801	1.289978	1.476657
H	2.666465	2.134706	0.382288
H	3.321686	0.072582	-0.724140
H	3.646762	-0.010891	0.990951
H	-1.287255	-2.350966	0.016519

1

(Lowest energy enamine conformation others given at end)

$E_0 = -634.5121219$

$E_{0+ZPE} = -634.232212$

$E_{298} = -634.219850$

$H_{298} = -634.218906$

$G_{298} = -634.271259$

NImag = 0

N	0.429174	0.556919	0.168744
C	0.850716	1.944364	0.339694
C	2.340376	1.912056	0.066273
C	2.438676	0.885663	-1.049497
C	1.406925	-0.170159	-0.640985
C	2.064270	-1.276208	0.174932
O	1.759830	-1.264690	1.460519
C	-0.941911	0.279354	0.042229
C	-1.295427	-1.129760	-0.351401
C	-3.357286	0.916966	0.242995
O	2.815424	-2.087093	-0.299844
H	0.966018	-0.642131	-1.514941
H	3.430182	0.462110	-1.181910
H	2.130320	1.328643	-1.994670
H	2.725562	2.887318	-0.219367
H	2.887764	1.579793	0.948610
H	0.340572	2.586772	-0.384865
H	0.602602	2.300074	1.337789
C	-1.885197	1.193108	0.310012
C	-2.734633	-1.478652	-0.010149
C	-3.674595	-0.382990	-0.475580
H	-3.770649	0.886469	1.256444
H	-3.858733	1.750867	-0.251586
H	-0.623357	-1.833225	0.141166
H	-1.597707	2.187035	0.622183
H	-1.135582	-1.259352	-1.424364
H	1.119188	-0.532801	1.559394
H	-2.992209	-2.434045	-0.466145
H	-3.556375	-0.244538	-1.552792
H	-4.713142	-0.664930	-0.303010
H	-2.832175	-1.604678	1.070323

(1-2)_{syn} (re-re)₁

$E_0 = -1148.5092603$

$E_{0+ZPE} = -1148.087470$

$E_{298} = -1148.065871$

$H_{298} = -1148.064927$

$G_{298} = -1148.138874$

3

$E_0 = -634.0150093$

$E_{0+ZPE} = -633.749534$

$E_{298} = -633.736878$

$H_{298} = -633.735934$

$G_{298} = -633.789857$

NImag = 0

N	0.418982	0.655406	-0.224225
C	0.935142	1.921720	0.232524
C	2.444671	1.804989	0.056914
C	2.599222	0.706644	-0.985279
C	1.464029	-0.256362	-0.640644
C	1.923809	-1.288747	0.419864
O	1.604456	-1.090171	1.605988
C	-0.901535	0.334616	-0.090458
C	-1.295435	-1.036417	-0.572939
C	-3.292624	0.891166	0.480485
O	2.607164	-2.227629	-0.043898
H	1.160170	-0.815283	-1.523991
H	3.570324	0.219315	-0.962149
H	2.444697	1.112162	-1.986331
H	2.900145	2.746748	-0.242988
H	2.902560	1.492609	0.993248
H	0.514853	2.740854	-0.362693
H	0.662560	2.110956	1.274165
C	-1.824648	1.195611	0.397831
C	-2.698575	-1.435222	-0.147881
H	-2.999663	-2.331259	-0.691335
H	-2.694600	-1.696163	0.912970
C	-3.680540	-0.302265	-0.375300
H	-4.698704	-0.620009	-0.146383
H	-3.664070	-0.017925	-1.430858
H	-3.590060	0.695638	1.517710
H	-3.869007	1.767800	0.174487
H	-0.580677	-1.767578	-0.198161
H	-1.509948	2.165348	0.757615
H	-1.215507	-1.063048	-1.663155

(1-2)_{syn} (re-re)₂

$E_0 = -1148.5076221$

$E_{0+ZPE} = -1148.084602$

$E_{298} = -1148.063300$

$H_{298} = -1148.062356$

$G_{298} = -1148.134683$

(1-2)_{syn-Conf} (re-re)₂

$E_0 = -1148.5002159$

$E_{0+ZPE} = -1148.077992$

$E_{298} = -1148.056521$

$H_{298} = -1148.055577$

$G_{298} = -1148.129008$

NImag = 1 (-438.0364)

C	-3.813497	0.296014	-0.934388
C	-2.883936	-0.486468	-0.248838
C	-3.319611	-1.260312	0.828676
C	-4.651651	-1.254845	1.203037
C	-5.572207	-0.481681	0.505014
C	-5.150144	0.291799	-0.565785
C	-1.492052	-0.497152	-0.711464
C	-0.800893	-1.699441	-0.742016
N	0.356835	-1.814679	-1.433583
O	0.953006	-2.894245	-1.463214
O	0.805942	-0.812929	-2.051561
C	-0.611683	0.856369	0.864644
C	0.713336	0.980231	0.460263
C	1.117160	2.107322	-0.447402
C	0.285272	3.365041	-0.252659
C	-1.194753	3.042980	-0.257034
C	-1.513525	2.062763	0.855017
N	1.649847	0.075906	0.812348
C	1.358866	-0.981676	1.785557
C	2.663440	-1.736102	1.883597
C	3.684146	-0.617370	1.809542
C	3.087683	0.361508	0.784403
C	3.831061	0.250131	-0.542630
O	4.976631	0.632906	-0.575751
O	3.271456	-0.257992	-1.607657
H	3.272400	1.381782	1.112793
H	4.678661	-0.942655	1.521836
H	3.760980	-0.116025	2.772296
H	2.734112	-2.313750	2.801128
H	2.769647	-2.416744	1.039770
H	1.094416	-0.529254	2.745980
H	0.530169	-1.595129	1.455441
H	-1.237315	0.228353	-1.468036
H	-2.554844	1.749335	0.803991
H	-1.408721	2.572713	1.817855
H	-1.784269	3.950395	-0.129847
H	-1.471767	2.618195	-1.224390
H	0.551428	3.836448	0.695376
H	0.535065	4.074866	-1.039916
H	-2.613641	-1.860702	1.384083
H	-4.974463	-1.854760	2.041412
H	-6.612014	-0.482135	0.797808
H	-5.859296	0.895373	-1.113233
H	-3.486435	0.899487	-1.769227
H	-0.819574	0.137810	1.643827
H	2.169321	2.346668	-0.326922
H	0.999811	1.747732	-1.472084
H	-1.109387	-2.595944	-0.236264
H	2.310597	-0.497230	-1.584775

(1-2)_{syn} (si-si)₁

E₀ = -1148.5040311
E_{0+ZPE} = -1148.081870
E₂₉₈ = -1148.060172
H₂₉₈ = -1148.059228
G₂₉₈ = -1148.133160
NImag = 1 (-399.6916)

C	-3.236013	0.000646	-0.356745
C	-1.917945	0.038424	-0.816632
C	-1.532497	-0.873489	-1.801294
C	-2.429806	-1.801837	-2.304880
C	-3.732123	-1.839118	-1.827821
C	-4.130216	-0.933449	-0.852912
C	-0.943194	1.049600	-0.378925
C	-1.378569	2.267955	0.140639
N	-0.645112	3.407328	0.035219
O	-1.050317	4.431318	0.595112
O	0.397074	3.446340	-0.666258

NImag = 1 (-446.8747)

C	3.941486	0.482896	0.694672
C	2.880524	-0.360545	0.363237
C	3.139270	-1.485079	-0.424636
C	4.422742	-1.755423	-0.864696
C	5.472887	-0.910848	-0.523289
C	5.229094	0.207353	0.258945
C	1.541597	-0.056259	0.884784
C	0.708441	-1.088497	1.295845
N	-0.444696	-0.783822	1.928563
O	-1.269441	-1.709700	2.171014
O	-0.702169	0.382180	2.239040
C	0.639830	0.951399	-0.862080
C	-0.740467	0.902757	-0.663906
C	-1.522889	2.115180	-0.237552
C	-0.794929	3.425989	-0.492032
C	0.658850	3.341415	-0.076410
C	1.357354	2.272376	-0.894267
N	-1.416986	-0.250276	-0.833356
C	-0.814844	-1.407266	-1.502163
C	-1.878609	-2.470075	-1.378503
C	-3.155509	-1.682295	-1.611757
C	-2.874938	-0.294170	-1.000362
C	-3.767989	-0.080435	0.217284
O	-4.793001	0.541135	0.066595
O	-3.509901	-0.656049	1.363215
H	-3.184115	0.478711	-1.698053
H	-4.034662	-2.152531	-1.179696
H	-3.337188	-1.562575	-2.677275
H	-1.744889	-3.271989	-2.099448
H	-1.860693	-2.900197	-0.378436
H	-0.624750	-1.158768	-2.550821
H	0.122306	-1.679088	-1.037121
H	1.442306	0.878902	1.414494
H	2.385619	2.140285	-0.556883
H	1.433522	2.608891	-1.932481
H	1.155290	4.300586	-0.221108
H	0.724131	3.106487	0.988140
H	-0.846749	3.671670	-1.554696
H	-1.312643	4.221913	0.041056
H	2.333455	-2.149353	-0.702375
H	4.607007	-2.627457	-1.475177
H	6.474341	-1.125766	-0.866572
H	6.039983	0.866551	0.532456
H	3.757662	1.349448	1.313922
H	1.059259	1.080633	-1.491657
H	-2.475219	2.129688	-0.763422
H	-1.757522	2.016045	0.820942
H	0.842804	-2.129407	1.069221
H	-2.622766	-1.065362	1.520944

(1-2)_{syn-Conf} (si-si)₁

E₀ = -1148.5042453
E_{0+ZPE} = -1148.081805
E₂₉₈ = -1148.060040
H₂₉₈ = -1148.059096
G₂₉₈ = -1148.133110
NImag = 1 (-387.2698)

C	-3.314588	0.303010	-0.491885
C	-1.970874	0.230759	-0.868234
C	-1.594296	-0.707580	-1.832245
C	-2.532637	-1.545798	-2.410633
C	-3.864605	-1.464604	-2.029019
C	-4.250528	-0.538982	-1.067842
C	-0.946998	1.122857	-0.325170
C	-1.289464	2.353452	0.212113
N	-0.345931	3.261428	0.586780
O	-0.702188	4.352577	1.028719
O	0.876587	2.977052	0.518266

NImag = 1 (-450.4469)

C	3.990305	0.176659	0.365876
C	2.784494	-0.524267	0.326377
C	2.765498	-1.791093	-0.262798
C	3.920039	-2.336693	-0.795984
C	5.115716	-1.629507	-0.749121
C	5.148129	-0.372996	-0.164055
C	1.587147	0.082571	0.924595
C	0.657896	-0.708300	1.584438
N	-0.327446	-0.094858	2.280801
O	-1.207313	-0.802419	2.842526
O	-0.371987	1.134653	2.344534
C	0.638704	0.997415	-0.810555
C	-0.726079	1.028904	-0.533835
C	-1.449894	2.328595	-0.285856
C	-0.622987	3.596602	-0.559977
C	0.830200	3.409761	-0.174769
C	1.416659	2.271062	-0.983320
N	-1.449301	-0.118615	-0.445643
C	-1.039372	-1.355122	-1.121293
C	-1.916189	-1.415773	-2.380311
C	-3.058230	-0.426820	-2.101858
C	-2.903454	-0.106427	-0.616202
C	-3.669060	-1.121964	0.236239
O	-4.714782	-1.562737	-0.173114
O	-3.239265	-1.458743	1.425214
H	-3.328520	0.851545	-0.338373
H	-4.041501	-0.824496	-2.325049
H	-2.920092	0.491524	-2.668350
H	-1.351615	-1.125159	-3.262781
H	-2.283781	-2.426194	-2.540277
H	0.021890	-1.376437	-1.321799
H	-1.259428	-2.187096	-0.455679
H	1.711544	1.083462	1.310074
H	2.458313	2.095276	-0.713364
H	1.432211	2.549458	-2.041183
H	1.383493	4.329178	-0.363866
H	0.910776	3.195119	0.892250
H	-0.671933	3.816660	-1.624413
H	-1.077834	4.416789	-0.032814
H	1.843843	-2.352572	-0.309831
H	3.888920	-3.316696	-1.249517
H	6.015539	-2.058749	-1.165108
H	6.074452	0.180761	-0.117035
H	4.024112	1.150524	0.833324
H	1.003914	0.159047	-1.381528
H	-2.321365	2.360647	-0.938890
H	-1.824642	2.332525	0.735043
H	0.601331	-1.780186	1.553361
H	-2.402754	-1.070289	1.780888

(1-2)_{syn} (si-si)₂

E₀ = -1148.5080359
E_{0+ZPE} = -1148.085376
E₂₉₈ = -1148.064082
H₂₉₈ = -1148.063138
G₂₉₈ = -1148.135171
NImag = 1 (-362.5786)

C	-0.396079	0.840425	-0.947527
C	0.792458	1.307585	-0.404490
N	1.873209	0.503925	-0.306239
C	2.168055	-0.514355	-1.319649
C	3.698883	-0.472032	-1.418441
C	4.128464	-0.116890	-0.006434
C	3.090207	0.905177	0.409549
C	1.747851	-1.960287	-1.083282
O	1.927239	-2.529824	0.088133
O	1.378355	-2.618204	-2.024980
H	4.119279	-1.404406	-1.786288

C	-0.173109	-2.345207	1.047917	C	-0.091232	-2.431142	1.063395	H	3.978019	0.320470	-2.110795
C	0.640516	-1.101889	0.860052	C	0.584977	-1.096807	0.943456	H	1.695675	-0.232390	-2.255087
C	0.134671	0.125197	1.310574	C	-0.043072	0.035911	1.444061	H	1.992749	-1.949540	0.884328
C	-0.839149	0.148777	2.461703	C	-1.172801	-0.064255	2.430626	C	-1.205684	0.004044	0.955919
C	-1.687394	-1.105278	2.602860	C	-1.935825	-1.376110	2.373606	C	-0.264015	-0.900329	1.424793
C	-0.851052	-2.353359	2.412997	C	-0.973784	-2.542226	2.295214	C	-1.445031	1.787450	-1.456931
N	1.825658	-1.218102	0.257464	N	1.762874	-1.070794	0.288253	H	-1.224887	0.972676	1.432168
C	2.311642	-2.423726	-0.398988	C	2.561344	-2.271671	0.001904	H	-0.263529	-1.948011	1.190390
C	3.568440	-1.978463	-1.111686	C	3.963939	-1.758146	-0.305810	C	-2.495017	-0.473686	0.442068
C	4.112814	-0.903209	-0.186254	C	3.983828	-0.350599	0.271285	C	-2.621436	-1.661792	-0.281160
C	2.857539	-0.188116	0.310582	C	2.549376	0.131293	0.064482	C	-3.863875	-2.089475	-0.714871
C	2.477281	0.986723	-0.572487	C	2.393339	0.632082	-1.371997	C	-5.001408	-1.342533	-0.431259
O	2.170037	0.870401	-1.732289	O	2.542786	-0.094601	-2.319960	C	-4.887199	-0.160485	0.284653
O	2.486041	2.126202	0.085814	O	2.149706	1.917317	-1.541894	C	-3.641575	0.273933	0.711719
H	2.963151	0.168877	1.331948	H	2.284732	0.908152	0.771840	H	-1.746444	-2.249812	-0.516989
H	4.808439	-0.224299	-0.672168	H	4.717684	0.300132	-0.197778	H	-3.946455	-3.008455	-1.276659
H	4.619152	-1.352118	0.666447	H	4.180872	-0.369323	1.341921	H	-5.969719	-1.680937	-0.770179
H	4.267203	-2.796831	-1.262197	H	4.722071	-2.394387	0.143274	H	-5.766136	0.425850	0.509785
H	3.318341	-1.552346	-2.080125	H	4.131503	-1.730627	-1.377325	H	-3.554978	1.194508	1.271435
H	2.545329	-3.192596	0.350519	H	2.575403	-2.910522	0.882179	N	0.792682	-0.480385	2.166502
H	1.559466	-2.833139	-1.073311	H	2.136719	-2.835348	-0.825380	O	0.854640	0.667622	6.211276
H	-0.058529	1.097204	-0.994523	H	0.014732	1.032981	-0.793969	O	1.724471	-1.300535	2.395934
H	-1.467037	-3.248088	2.495589	H	-1.512266	-3.488593	2.259182	H	-0.379905	-0.130121	-1.424494
H	-0.089703	-2.418587	3.193061	H	-0.346486	-2.567629	3.188791	C	0.853833	2.701460	0.157145
H	-2.163662	-1.111212	3.583204	H	-2.579353	-1.465371	3.248594	H	0.581632	2.661734	1.211896
H	-2.487148	-1.104866	1.864146	H	-2.585430	-1.393377	1.498603	H	1.872689	3.075458	0.119866
H	-0.261389	0.290196	3.379992	H	-0.762408	0.067432	3.436562	C	-0.065128	3.662755	-0.583890
H	-1.473349	1.033601	2.382409	H	-1.852898	0.778990	2.285068	C	-1.468776	3.105212	-0.705653
H	-0.522325	-0.841200	-2.184713	H	-0.558975	-0.765920	-2.137606	H	-1.246192	1.977686	-2.516076
H	-2.112605	-2.491135	-3.073999	H	-2.224640	-2.257716	-3.162418	H	-2.421505	1.306279	-1.424469
H	-4.435081	-2.560272	-2.218850	H	-4.599195	-2.115760	-2.480022	H	0.336814	3.854374	-1.580890
H	-5.145640	-0.947741	-0.484092	H	-5.286061	-0.471183	-0.767647	H	-0.069711	4.616579	-0.057528
H	-3.575235	-0.705197	0.387499	H	-3.635967	1.012761	0.255535	H	-1.888763	2.959137	0.291602
H	0.449100	-3.227255	0.935200	H	0.637168	-3.235066	1.057826	H	-2.118965	3.812359	-1.219865
H	0.832016	0.950512	1.325764	H	0.564104	0.922646	1.549330	H	5.133377	0.294475	0.034463
H	-2.295600	2.409336	0.681034	H	-2.293778	2.673406	0.415256	H	4.103197	-0.989205	0.643616
H	1.858902	2.761453	-0.335426	H	1.777304	2.346991	-0.741928	H	3.403693	1.898181	0.091860
H	-0.931315	-2.388373	0.262575	H	-0.695181	-2.564544	0.159995	H	2.894031	0.928787	1.479605

(1-2)_{syn} (si-re)₁

$E_0 = -1148.5103668$
 $E_{0+ZPE} = -1148.087948$
 $E_{298} = -1148.066385$
 $H_{298} = -1148.065440$
 $G_{298} = -1148.138698$
 $N\text{Imag} = 1 (-384.9677)$

C	2.588149	1.853941	0.172717
C	2.444557	0.486878	0.418637
C	3.565971	-0.335630	0.292306
C	4.793485	0.197874	-0.064553
C	4.923789	1.559389	-0.302911
C	3.815929	2.387209	-0.181677
C	1.125319	-0.012474	0.826789
C	1.014783	-1.178289	1.580260
N	-0.112285	-1.461839	2.285580
O	-0.120067	-2.438305	3.042917
O	-1.139351	-0.753054	2.167570
C	-0.975806	-2.246830	-0.863065
C	-0.992209	-0.754026	-0.911512
C	0.199734	-0.086244	-1.200362
C	1.213991	-0.741245	-2.101719
C	1.294330	-2.243898	-1.915719
C	-0.091201	-2.855530	-1.943532
N	-2.134445	-0.116623	-0.621752
C	-3.354276	-0.791900	-0.170610
C	-4.351827	0.337832	0.015272
C	-3.889531	1.374825	-0.994260
C	-2.364615	1.290463	-0.890794
C	-1.873373	2.251308	0.182071

(1-2)_{syn} (si-re)₂

$E_0 = -1148.5065383$
 $E_{0+ZPE} = -1148.083925$
 $E_{298} = -1148.062430$
 $H_{298} = -1148.061486$
 $G_{298} = -1148.134102$
 $N\text{Imag} = 1 (-401.1022)$

C	-3.089404	0.909040	-0.659696
C	-1.723234	0.750391	-0.890926
C	-1.309674	-0.144283	-1.880666
C	-2.241703	-0.862245	-2.611760
C	-3.600367	-0.694875	-2.374801
C	-4.021580	0.196848	-1.399137
C	-0.762205	1.555615	-0.121725
C	0.330050	2.086195	-0.802496
N	1.150476	2.991908	-0.217029
O	2.190547	3.330120	-0.840371
O	0.906347	3.444648	0.906104
C	-1.357437	-1.697191	1.346802
C	-0.077505	-0.956093	1.103604
C	0.042887	0.365594	1.537834
C	-0.763398	0.842655	2.719820
C	-2.124801	0.181849	2.827682
C	-1.999556	-1.320580	2.676650
N	0.892837	-1.592696	0.436211
C	0.750735	-2.938445	-0.129926
C	2.089219	-3.202357	-0.789268
C	3.057544	-2.435612	0.095246
C	2.286530	-1.160742	0.436977
C	2.553079	-0.083582	-0.599779

(1-2)_{syn}-Conf (si-re)₂

$E_0 = -1148.498735$
 $E_{0+ZPE} = -1148.076647$
 $E_{298} = -1148.054972$
 $H_{298} = -1148.054028$
 $G_{298} = -1148.127817$
 $N\text{Imag} = 1 (-388.7306)$

C	-3.337082	-0.987570	0.110049
C	-1.977015	-1.024433	0.423682
C	-1.578604	-0.736261	1.731628
C	-2.520672	-0.427443	2.697984
C	-3.872303	-0.404467	2.377500
C	-4.278397	-0.686190	1.080705
C	-1.026937	-1.402534	-0.621566
C	0.099131	-2.149514	-0.324995
N	0.913395	-2.583597	-1.328491
O	2.023084	-3.090122	-1.017848
O	0.596067	-2.448665	-2.509216
C	-0.854219	2.458065	-0.145004
C	0.116248	1.391020	-0.566021
C	-0.244947	0.514511	-1.577971
C	-1.339591	0.870699	-2.553916
C	-2.381420	1.830192	-2.008624
C	-1.710842	2.978142	-1.285895
N	1.273914	1.334878	0.126605
C	1.842564	2.504976	0.817575
C	3.347459	2.245047	0.877962
C	3.584245	1.119718	-0.119122
C	2.289937	0.311311	-0.014134
C	2.375873	-0.548885	1.243114

O	-1.817423	3.432633	-0.044829	O	2.259674	-0.182161	-1.764344	O	2.103379	-0.118738	2.333928
O	-1.562911	1.779082	1.371644	O	3.162483	0.956488	-0.067710	O	2.879225	-1.762784	1.106815
H	-1.878484	1.587180	-1.817082	H	2.547718	-0.771214	1.416701	H	2.122320	-0.301192	-0.892707
H	-4.259189	2.377240	-0.801610	H	4.011273	-2.226059	-0.382166	H	4.473383	0.531811	0.094905
H	-4.185255	1.087424	-2.001669	H	3.252547	-2.982328	1.016283	H	3.662269	1.501476	-1.135531
H	-5.371581	0.005447	-0.157022	H	2.312191	-4.265006	-0.833402	H	3.911508	3.139264	0.626849
H	-4.298887	0.735872	1.027722	H	2.101141	-2.802533	-1.799972	H	3.638518	1.934986	1.877396
H	-3.700002	-1.486254	-0.935966	H	0.573929	-3.658922	0.669912	H	1.634394	3.399318	0.235960
H	-3.156105	-1.346831	0.744043	H	-0.085123	-2.976218	-0.822804	H	1.411562	2.624597	1.808014
H	0.424070	0.768886	1.060340	H	-1.184066	2.161259	0.666564	H	-1.435265	-1.511349	-1.614068
H	-0.043755	-3.932815	-1.789574	H	-2.975704	-1.800083	2.741641	H	-2.450146	3.671677	-0.886937
H	-0.548534	-2.694933	-2.921905	H	-1.396106	-1.721205	3.493862	H	-1.087707	3.543789	-1.981859
H	1.921363	-2.680447	-2.692665	H	-2.580026	0.431038	3.785839	H	-3.004148	2.196100	-2.824759
H	1.767590	-2.471308	-0.959395	H	-2.788609	0.566338	2.053469	H	-3.041252	1.311516	-1.313042
H	0.938175	-0.520635	-3.137993	H	-0.190121	0.635721	3.628954	H	-0.868532	1.319307	-3.434281
H	2.190524	-0.283111	-1.953983	H	-0.863036	1.927399	2.679550	H	-1.822896	-0.035864	-0.2923471
H	3.487570	-1.397587	0.470523	H	-0.255476	-0.288499	-2.070190	H	-0.530643	-0.737399	1.993338
H	5.651383	-0.452232	-0.156194	H	-1.906593	-1.552849	-3.372341	H	-2.199284	-0.203255	3.704724
H	5.882967	1.972320	-0.579402	H	-4.324745	-1.253238	-2.949838	H	-4.604349	-0.167380	3.135740
H	3.908481	3.448689	-0.359373	H	-5.076159	0.340570	-1.213070	H	-5.327887	-0.672772	0.824941
H	1.729883	2.503978	0.273157	H	-3.423959	1.608462	0.093153	H	-3.655058	-1.213253	-0.898056
H	-1.979555	-2.654135	-0.921635	H	-1.187364	-2.768654	1.314088	H	-0.346185	3.279663	0.346399
H	0.150578	0.990916	-1.295092	H	1.020137	0.821916	1.466591	H	0.531200	-0.097294	-2.014017
H	1.796181	-1.902714	1.710919	H	0.654196	1.758410	-1.771253	H	0.443991	-2.369771	0.667515
H	-1.528485	0.803650	1.449053	H	3.115576	1.743094	-0.648498	H	2.712219	-2.180998	0.231310
H	-0.577010	-2.534120	0.115573	H	-2.042311	-1.467723	0.526616	H	-1.493779	2.002214	0.617708

(1-2)_{syn} (re-si)₁

E₀ = -1148.5082867
E_{0+ZPE} = -1148.086624
E₂₉₈ = -1148.064798
H₂₉₈ = -1148.063854
G₂₉₈ = -1148.139046
NImag = 1 (-438.9753)

C	3.807977	-0.722045	-0.122601
C	2.840034	0.151731	-0.624094
C	3.222025	1.456532	-0.944614
C	4.530331	1.876546	-0.776744
C	5.483172	0.997702	-0.279126
C	5.116833	-0.301279	0.045947
C	1.450096	-0.248694	-0.858613
C	1.099771	-1.585886	-1.012723
N	-0.069578	-1.907597	-1.619816
O	-0.352423	-3.089196	-1.830029
O	-0.848857	-0.985125	-1.977050
C	0.560056	0.723800	0.963033
C	-0.768974	0.302009	0.963711
C	-1.123994	-0.973029	1.660975
C	-0.311921	-1.221189	2.922873
C	1.168783	-1.061531	2.645920
C	1.455245	0.327392	2.109842
N	-1.732028	0.952194	0.290855
C	-1.450975	2.157287	-0.484254
C	-2.799200	2.547505	-1.052465
C	-3.754298	2.117089	0.045101
C	-3.160361	0.791131	0.535822
C	-3.867731	-0.382477	-0.133206
O	-4.999006	-0.634325	0.203899
O	-3.279579	-1.085340	-1.067555
H	-3.352781	0.666862	1.598273
H	-4.783407	2.003275	-0.280548
H	-3.734729	2.833526	0.864375
H	-2.856411	3.610043	-1.271641
H	-2.997647	2.001486	-1.974101
H	-1.059595	2.936725	0.173876
H	-0.710444	1.949693	-1.250247
H	0.868656	0.440863	-1.446917
H	2.499599	0.413941	1.814032
H	1.318303	1.055774	2.915912

(1-2)_{syn} (re-si)₂

E₀ = -1148.5079508
E_{0+ZPE} = -1148.084917
E₂₉₈ = -1148.063728
H₂₉₈ = -1148.062784
G₂₉₈ = -1148.134488
NImag = 1 (-386.2723)

C	-2.502911	0.386167	1.475285
C	-2.400638	0.875584	0.169042
C	-3.570838	1.025225	-0.578130
C	-4.802898	0.673505	-0.050189
C	-4.887096	0.167890	1.238704
C	-3.733065	0.032894	2.001014
C	-1.128262	1.296036	-0.425378
C	-0.073072	1.709502	0.387174
N	0.939451	2.448152	-0.110389
O	1.966328	2.615468	0.609110
O	0.889465	2.947574	-1.240896
C	-0.461202	-0.435829	-1.634631
C	0.422731	-1.008306	-0.720242
C	-0.096211	-2.041061	0.228514
C	-1.073938	-2.985838	-0.459611
C	-2.204381	-2.216622	-1.113396
C	-1.674319	-1.193406	-2.104291
N	1.684393	-0.572627	-0.611491
C	2.342547	0.181362	-1.689698
C	3.745750	0.415503	-1.175556
C	4.028470	-0.831758	-0.359680
C	2.676991	-1.183498	0.276625
C	2.623618	-0.757246	1.738621
O	2.787653	-1.589829	2.596950
O	2.474081	0.504707	2.063910
H	2.552762	-2.259964	0.297326
H	4.810901	-0.699982	0.383090
H	4.323243	-1.652348	-1.010640
H	4.453719	0.551805	-1.988469
H	3.770477	1.309678	-0.555692
H	2.341822	-0.436050	-2.589748
H	1.822338	1.107899	-1.906685
H	-1.218209	1.810653	-1.369762
H	-2.463459	-0.495041	-2.383050
H	-1.395962	-1.701108	-3.032868

H	1.748465	-1.236116	3.551972	H	-2.881065	-2.899621	-1.626401
H	1.481706	-1.812191	1.917977	H	-2.786978	-1.719026	-0.339121
H	-0.620800	-0.519058	3.699650	H	-0.537221	-3.576476	-1.204818
H	-0.535470	-2.221000	3.291896	H	-1.463655	-3.686461	0.277483
H	2.484128	2.143379	-1.335835	H	-3.512639	1.434609	-1.576622
H	4.807538	2.887515	-1.037683	H	-5.696728	0.800308	-0.643494
H	6.505241	1.322013	-0.147815	H	-5.845977	-0.108143	1.652667
H	5.853113	-0.990852	0.432407	H	-3.793015	-0.345343	3.011143
H	3.547475	-1.736674	0.138265	H	-1.622137	0.283833	2.091276
H	0.751214	1.709923	0.563590	H	-0.027502	0.204981	-2.388126
H	-2.185403	-1.032260	1.880717	H	0.706896	-2.608752	0.685185
H	-0.911840	-1.776171	0.945229	H	-0.606270	-1.519159	1.043282
H	1.689461	-2.432028	-0.715016	H	0.058571	1.406831	1.408762
H	-2.337430	-0.894525	-1.288462	H	2.315304	1.184225	1.360790

(1-2)_{syn} (re-re)₁ (down)

E₀ = -1148.5099153
E_{0+ZPE} = -1148.088052
E₂₉₈ = -1148.066395
H₂₉₈ = -1148.065451
G₂₉₈ = -1148.139372
NImag = 1 (-406.1622)

C	-3.357497	-1.246922	0.761676
C	-2.889172	-0.471983	-0.301854
C	-3.789968	0.342437	-0.988866
C	-5.130731	0.367917	-0.636676
C	-5.585140	-0.407074	0.419679
C	-4.693263	-1.211440	1.119908
C	-1.494279	-0.509137	-0.747243
C	-0.607807	0.807127	0.886530
C	-1.483450	2.030602	0.918104
C	-0.801265	-1.708114	-0.743043
N	0.367709	-1.830705	-1.413354
O	0.992546	-2.893742	-1.374044
C	0.731110	0.910546	0.526385
C	1.202408	2.095390	-0.271437
N	1.636599	-0.044765	0.824400
C	3.085371	0.157336	0.699991
C	3.681702	-1.102275	1.327661
C	2.703055	-1.401257	2.442698
C	1.361316	-1.114164	1.798600
C	3.723845	0.384271	-0.660928
O	3.190020	-0.090156	-1.753755
O	4.792188	0.948842	-0.691795
O	0.796409	-0.854405	-2.085508
H	2.873004	-0.727085	3.281438
H	2.768791	-2.423275	2.805730
H	3.693627	-1.915339	0.602014
H	4.697976	-0.925925	1.665339
H	3.380268	1.019409	1.298608
H	0.622293	-0.779760	2.520844
H	0.976805	-1.995724	1.292729
H	-1.102832	-2.590400	-0.209244
H	-1.214090	0.211903	-1.498638
H	-3.436856	0.947412	-1.811955
H	-5.817620	0.995719	-1.185185
H	-6.628171	-0.384599	0.699857
H	-5.041818	-1.812357	1.947168
H	-2.674110	-1.871208	1.319086
H	2.267882	-0.461935	-1.718241
H	-0.872891	0.037231	1.594518
H	1.158911	1.822921	-1.327962
H	2.243967	2.312689	-0.050712
C	0.378788	3.352372	-0.037474
C	-1.104561	3.062263	-0.125342
H	-1.406357	2.485166	1.911058
H	-2.527693	1.741162	0.811552
H	-1.347683	2.694228	-1.124563

(1-2)_{syn} (si-si)₂ (down)

E₀ = -1148.5062518
E_{0+ZPE} = -1148.083749
E₂₉₈ = -1148.062402
H₂₉₈ = -1148.061457
G₂₉₈ = -1148.134015
NImag = 1 (-366.2775)

C	-0.346091	0.829095	-0.898262
C	0.847663	1.243040	-0.322191
N	1.869915	0.371641	-0.177300
C	2.183556	-0.612100	-1.221275
C	3.731243	-0.619253	-1.305224
C	4.170688	0.586204	-0.487957
C	3.089281	0.672615	0.565790
C	1.727159	-2.051783	-1.054246
O	1.815412	-2.647521	0.115033
O	1.409546	-2.682402	-2.032839
H	4.169733	1.490579	-1.095755
H	5.162104	0.458564	-0.061375
H	4.129599	-1.530622	-0.862435
H	4.055318	-0.586436	-2.340726
H	1.745164	-0.271783	-2.153961
H	3.024794	1.622844	1.075639
H	3.218973	-0.095533	1.331992
H	1.871839	-2.084408	0.923699
C	-1.237816	0.016727	0.947291
C	-0.349315	-0.938402	1.422724
C	-1.337321	1.818701	-1.440438
H	-1.235829	0.971542	1.451655
H	-0.385702	-1.979566	1.163033
C	-2.534046	-0.403697	0.396645
C	-2.682270	-1.561963	-0.369108
C	-3.929120	-1.938931	-0.836321
C	-5.049422	-1.169490	-0.544580
C	-4.913087	-0.016257	0.213188
C	-3.662660	0.367323	0.673999
H	-1.820086	-2.166555	-0.610999
H	-4.028503	-2.835598	-1.430529
H	-6.021411	-1.468216	-0.909305
H	-5.778566	0.587339	0.444858
H	-3.559469	1.265531	1.266113
N	0.700225	-0.581880	2.205259
O	0.801848	0.553931	2.672226
O	1.582327	-1.452688	2.447927
H	-0.355682	-0.142310	-1.374031
C	0.975596	2.645793	0.208586
H	0.722648	2.647217	1.268788
H	2.009982	2.971708	0.135177
C	0.095070	3.635376	-0.542889
C	-1.326682	3.131551	-0.682030
H	-1.097326	2.004119	-2.491759
H	-2.332796	1.377362	-1.439411
H	0.513311	3.809072	-1.536363

(1-2)_{syn} (si-re)₁ (down)

E₀ = -1148.5063462
E_{0+ZPE} = -1148.083829
E₂₉₈ = -1148.062175
H₂₉₈ = -1148.061231
G₂₉₈ = -1148.134891
NImag = 1 (-381.7990)

C	0.140086	-0.031686	-1.151012
C	-1.037804	-0.726655	-0.851500
C	-0.981778	-2.220116	-0.850236
N	-2.175900	-0.103263	-0.518487
C	-2.401051	1.315847	-0.748060
C	-3.934307	1.491589	-0.662938
C	-4.482474	0.075483	-0.717484
C	-3.400434	-0.730932	-0.033484
C	-1.770542	2.266052	0.250416
O	-1.472838	1.816853	1.452744
O	-1.628466	3.429773	-0.025508
H	-4.592406	-0.258804	-1.748224
H	-5.444154	-0.017406	-0.220241
H	-4.209348	1.959639	0.280878
H	-4.292156	2.130737	-1.463569
H	-2.024687	1.589700	-1.731009
H	-3.438191	-1.784811	-0.271230
H	-3.449380	-0.634239	1.053451
H	-1.462892	0.842212	1.559831
H	-0.554206	-2.525188	0.110889
C	1.138112	-0.023561	0.836736
H	0.474957	0.778134	1.108622
C	1.012030	-1.197553	1.577763
H	0.074674	1.047189	-1.212494
N	-0.098238	-1.453475	2.317657
O	-0.118561	-2.447976	3.051402
O	-1.100051	-0.700822	2.259428
C	2.461446	0.438879	0.397219
C	2.639697	1.803250	0.158527
C	3.871973	2.302583	-0.228184
C	4.950201	1.443091	-0.388819
C	4.785929	0.084308	-0.155979
C	3.553936	-0.415183	0.233132
H	1.804723	2.477776	0.287558
H	3.991023	3.362278	-0.400748
H	5.912735	1.829194	-0.691255
H	5.620726	-0.590588	-0.276903
H	3.450709	-1.475631	0.407063
H	1.768518	-1.954188	1.665281
C	1.131375	-0.635193	-2.112758
H	-1.970694	-2.659220	-0.903270
C	-0.113829	-2.779420	-1.970403
C	1.257470	-2.138805	-1.972203
H	0.807155	-0.394690	-3.130422
H	2.100214	-0.153953	-1.991469
H	1.769024	-2.381386	-1.039609

H -1.682205 3.973651 0.025961
H 0.678067 4.104692 -0.765821
H 0.608504 3.758031 0.949705

H 0.121532 4.590329 -0.019335
H -1.764794 2.993497 0.308497
H -1.943434 3.865147 -1.200169

H 1.866602 -2.538334 -2.782680
H -0.039789 -3.858782 -1.843378
H -0.605077 -2.606946 -2.930189

(1-2)_{syn} (re-si)₁ (down)

E₀ = -1148.5077487
E_{0+ZPE} = -1148.085944
E₂₉₈ = -1148.064211
H₂₉₈ = -1148.063267
G₂₉₈ = -1148.137446
NImag = 1 (-422.8741)
C 3.811250 -0.699519 -0.212547
C 2.822384 0.223890 -0.560227
C 3.173590 1.572146 -0.662298
C 4.473610 1.987126 -0.430867
C 5.447166 1.059182 -0.085029
C 5.111423 -0.283512 0.022178
C 1.442288 -0.164994 -0.859470
C 1.122125 -1.461583 -1.241964
N -0.045711 -1.699583 -1.886093
O -0.319883 -2.837279 -2.272834
O -0.834612 -0.738763 -2.099856
C 0.551737 0.427014 1.127758
C -0.815811 0.177326 1.005065
C -1.383164 -1.110082 1.525104
C -0.630895 -1.666827 2.723626
C 0.858076 -1.700621 2.454696
C 1.359393 -0.298315 2.171378
N -1.654968 1.024714 0.390256
C -1.235060 2.344647 -0.079873
C -2.518150 3.149379 -0.142557
C -3.562622 2.100722 -0.463966
C -3.112004 0.901933 0.373809
C -3.762656 -0.353378 -0.183888
O -4.852107 -0.664986 0.233659
O -3.205357 -1.026438 -1.157238
H -3.498318 0.999607 1.388157
H -3.529608 1.847403 -1.523708
H -4.576912 2.394724 -0.213396
H 0.832944 0.603593 -1.303768
H 2.408148 -0.319504 1.876902
H 1.329346 0.282727 3.098880
H 1.392598 -2.121074 3.306140
H 1.057276 -2.350501 1.600497
H -0.830628 -1.046314 3.599358
H -1.015631 -2.661378 2.944339
H 2.418516 2.296156 -0.935970
H 4.728683 3.032801 -0.523072
H 6.462675 1.379966 0.096358
H 5.865023 -1.010207 0.288259
H 3.571356 -1.748793 -0.128581
H 0.880501 1.434940 0.926368
H -2.431403 -0.988038 1.784901
H -1.345900 -1.842030 0.712912
H 1.726870 -2.334421 -1.083762
H -2.285525 -0.792122 -1.442194
H -2.724378 3.603106 0.825970
H -2.468726 3.940017 -0.886183
H -0.513528 2.778029 0.607992
H -0.769041 2.258221 -1.060970

(1-2)_{syn} (re-si)₂ (down)

E₀ = -1148.5095408
E_{0+ZPE} = -1148.086568
E₂₉₈ = -1148.065348
H₂₉₈ = -1148.064404
G₂₉₈ = -1148.136284
NImag = 1 (-372.4791)
C 3.577068 -0.960206 -0.724046
C 2.425268 -0.871341 0.060245
C 2.554763 -0.453751 1.389002
C 3.794609 -0.122641 1.905599
C 4.931039 -0.203140 1.109577
C 4.818991 -0.628541 -0.205675
C 1.142670 -1.272059 -0.526019
C 0.123168 -1.757130 0.289857
N -0.931524 -2.417216 -0.228065
O -0.951899 -2.797447 -1.403739
O -1.930106 -2.634615 0.522323
C 0.391108 0.516005 -1.599919
C 1.573011 1.337458 -2.036051
C -0.506289 1.009792 -0.653912
C -0.031423 2.015633 0.345507
N -1.753905 0.530122 -0.569085
C -2.727463 0.955096 0.445379
C -4.038307 0.318658 -0.013206
C -3.896820 0.319148 -1.521345
C -2.446605 -0.072786 -1.719783
C -2.414978 0.589806 1.889749
O -2.146448 -0.657250 2.192966
O -2.486129 1.430805 2.751961
H -4.080288 1.316256 -1.919844
H -4.573963 -0.376590 -2.009145
H -4.117755 -0.703881 0.353215
H -4.892725 0.880018 0.352913
H -2.825251 2.038351 0.427320
H -2.026409 0.322700 -2.639361
H -2.324342 -1.154084 -1.726323
H 1.209338 -1.709411 -1.510201
H 0.048762 -1.553045 1.340700
H 1.687184 -0.385166 2.028108
H 3.875732 0.198179 2.933953
H 5.897636 0.055684 1.516644
H 5.698607 -0.708500 -0.827626
H 3.497938 -1.309406 -1.743826
H -0.024826 -0.115002 -2.372348
H 0.477007 1.485417 1.155758
H -2.128421 -1.331842 1.460282
H -0.865846 2.542616 0.797551
C 0.927044 3.015304 -0.291790
C 2.077257 2.310616 -0.983373
H 2.381477 0.682432 -2.360526
H 1.273627 1.894132 -2.929651
H 1.297496 3.687678 0.480796
H 0.377230 3.629012 -1.008237
H 2.741316 3.038153 -1.449353
H 2.666459 1.778488 -0.237610

(1-2)_{anti} (re-re)₁ (down)

E₀ = -1148.5129632
E_{0+ZPE} = -1148.090506
E₂₉₈ = -1148.068835
H₂₉₈ = -1148.067891
G₂₉₈ = -1148.141457

(1-2)_{anti} (re-re)₂ (down)

E₀ = -1148.5007194
E_{0+ZPE} = -1148.078250
E₂₉₈ = -1148.056539
H₂₉₈ = -1148.055595
G₂₉₈ = -1148.129445

(1-2)_{anti} (si-si)₁ (down)

E₀ = -1148.5063521
E_{0+ZPE} = -1148.083262
E₂₉₈ = -1148.061829
H₂₉₈ = -1148.060884
G₂₉₈ = -1148.133562

NImag = 1 (-367.9061)

C	-2.430202	-0.316931	-0.586898
N	-1.482351	-1.366281	-0.249224
C	-1.760624	-2.598026	-0.986582
C	-2.604276	-2.118259	-2.150163
C	-3.421765	-0.996358	-1.535769
C	-0.445715	-1.188275	0.576033
C	-0.107571	-0.062870	1.085783
C	0.823131	0.201581	2.256785
C	1.768295	-0.975657	2.431810
C	1.019397	-2.284042	2.289157
C	0.379300	-2.393412	0.913660
C	-3.165944	0.230651	0.632242
O	-3.280870	1.544027	0.695116
O	-3.673423	-0.482424	1.456274
C	0.902696	1.143063	-0.608036
C	0.784895	2.471535	-0.217850
N	-0.393156	3.135188	-0.337562
O	-1.373427	2.569788	-0.892504
C	2.216494	0.506980	-0.719991
C	2.350217	-0.609921	-1.548399
C	3.578169	-1.226682	-1.718318
C	4.697085	-0.738662	-1.057231
C	4.578440	0.372807	-0.233394
C	3.351843	0.993723	-0.067017
O	-0.496468	4.284668	0.093999
H	-1.913580	0.497971	-1.088000
H	-4.250481	-1.409464	-0.963665
H	-3.819633	-0.295367	-2.263483
H	0.153097	0.767704	-1.285577
H	1.385971	1.133171	2.163158
H	0.221043	0.315175	3.163208
H	2.250199	-0.914117	3.407269
H	2.560126	-0.935932	1.683782
H	0.243205	-2.353433	3.053710
H	1.687074	-3.131972	2.436352
H	3.285525	1.857432	0.576967
H	5.446380	0.760756	0.279595
H	5.656638	-1.217472	-1.187706
H	3.663391	-2.084265	-2.369720
H	1.483052	-0.986136	-2.073151
H	-0.861500	0.830779	1.026600
H	-0.241044	-3.284660	0.863006
H	1.156955	-2.507371	0.152849
H	1.551016	3.040205	0.274094
H	-2.678935	2.001138	0.068573
H	-1.963218	-1.735150	-2.943354
H	-3.222236	-2.911230	-2.562518
H	-0.838811	-3.073981	-1.304930
H	-2.315380	-3.296512	-0.357572

(1-2)_{anti} (si-si)₂ (down)

E₀ = -1148.4998357
E_{0+ZPE} = -1148.077054
E₂₉₈ = -1148.055419
H₂₉₈ = -1148.054475
G₂₉₈ = -1148.127891
NImag = 1 (-346.4158)

C	2.538478	-1.071148	-0.249867
N	1.289851	-0.536422	-0.801829
C	0.638792	-1.628845	-1.540688
C	1.704876	-2.712922	-1.695416
C	3.007854	-2.019401	-1.331927
C	0.760426	0.694052	-0.774704
C	1.633844	1.887524	-0.489267
C	1.022944	3.190242	-0.987406
C	-0.434969	3.306300	-0.593953
C	-1.222852	2.186674	-1.245964
C	-0.607684	0.837585	-1.017117

NImag = 1 (-362.7945)

C	-2.604238	0.001165	-0.224969
N	-1.741188	-1.141664	-0.472435
C	-2.306832	-2.016621	-1.505488
C	-3.399710	-1.174308	-2.131283
C	-3.898695	-0.343526	-0.964687
C	-0.535385	-1.314067	0.069909
C	0.070121	-0.360267	0.894379
C	1.096288	-0.783684	1.910053
C	1.901151	-2.005355	1.503912
C	0.992448	-3.087211	0.957859
C	0.197774	-2.585991	-0.241019
C	-2.901802	0.236075	1.248305
O	-2.920173	1.492608	1.663791
O	-3.190870	-0.656791	1.998390
C	1.042909	1.093280	-0.518556
C	0.546085	2.280475	0.023957
N	-0.662553	2.727392	-0.382862
O	-1.152440	2.360159	-1.465636
C	2.457782	0.726850	-0.466543
C	2.957075	-0.133800	-1.447918
C	4.298234	-0.475277	-1.478791
C	5.164602	0.030848	-0.519124
C	4.682607	0.891522	0.458323
C	3.343188	1.243398	0.482519
O	-1.328864	3.476785	0.377091
H	-2.166346	0.890596	-0.686097
H	-4.544613	-0.940416	-0.322683
H	-4.434247	0.553035	-1.262857
H	0.521696	0.742868	-1.395778
H	1.761414	0.050085	2.136388
H	0.565687	-0.997717	2.843069
H	2.457963	-2.375369	2.364311
H	2.634254	-1.734778	0.744599
H	0.298360	-3.415831	1.733716
H	1.568478	-3.961543	0.657034
H	2.992307	1.929227	1.239025
H	5.354775	1.297198	1.200402
H	6.211331	-0.235674	-0.537775
H	4.667858	-1.134184	-2.250955
H	2.285086	-0.524366	-2.199263
H	-0.557158	0.441056	1.246574
H	-0.499613	-3.352846	-0.563805
H	0.873545	-2.400318	-1.080070
H	0.908942	2.743864	0.923419
H	-2.534447	2.142745	1.049191
H	-2.983194	-0.530647	-2.904656
H	-4.178528	-1.786270	-2.577843
H	-1.543465	-2.308462	-2.219678
H	-2.716725	-2.915492	-1.043315

(1-2)_{anti} (si-re)₁ (down)

E₀ = -1148.5010017
E_{0+ZPE} = -1148.078307
E₂₉₈ = -1148.056717
H₂₉₈ = -1148.055772
G₂₉₈ = -1148.129033
NImag = 1 (-347.9318)

C	2.719625	0.958100	-0.445027
N	1.557300	1.108098	0.432232
C	1.119364	2.503757	0.360133
C	2.302869	3.273396	-0.227974
C	3.446982	2.271646	-0.246169
C	0.774457	0.158540	0.968979
C	1.334860	-1.189483	1.305949
C	0.695922	-1.784518	2.554604
C	-0.812690	-1.803084	2.433643
C	-1.335533	-0.390867	2.253246
C	-0.568644	0.407763	1.240336

NImag = 1 (-283.6481)

C	2.774020	-0.636211	-0.271735
N	1.486485	-0.239120	-0.846919
C	1.148967	-1.187891	-1.920189
C	2.396611	-2.043106	-2.113545
C	3.503804	-1.241879	-1.452498
C	0.706183	0.829330	-0.603124
C	1.244158	2.035046	0.118006
C	0.514907	3.316797	-0.260118
C	-0.985541	3.146742	-0.151673
C	-1.443429	2.061250	-1.105385
C	-0.619344	0.811915	-1.013534
C	3.609247	0.390106	0.485924
O	3.352720	0.496438	1.771945
O	4.518354	0.992395	-0.024142
C	-1.421996	-0.336551	0.822208
C	-0.658124	-1.478991	0.982835
N	0.509820	-1.451837	1.669986
O	1.183288	-2.483856	1.780191
C	-2.814344	-0.431305	0.375554
C	-3.251712	-1.410311	-0.520298
C	-4.583870	-1.482174	-0.886114
C	-5.504686	-0.580685	-0.363599
C	-5.081956	0.396621	0.524189
C	-3.745361	0.474551	0.885454
O	0.908944	-0.378145	2.188210
H	2.570420	-1.442793	0.444650
H	3.872887	-0.447673	-2.098319
H	4.345764	-1.851749	-1.136597
H	-1.182821	0.502450	1.457019
H	0.867944	4.118047	0.387891
H	0.774784	3.598769	-1.282553
H	-1.497703	4.081687	-0.377320
H	-1.248436	2.880272	0.874516
H	-1.387194	2.436155	-2.132514
H	-2.493508	1.819173	-0.942716
H	-3.418624	1.236309	1.579122
H	-5.790355	1.101312	0.934709
H	-6.544298	-0.640767	-0.650935
H	-4.907535	-2.242312	-1.582142
H	-2.546804	-2.113160	-0.940940
H	2.297088	1.159900	-0.114281
H	-0.939852	0.004255	-1.652505
H	-0.909445	-2.445845	0.587549
H	2.514999	0.034889	2.014379
H	2.279939	-3.000543	-1.609554
H	2.584950	-2.240610	-3.165209
H	0.283003	-1.790356	-1.658684
H	0.905604	-0.613088	-2.812795
H	1.163406	1.878184	1.192033

(1-2)_{anti} (si-re)₂ (down)

E₀ = -1148.4969086
E_{0+ZPE} = -1148.073859
E₂₉₈ = -1148.052552
H₂₉₈ = -1148.051608
G₂₉₈ = -1148.123853
NImag = 1 (-354.4435)

C	2.875571	-0.415913	-0.199206
N	1.679714	-0.131845	-1.000101
C	1.575697	-1.176799	-2.025035
C	2.942971	-1.855334	-2.067237
C	3.842481	-0.959732	-1.232310
C	0.675286	0.714238	-0.773052
C	0.873160	1.874202	0.147126
C	-0.003886	3.069407	-0.201836
C	-1.451566	2.662731	-0.363637
C	-1.578891	1.615458	-1.451170
C	-0.601307	0.484051	-1.301173

C	3.616458	-0.118088	0.245273	C	3.630208	-0.248018	-0.242391	C	3.494648	0.703873	0.627423
O	3.599906	0.127718	1.539353	O	3.409075	-1.274439	-1.035029	O	3.248003	0.676228	1.918736
O	4.489473	0.311714	-0.461630	O	4.553746	-0.240847	0.529934	O	4.235533	1.524617	0.150567
C	-1.480158	0.140361	0.902303	C	-1.316379	-0.185117	-0.799397	C	-1.306800	-0.885240	0.330249
C	-0.628603	-0.790744	1.488738	C	-1.016650	-1.496758	-1.159503	C	-0.609448	-0.675860	1.525495
N	0.484357	-0.340980	2.112396	N	0.148692	-1.805792	-1.775856	N	0.532063	-1.353776	1.763043
O	1.349025	-1.164479	2.519027	O	0.988294	-0.894421	-2.017173	O	1.285917	-0.955836	2.700839
C	-2.819207	-0.249321	0.441974	C	-2.706722	0.223272	-0.563868	C	-2.746662	-0.646862	0.204227
C	-3.095235	-1.511625	-0.088525	C	-3.046962	1.567780	-0.729486	C	-3.434467	-1.265790	-0.842849
C	-4.378915	-1.846694	-0.480693	C	-4.351390	1.997453	-0.558284	C	-4.802375	-1.110034	-0.986364
C	-5.413310	-0.926668	-0.352394	C	-5.341290	1.089148	-0.206517	C	-5.509345	-0.325409	-0.085098
C	-5.152875	0.329608	0.172504	C	-5.016073	-0.248975	-0.034040	C	-4.838644	0.292914	0.961648
C	-3.865360	0.666115	0.564067	C	-3.711533	-0.680524	-0.211346	C	-3.470617	0.133415	1.108051
O	0.684161	0.872892	2.246380	O	0.381462	-2.971445	-2.109433	O	0.865329	-2.345841	1.096193
H	2.243958	-1.666316	0.621250	H	2.342326	0.906728	-1.468805	H	2.598466	-1.233493	0.476228
H	3.415059	-1.449833	-2.164903	H	3.974429	2.243389	0.704567	H	4.245738	-1.32932	-1.812891
H	3.770312	-2.703916	-0.970410	H	4.168344	2.459210	-1.036766	H	4.666825	-1.493878	-0.767911
H	-1.392731	1.150626	1.270746	H	-0.677957	0.572395	-1.226973	H	-0.943827	-1.722689	-0.244711
H	1.606130	4.019374	-0.589336	H	1.089362	-2.789936	2.696914	H	0.108575	3.818940	0.580235
H	1.104248	3.240413	-2.075312	H	0.991237	-1.200916	3.428756	H	0.357616	3.521409	-1.127265
H	-0.839604	4.271192	-0.898013	H	-1.263991	-2.255265	3.316363	H	-2.068898	3.527556	-0.604944
H	-0.525761	3.248383	0.492640	H	-1.096749	-2.420702	1.580282	H	-1.823468	2.261022	0.579846
H	-1.288973	2.371423	-2.322414	H	-1.281018	0.138478	3.210081	H	-1.412505	2.083849	-2.426892
H	-2.253819	2.177682	-0.890056	H	-2.392536	-0.399403	1.986016	H	-2.592702	1.218571	-1.485910
H	-3.670680	1.641401	0.987270	H	-3.482834	-1.726894	-0.075922	H	-2.971827	0.610577	1.938029
H	-5.950950	1.049631	0.280800	H	-5.781190	-0.961298	0.238049	H	-5.384253	0.897522	1.671448
H	-6.414766	-1.190777	-0.659543	H	-6.360045	1.421762	-0.070472	H	-6.576902	-0.200951	-0.193831
H	-4.574987	-2.827381	-0.889368	H	-4.596640	3.039847	-0.700593	H	-5.316917	-1.602140	-1.798743
H	-2.300861	-2.234729	-0.200877	H	-2.279232	2.277838	-1.004376	H	-2.886492	-1.876932	-1.546739
H	2.588652	1.734689	-0.984638	H	2.406543	-1.124363	1.457053	H	1.908180	2.193504	0.137087
H	-1.109420	0.015598	-1.503131	H	-0.920061	1.419640	1.111257	H	-0.695729	-0.289393	-2.048424
H	-0.718079	-1.859159	1.421557	H	-1.661467	-2.341130	-1.005891	H	-0.829575	0.085179	2.251086
H	2.833689	-0.284344	1.993015	H	2.552613	-1.191468	-1.519378	H	2.569335	0.007585	2.177732
H	1.516123	-3.530817	-1.002936	H	2.071487	3.596898	-1.240340	H	2.881972	-2.845140	-1.621446
H	1.709851	-3.122774	-2.701512	H	2.536402	4.159030	0.356363	H	3.301179	-1.970322	-3.086359
H	-0.236294	-1.992077	-1.009552	H	0.236748	2.606267	-0.270639	H	0.792829	-1.885584	-1.763015
H	0.315261	-1.237323	-2.502883	H	0.856082	2.835418	1.362578	H	1.313194	-0.704676	-2.968773
H	1.826630	1.960059	0.576983	H	1.163066	-1.873515	0.473529	H	0.643662	1.538514	1.163367

(1-2)*anti* (re-si)₁ (down)

$E_0 = -1148.5095723$
 $E_{0+ZPE} = -1148.086699$
 $E_{298} = -1148.065046$
 $H_{298} = -1148.064102$
 $G_{298} = -1148.137613$
 $N_{\text{Imag}} = 1 (-332.0332)$

C	2.564763	-0.000329	0.279226
N	1.478989	-0.827768	0.793285
C	1.783575	-1.313749	2.142178
C	2.929018	-0.429518	2.587488
C	3.688636	-0.204495	1.293932
C	0.380713	-1.183197	0.111024
C	-0.006872	-0.570006	-1.071901
C	-0.963187	-1.241419	-2.020261
C	-1.886649	-2.250389	-1.357947
C	-1.118796	-3.124280	-0.389410
C	-0.458599	-2.282819	0.692812
C	3.029631	-0.397550	-1.117353
O	3.100206	0.585005	-1.998366
C	3.388366	-1.510336	-1.392244
C	-1.085266	1.324250	-0.471017
C	-0.269880	2.113174	0.326743
N	0.851415	2.684637	-0.179963
O	1.196259	2.437489	-1.362170
C	-2.401413	0.908781	0.017039
C	-2.637672	0.600899	1.359394
C	-3.906774	0.252484	1.787422
C	-4.963018	0.210253	0.885080
C	-4.742004	0.522159	-0.448410

(1-2)*anti* (re-si)₂ (down)

$E_0 = -1148.5061413$
 $E_{0+ZPE} = -1148.083232$
 $E_{298} = -1148.061614$
 $H_{298} = -1148.060669$
 $G_{298} = -1148.133956$
 $N_{\text{Imag}} = 1 (-350.3195)$

C	-2.221166	-0.457940	-0.664223
N	-1.040360	-1.264260	-0.372895
C	-0.947606	-2.404103	-1.291909
C	-1.894018	-2.037253	-2.414690
C	-2.996562	-1.295412	-1.685690
C	-0.160507	-1.047637	0.615864
C	-0.123175	0.116754	1.374344
C	0.587350	0.160747	2.700848
C	1.726278	-0.834742	2.822825
C	1.290189	-2.194045	2.320330
C	0.853862	-2.126032	0.864454
C	-3.110214	-0.186461	0.539030
O	-3.658340	1.015551	0.573237
O	-3.380156	-1.019559	1.361330
C	0.976611	1.549320	0.032243
C	-0.017187	2.000557	-0.826645
N	-1.088619	2.654176	-0.313027
O	-1.083765	3.083253	0.844248
C	2.182466	0.906261	-0.494778
C	2.182080	0.168112	-1.681043
C	3.355120	-0.383691	-2.167197
C	4.549751	-0.205971	-1.480686
C	4.562744	0.524984	-0.301347

C -3.470392 0.865491 -0.879503
O 1.556888 3.395173 0.543554
H 2.288848 1.047702 0.283913
H 4.259115 -1.093660 1.030966
H 4.360584 0.648597 1.318808
H -1.008171 1.478163 -1.536215
H -1.548852 -0.488748 -2.551846
H -0.373384 -1.746166 -2.791375
H -2.369973 -2.858485 -2.122330
H -2.678751 -1.733378 -0.816433
H -0.351777 -3.689849 -0.922238
H -1.778870 -3.851365 0.082155
H -3.302723 1.114787 -1.917450
H -5.559313 0.498860 -1.154447
H -5.952854 -0.061121 1.222132
H -4.074536 0.013777 2.827571
H -1.825674 0.629165 2.071462
H 0.701405 0.089368 -1.548905
H 0.150040 -2.918104 1.329619
H -1.225316 -1.837837 1.332581
H -0.435929 2.316248 1.368699
H 2.594089 1.368730 -1.707208
H 2.551593 0.514644 2.978145
H 3.533709 -0.902582 3.356375
H 0.909813 -1.234848 2.782654
H 2.095478 -2.358681 2.104698

C 3.388043 1.072335 0.188936
O -2.130591 2.727375 -1.019866
H -1.944599 0.483357 -1.127706
H -3.643890 -2.001195 -1.167463
H -3.608158 -0.669348 -2.328872
H 1.102443 2.087915 0.958803
H 0.944515 1.173489 2.895014
H -0.150762 -0.039312 3.483751
H 2.049856 -0.895415 3.861658
H 2.584730 -0.498046 2.241823
H 0.461008 -2.562662 2.927220
H 2.097136 -2.920230 2.411091
H 3.403271 1.648389 1.103319
H 5.488205 0.672273 0.236063
H 5.464423 -0.633420 -1.864894
H 3.338791 -0.951894 -3.085929
H 1.261542 0.018534 -2.225770
H -0.969632 0.785622 1.327966
H 0.452098 -3.088886 0.562293
H 1.720594 -1.933388 0.225303
H -0.125139 1.702285 -1.852812
H -3.247332 1.640123 -0.057132
H -1.400840 -1.381337 -3.131062
H -2.254751 -2.913959 -2.945674
H 0.074827 -2.543539 -1.629065
H -1.277037 -3.316416 -0.792057

(1-2)_{anti} (re-re)₁

E₀ = -1148.5120821
E_{0+ZPE} = -1148.089532
E₂₉₈ = -1148.067745
H₂₉₈ = -1148.066801
G₂₉₈ = -1148.141151
NImag = -377.3295 24.2072
C -2.335677 -0.175025 -0.655094
N -1.525938 -1.313950 -0.270738
C -1.996006 -2.556014 -0.887548
C -3.345931 -2.184875 -1.472957
C -3.200844 -0.708682 -1.799126
C -0.461140 -1.200927 0.531166
C -0.063310 0.025526 1.062003
C 0.879170 0.092745 2.231614
C 1.782801 -1.121555 2.369404
C 0.990897 -2.399147 2.187184
C 0.338683 -2.435606 0.814043
C -3.206540 0.330998 0.490809
O -3.297180 1.644464 0.601531
O -3.822469 -0.400883 1.219333
C 0.993273 1.158937 -0.576125
C 0.927077 2.464940 -0.107590
N -0.224581 3.180445 -0.192701
O -1.222048 2.687799 -0.784003
C 2.275461 0.469859 -0.725782
C 2.354435 -0.608646 -1.610511
C 3.551954 -1.272174 -1.817119
C 4.693760 -0.871214 -1.136608
C 4.629456 0.202041 -0.257907
C 3.433528 0.870036 -0.054905
O -0.285075 4.305853 0.304681
H -1.702201 0.638493 -0.991350
H -4.150876 -0.187342 -1.882765
H -2.660616 -0.571393 -2.734410
H 0.233391 0.857591 -1.277299
H 1.475346 1.005973 2.167059
H 0.283957 0.199318 3.143398
H 2.266802 -1.105890 3.345661
H 2.575560 -1.086572 1.622299
H 0.218362 -2.472607 2.955098
H 1.632484 -3.272521 2.297201

(1-2)_{anti} (re-si)₂

E₀ = -1148.5043884
E_{0+ZPE} = -1148.081770
E₂₉₈ = -1148.059980
H₂₉₈ = -1148.059036
G₂₉₈ = -1148.133042
NImag = 1 (-387.6945)
C -2.099322 -0.270999 -0.688241
N -1.109255 -1.283603 -0.360175
C -1.291457 -2.496043 -1.166464
C -2.627962 -2.289319 -1.853329
C -2.729887 -0.781860 -1.987258
C -0.162419 -1.127499 0.575534
C -0.045330 0.020585 1.357143
C 0.705503 -0.020448 2.664564
C 1.818907 -1.050657 2.709132
C 1.330214 -2.377623 2.169658
C 0.840794 -2.230725 0.737373
C -3.168412 -0.099551 0.380897
O -3.677556 1.117687 0.471716
O -3.582244 -1.001166 1.059068
C 1.080293 1.537046 0.134875
C 0.110481 2.150470 -0.649126
N -0.926989 2.785766 -0.046517
O -0.893361 3.071695 1.152929
C 2.232942 0.883211 -0.491230
C 2.144225 0.225675 -1.720488
C 3.267724 -0.340747 -2.298269
C 4.499812 -0.257181 -1.661844
C 4.600199 0.393365 -0.440474
C 3.474696 0.954029 0.142136
O -1.969159 2.986030 -0.727393
H -1.622152 0.679975 -0.865248
H -3.746732 -0.423734 -2.124942
H -2.133157 -0.426871 -2.825705
H -2.672747 -2.799435 -2.811687
H -3.431807 -2.669407 -1.226916
H -0.478313 -2.590189 -1.886750
H -1.299368 -3.381063 -0.537564
H 1.255728 1.961928 1.110945
H 1.097511 0.970129 2.900623
H -0.015825 -0.239703 3.457727

(1-2)_{anti} (re-re)₁ (down

Cyhex_{Conf})
E₀ = -1148.5122525
E_{0+ZPE} = -1148.089708
E₂₉₈ = -1148.068027
H₂₉₈ = -1148.067083
G₂₉₈ = -1148.140584
NImag = -368.3149 33.1307
C -2.418891 -0.397802 -0.587949
N -1.422821 -1.389993 -0.211358
C -1.686732 -2.678670 -0.846094
C -2.559446 -2.307713 -2.027203
C -3.398546 -1.166719 -1.479913
C -0.389252 -1.131115 0.596270
C -0.125722 0.151511 1.069635
C 0.751309 0.374497 2.273171
C 1.173005 -0.923523 2.942043
C 1.636885 -1.911671 1.891344
C 0.496268 -2.283016 0.957016
C -3.160682 0.188553 0.609794
O -3.306632 1.500459 0.614229
O -3.648773 -0.498416 1.466925
C 0.882236 1.139022 -0.654539
C 0.757133 2.484435 -0.324389
N -0.429927 3.124954 -0.468846
O -1.404799 2.518770 -0.991390
C 2.194748 0.495749 -0.736283
C 2.331777 -0.640554 -1.538080
C 3.555575 -1.272722 -1.672332
C 4.667872 -0.781913 -1.000886
C 4.546931 0.348298 -0.204537
C 3.323455 0.985870 -0.074376
O -0.549454 4.291998 -0.090046
H -1.941326 0.406678 -1.141969
H -4.210598 -1.561728 -0.872408
H -3.821759 -0.526788 -2.248400
H 0.136528 0.738375 -1.322395
H 1.646687 0.938001 1.996869
H 0.212113 1.002573 2.982222
H 3.256709 1.870731 0.540380
H 5.410015 0.739935 0.313772
H 5.624424 -1.273262 -1.103855

H 3.408369 1.704028 0.629524
H 5.515878 0.522793 0.269746
H 5.629647 -1.386900 -1.295300
H 3.595767 -2.098558 -2.511628
H 1.468850 -0.916695 -2.149264
H -0.798836 0.814546 1.045082
H -0.284243 -3.319476 0.719822
H 1.110132 -2.517368 0.042299
H 1.710836 2.971584 0.423808
H -2.621289 2.112372 0.067424
H -3.586907 -2.785071 -2.346112
H -4.125569 -2.332366 -0.729435
H -1.294914 -2.876501 -1.659513
H -2.078395 -3.348070 -0.149319

H 2.175497 -1.159399 3.733124
H 2.665938 -0.715120 2.110852
H 0.516789 -2.755171 2.792278
H 2.123056 -3.124232 2.195383
H 3.558093 1.466563 1.090031
H 5.555200 0.466635 0.059093
H 5.375639 -0.696527 -2.116675
H 3.182865 -0.848338 -3.248183
H 1.192427 0.146989 -2.224691
H -0.891082 0.692335 1.381476
H 0.439700 -3.175271 0.387404
H 1.684673 -1.992741 0.082193
H -0.021668 1.984340 -1.702579
H -3.163989 1.788821 -0.021435

H 3.643914 -2.145139 -2.303302
H 1.469731 -1.020138 -2.068668
H -0.907770 0.879866 0.941762
H -0.137044 -3.043465 1.420075
H 0.893897 -2.735978 0.047832
H 1.517835 3.079533 0.144658
H -2.710003 1.945834 -0.025467
H -1.940189 -1.966349 -2.855985
H -3.162282 -3.143670 -2.371481
H -0.761774 -3.163110 -1.140227
H -2.215176 -3.335939 -0.153059
H 0.331669 -1.347025 3.495017
H 1.964963 -0.728888 3.664234
H 2.024278 -2.821211 2.348176
H 2.454132 -1.471159 1.319752

(1-2)_{anti} (si-si)₁ (down

Cyhex_{Conf})

E₀ = -1148.5041882
E_{0+ZPE} = -1148.081057
E₂₉₈ = -1148.059635
H₂₉₈ = -1148.058691
G₂₉₈ = -1148.131203
NImag = 1 (-308.7150)

C -2.767993 -0.616209 0.291850
N -1.476103 -0.210335 0.850902
C -1.151021 -1.117448 1.964913
C -2.408880 -1.948708 2.192129
C -3.505358 -1.161136 1.498241
C -0.688575 0.835611 0.559981
C -1.222088 2.016237 -0.198937
C -0.173636 3.082218 -0.473514
C 0.663155 3.336692 0.761021
C 1.452394 2.083809 1.097905
C 0.638875 0.823289 0.979574
C -3.592170 0.396134 -0.493932
O -3.425413 0.364831 -1.802077
O -4.418266 1.104914 0.016275
C 1.397030 -0.334672 -0.794564
C 0.647166 -1.496692 -0.931574
N -0.519123 -1.510951 -1.615062
O -1.176351 -2.558885 -1.694111
C 2.800326 -0.427392 -0.372068
C 3.240103 -1.369785 0.560981
C 4.577287 -1.445427 0.906570
C 5.501790 -0.583836 0.326090
C 5.077561 0.354530 -0.601475
C 3.735495 0.435395 -0.943842
O -0.942848 -0.460994 -2.164893
C -2.573934 -1.453931 -0.388522
H -3.861593 -0.334159 2.109323
H -4.356366 -1.771665 1.208659
H 1.161401 0.478156 -1.464078
H 1.847188 2.144582 2.112922
H 2.330207 2.027120 0.450438
H 3.409493 1.162760 -1.673778
H 5.788794 1.026223 -1.059710
H 6.545400 -0.645988 0.598117
H 4.902219 -2.177004 1.632013
H 2.532780 -2.042244 1.025438
H -2.026688 2.447748 0.399875
H 0.944377 0.221167 1.631378
H 0.916885 -2.446559 -0.508445
H -2.603545 -0.123648 -2.042260
H -2.303510 -2.926841 1.727075
H -2.600163 -2.100826 3.250742
H -0.293704 -1.741400 1.727919
H -0.900866 -0.508506 2.832519
H -1.657194 1.706707 -1.141001

(1-2)_{syn} (re-re)₁ (Cyhex_{Conf})

E₀ = -1148.5084315
E_{0+ZPE} = -1148.086206
E₂₉₈ = -1148.064708
H₂₉₈ = -1148.063764
G₂₉₈ = -1148.137012
NImag = 1 (-445.9680)

C -3.930132 0.272773 -0.851225
C -2.892947 -0.458745 -0.273716
C -3.185175 -1.319882 0.786087
C -4.481624 -1.445330 1.252735
C -5.509693 -0.716887 0.665150
C -5.231221 0.139550 -0.388798
C -1.533640 -0.339112 -0.823533
C -0.810826 -1.507590 -1.024170
N 0.343128 -1.493162 -1.727491
O 0.954226 -2.544326 -1.940029
O 0.786604 -0.392027 -2.152298
C -0.638832 0.943541 0.731989
C 0.724320 1.004512 0.444600
C 1.319791 2.194360 -0.247750
C 0.283206 3.186092 -0.738828
C -0.717604 3.457436 0.364657
C -1.496085 2.188106 0.667855
N 1.565307 0.019407 0.811850
C 1.136291 -1.063398 1.706073
C 2.406795 -1.840995 1.962324
C 3.447133 -0.739163 2.012112
C 3.017102 0.203367 0.883807
C 3.851068 -0.044875 -0.373142
O 5.051068 0.051112 -0.276923
O 3.301751 -0.320636 -1.526299
H 3.250579 1.231686 1.151571
H 4.468427 -1.078492 1.879447
H 3.383596 -0.208291 2.960350
H 2.351676 -2.418102 2.881203
H 2.608674 -2.525266 1.138789
H 0.752823 -0.630500 2.634244
H 0.351088 -1.654158 1.250571
H -1.365706 0.465034 -1.523034
H 0.789809 4.098271 -1.049840
H -0.229370 2.792354 -1.618119
H -2.391925 -1.884655 1.255429
H -4.692820 -2.110660 2.077254
H -6.521516 -0.817308 1.030037
H -6.025335 0.706031 -0.852881
H -3.718371 0.934487 -1.679199
H -0.928495 0.217979 1.476166
H 1.968896 2.698379 0.473668
H 1.962856 1.874199 -1.064390
H -1.093114 -2.472566 -0.645032
H 2.316208 -0.355800 -1.601033
H -2.274095 2.077984 -0.090029

(1-2)_{syn} (re-re)₁ (down

Cyhex_{Conf})

E₀ = -1148.5087312
E_{0+ZPE} = -1148.086919
E₂₉₈ = -1148.065206
H₂₉₈ = -1148.064261
G₂₉₈ = -1148.138432
NImag = 1 (-414.7419)

C -3.337911 -1.204388 0.788708
C -2.905967 -0.458869 -0.310744
C -3.838809 0.302835 -1.014530
C -5.174503 0.308111 -0.640643
C -5.591985 -0.436439 0.451593
C -4.668345 -1.190399 1.166952
C -1.513064 -0.480182 -0.774067
C -0.631720 0.867792 0.771653
C -1.480389 2.117847 0.743605
C -0.817514 -1.680550 -0.761075
N 0.355669 -1.807813 -1.417880
O 0.981449 -2.871312 -1.365751
C 0.724354 0.921077 0.457275
C 1.294419 2.097103 -0.281662
N 1.591656 -0.051004 0.805178
C 3.045542 0.134340 0.726027
C 3.611987 -1.088019 1.449253
C 2.573238 -1.345130 2.519807
C 1.271393 -1.103896 1.782821
C 3.743504 0.272673 -0.618436
O 3.238719 -0.236417 -1.710803
O 4.832141 0.796781 -0.629031
O 0.795930 -0.832797 -2.086682
H 2.686868 -0.630515 3.334432
H 2.626376 -2.348759 2.932980
H 3.671991 -1.935379 0.766296
H 4.605807 -0.885413 1.835013
H 3.321695 1.031341 1.279783
H 0.476704 -0.773694 2.444641
H 0.945946 -2.006098 1.271581
H -1.121662 -2.556649 -0.218757
H -1.257366 0.226465 -1.547987
H -3.516602 0.878584 -1.870624
H -5.886197 0.895371 -1.202333
H -6.630791 -0.430023 0.747890
H -4.987891 -1.767919 2.022121
H -2.629331 -1.788271 1.358627
H 2.290705 -0.542590 -1.707476
H -0.933118 0.125041 1.491928
H 1.820329 1.757741 -1.171409
H 2.046800 2.556151 0.364872
C 0.265227 3.144995 -0.665634
C -0.684495 3.384759 0.487459
H -2.014438 2.190004 1.691142
H -2.255466 2.040029 -0.021308

H	0.006821	3.603279	1.592422	H	-2.027674	2.288548	1.614013	H	-0.113829	3.662498	1.376738
H	1.342098	4.174809	0.609536	H	-0.184973	3.799363	1.255051	H	-1.362118	4.209873	0.271474
H	-0.682223	3.986590	-0.803743	H	-1.407034	4.252227	0.082276	H	0.787129	4.056387	-0.952451
H	0.472969	2.768030	-1.295359					H	-0.298502	2.815528	-1.540321

(1-2)'_{anti}(re-re)₆₀

E₀ = -1148.5133564
E_{0+ZPE} = -1148.091038
E₂₉₈ = -1148.069015
H₂₉₈ = -1148.068070
G₂₉₈ = -1148.143008
NImag = 1 (-366.4135)

C	2.519453	-1.655918	0.145962
C	2.513018	-0.299656	0.476676
C	3.708332	0.412843	0.392257
C	4.882335	-0.215121	0.000199
C	4.876563	-1.563270	-0.322935
C	3.688807	-2.281551	-0.249757
C	1.291630	0.386115	0.939522
C	0.468312	-0.273259	1.843839
N	-0.449914	0.403718	2.593884
O	-1.128140	-0.229317	3.419224
O	-0.592978	1.627131	2.451793
C	0.341905	0.639404	-1.009763
C	-0.922752	1.037462	-0.581289
C	-1.299335	2.491778	-0.544771
C	-0.513125	3.332599	-1.538005
C	0.970351	3.039521	-1.451468
C	1.225630	1.580394	-1.780002
N	-1.800823	0.151763	-0.101986
C	-3.046600	0.507859	0.578756
C	-3.778143	-0.813283	0.753082
C	-2.668968	-1.851557	0.735041
C	-1.681477	-1.280730	-0.283865
C	-2.058195	-1.695711	-1.695455
O	-2.639974	-1.003859	-2.494628
O	-1.680532	-2.936202	-1.945731
H	-0.673555	-1.631984	-0.091772
H	-3.007480	-2.849942	0.473074
H	-2.172806	-1.894690	1.702104
H	-4.351936	-0.835357	1.675119
H	-4.466591	-0.975112	-0.074540
H	-2.801207	0.973507	1.534750
H	-3.626334	1.214349	-0.008436
H	1.374520	1.455460	1.064090
H	2.270141	1.323589	-1.603064
H	1.061177	1.419680	-2.849827
H	1.529125	3.675738	-2.137419
H	1.328418	3.268009	-0.445440
H	-0.862121	3.122592	-2.551046
H	-0.716934	4.385164	-1.344985
H	3.720874	1.462859	0.648622
H	5.800492	0.351869	-0.053230
H	5.788498	-2.052808	-0.632455
H	3.674578	-3.331381	-0.504951
H	1.600179	-2.223570	0.188308
H	0.481487	-0.401985	-1.256235
H	-2.363022	2.590976	-0.747092
H	0.504705	-1.328620	2.042021
H	-1.970485	-3.172179	-2.834020
H	-1.140031	2.855932	0.469728

(1-2)'_{anti}(re-re)₁₈₀

E₀ = -1148.5095751
E_{0+ZPE} = -1148.087622
E₂₉₈ = -1148.065304
H₂₉₈ = -1148.064360
G₂₉₈ = -1148.142531
NImag = 1 (-401.7586)

C	3.437854	0.537264	-0.051796
C	2.236341	0.287303	-0.718171
C	2.189629	-0.767455	-1.631169
C	3.307870	-1.549176	-1.876235
C	4.494420	-1.292894	-1.204549
C	4.553547	-0.247324	-0.292031
C	1.037818	1.120198	-0.539663
C	1.174786	2.465132	-0.212689
N	0.108919	3.310135	-0.319533
O	0.254080	4.499941	-0.006019
O	-0.985185	2.880880	-0.726814
C	-0.087370	0.293077	1.115140
C	-0.442919	-0.966914	0.635018
C	0.342443	-2.172371	1.050923
C	0.850332	-2.051487	2.480508
C	1.622898	-0.763047	2.670737
C	0.753594	0.442816	2.352240
N	-1.427196	-1.135434	-0.254948
C	-1.747057	-2.402751	-0.918742
C	-2.991168	-2.098987	-1.743015
C	-2.954615	-0.591534	-1.932266
C	-2.374704	-0.099256	-0.608290
C	-3.443791	0.033608	0.459012
O	-3.562962	-0.669574	1.426002
O	-4.264481	1.041752	0.189969
H	-1.900515	0.875254	-0.717301
H	-3.923570	-0.154308	-2.151996
H	-2.268918	-0.314725	-2.730737
H	-2.993235	-2.641205	-2.684416
H	-3.884835	-2.387326	-1.191798
H	-0.909678	-2.709947	-1.543983
H	-1.935515	-3.188570	-0.191919
H	0.224444	0.875982	-1.206227
H	1.365042	1.344185	2.260394
H	0.083064	0.633370	3.195260
H	1.991501	-0.686166	3.693540
H	2.496733	-0.778741	2.020676
H	0.002236	-2.085204	3.167356
H	1.476310	-2.913901	2.706896
H	1.269889	-0.963567	-2.165057
H	3.253201	-2.354513	-2.594538
H	5.368798	-1.898516	-1.393810
H	5.474445	-0.040512	0.233938
H	3.504990	1.342973	0.663981
H	-0.816133	1.080470	0.984381
H	-0.260775	-3.069034	0.947225
H	2.058671	2.921609	0.191054
H	-4.927234	1.092062	0.887583
H	1.187956	-2.283780	0.365990

(1-2)'_{anti}(re-re)₃₀₀

E₀ = -1148.5042057
E_{0+ZPE} = -1148.082215
E₂₉₈ = -1148.060118
H₂₉₈ = -1148.059174
G₂₉₈ = -1148.134908
NImag = 1 (-370.1873)

C	0.235804	2.296547	1.001999
C	-0.329567	1.989051	-0.236249
C	0.224127	2.565429	-1.382010
C	1.309596	3.420807	-1.296391
C	1.867248	3.714701	-0.058780
C	1.323582	3.151936	1.087481
C	-1.512714	1.121944	-0.383186
C	-2.433176	1.029277	0.655303
N	-3.755712	0.762394	0.417168
O	-4.530053	0.742186	1.385720
O	-4.165361	0.566157	-0.734232
C	-0.532001	-0.726196	-0.998621
C	-0.126405	-1.240860	0.234258
C	-1.138142	-1.995473	1.025418
C	-1.913654	-2.976866	0.154468
C	-2.572981	-2.259873	-1.005830
C	-1.559520	-1.471787	-1.818428
N	1.078784	-1.008673	0.763868
C	1.519049	-1.473352	2.083746
C	3.025773	-1.282176	2.065262
C	3.234452	-0.142976	1.083962
C	2.163494	-0.398191	0.021087
C	2.687343	-1.330450	-0.052913
O	2.520929	-2.518969	-1.097382
O	3.408064	-0.663655	-1.948998
H	1.857342	0.530626	-0.449314
H	4.235354	-0.104121	0.663474
H	3.027680	0.815601	1.553879
H	3.416389	-1.059601	3.054283
H	3.512961	-2.187533	1.708209
H	1.044531	-1.077656	2.863107
H	1.252949	-2.514726	2.237180
H	-1.948203	1.115028	-1.371991
H	-2.073618	-0.781404	-2.487306
H	-1.009925	-2.160876	-2.467691
H	-3.076306	-2.975847	-1.655896
H	-3.341261	-1.586568	-0.630767
H	-1.233007	-3.748053	-0.212006
H	-2.660689	-3.478737	0.768273
H	-0.208908	2.342970	-2.347587
H	1.718096	3.861334	-2.194384
H	2.712941	4.383235	0.012036
H	1.745453	3.383071	2.055078
H	-0.174687	1.876837	1.908109
H	0.224101	-0.244065	-1.602856
H	-0.697072	-2.503802	1.874821
H	-2.217996	1.222834	1.689481
H	3.764539	-1.293832	-2.585206
H	-1.834650	-1.245459	1.425511

(1-2)'_{anti}(si-si)₆₀

E₀ = -1148.5047883
E_{0+ZPE} = -1148.082345
E₂₉₈ = -1148.060409
H₂₉₈ = -1148.059465
G₂₉₈ = -1148.134731

(1-2)'_{anti}(si-si)₁₈₀

E₀ = -1148.5090886
E_{0+ZPE} = -1148.087005
E₂₉₈ = -1148.064817
H₂₉₈ = -1148.063873
G₂₉₈ = -1148.140591

(1-2)'_{anti}(si-si)₃₀₀

E₀ = -1148.5127062
E_{0+ZPE} = -1148.090303
E₂₉₈ = -1148.068381
H₂₉₈ = -1148.067437
G₂₉₈ = -1148.142186

NImag = 1 (-381.5208)

C	-0.631972	2.245367	-1.103873
C	-1.369119	1.837826	0.008256
C	-1.526701	2.735167	1.066900
C	-0.958388	3.996970	1.022272
C	-0.213630	4.385610	-0.083987
C	-0.057148	3.506411	-1.146500
C	-2.024488	0.519677	0.093205
C	-2.397299	-0.140366	-1.074802
N	-3.459708	-1.003087	-1.103277
O	-3.757178	-1.526328	-2.188298
O	-4.114083	-1.238738	-0.078953
C	0.158990	-2.093522	-0.329120
C	0.373883	-0.858533	0.476928
C	-0.621879	-0.505067	1.389117
C	-1.422703	-1.584040	2.079694
C	-1.616328	-2.850609	1.262780
C	-0.345512	-3.242930	0.536529
N	1.439226	-0.086731	0.247987
C	1.824972	1.031663	1.114112
C	3.211976	1.420591	0.630413
C	3.214984	0.983246	-0.824759
C	2.427557	-0.328353	-0.783321
C	3.355936	-1.471891	-0.421825
O	3.472580	-1.962479	0.668029
O	4.069887	-1.856216	-1.474079
H	1.966179	-0.546332	-1.742700
H	4.208492	0.857776	-1.245350
H	2.669677	1.692476	-1.443436
H	3.395812	2.484847	0.747477
H	3.975768	0.884136	1.190457
H	1.121890	1.852308	0.998485
H	1.813843	0.711130	2.153943
H	-2.722830	0.144531	0.911341
H	-0.520706	-4.111106	-0.097638
H	0.430515	-3.522389	1.251446
H	-1.938083	-3.658005	1.920824
H	-2.417288	-2.699772	0.542148
H	-0.892779	-1.832716	3.004569
H	-2.390242	-1.189150	2.389403
H	-2.104864	2.437358	1.930883
H	-1.098798	4.678682	1.848618
H	0.231803	5.369116	-0.121880
H	0.509661	3.805412	-2.016577
H	-0.507430	1.582763	-1.946964
H	1.045651	-2.395428	-0.875981
H	-0.419794	0.353678	2.013843
H	-1.945620	0.008224	-2.037723
H	4.672394	-2.556295	-1.198317
H	-0.608300	-1.845748	-1.075545

(1-2)'*anti* (si-re)₆₀

E₀ = -1148.5093733
E_{0+ZPE} = -1148.087485
E₂₉₈ = -1148.065353
H₂₉₈ = -1148.064408
G₂₉₈ = -1148.140467

NImag = 1 (-376.8640)

C	3.052266	1.775847	0.327850
C	2.806761	0.402540	0.375401
C	3.845527	-0.469706	0.044773
C	5.090798	0.020173	-0.316467
C	5.322699	1.387971	-0.354555
C	4.297579	2.265825	-0.028587
C	1.475552	-0.064496	0.800098
C	1.333367	-1.309101	1.408565
N	0.264411	-1.574018	2.215204
O	0.230964	-2.656498	2.822078
O	-0.648542	-0.739364	2.340477

NImag = 1 (-415.7588)

C	-3.036218	-1.501386	-0.210331
C	-1.985739	-0.802070	-0.807856
C	-1.190121	-1.470077	-1.739877
C	-1.432073	-2.795701	-2.066367
C	-2.475120	-3.480707	-1.460304
C	-3.275255	-2.827209	-0.531808
C	-1.718385	0.620731	-0.537011
C	-2.773955	1.463814	-0.195500
N	-2.606187	2.817552	-0.221264
O	-3.554525	3.544475	0.111325
O	-1.516111	3.300001	-0.572084
C	0.841039	-1.416406	1.193219
C	0.708130	0.003987	0.735685
C	-0.395014	0.760652	1.133409
C	-1.175636	0.389392	2.363233
C	-1.103536	-1.083774	2.729861
C	0.314239	-1.603764	2.609752
N	1.616474	0.503255	-0.106864
C	1.684350	1.924950	-0.460033
C	2.922090	2.038465	-1.336851
C	3.099940	0.636517	-1.896825
C	2.691642	-0.248948	-0.716867
C	3.862579	-0.435028	0.228859
O	4.004650	0.116982	1.285611
O	4.748532	-1.288650	-0.272879
H	2.360370	-1.229940	-1.047722
H	4.106803	0.427852	-2.246084
H	2.409197	0.456140	-2.718213
H	2.799291	2.786544	-2.114788
H	3.786828	2.318882	-0.738200
H	0.781746	2.228270	-0.985477
H	1.757324	2.524627	0.445303
H	-0.960494	1.054941	-1.169969
H	0.360488	-2.661834	2.865008
H	0.967589	-1.078358	3.308824
H	-1.475550	-1.226699	3.744198
H	-1.747503	-1.666414	2.072423
H	-0.796317	0.986158	3.197696
H	-2.214208	0.702620	2.231030
H	-0.384359	-0.936886	-2.225121
H	-0.809639	-3.290539	-2.798011
H	-2.668156	-4.513214	-1.712787
H	-4.092365	-3.351846	-0.058011
H	-3.672056	-1.012413	0.512633
H	1.873735	-1.746947	1.141261
H	-0.325496	1.825369	0.956623
H	-3.731486	1.144275	0.169964
H	5.489203	-1.359688	0.339886
H	0.274929	-2.049646	0.504321

NImag = 1 (-379.1476)

C	-3.077736	-1.246760	-0.899908
C	-2.854179	-0.352265	0.148665
C	-3.921565	0.419898	0.604811
C	-5.182148	0.294343	0.037848
C	-5.392355	-0.599351	-1.000722
C	-4.333634	-1.369203	-1.468326
C	-1.538275	-0.227229	-0.805179
C	-0.834429	-1.394137	1.084482
N	0.171887	-1.420204	2.003870
O	0.709421	-2.509329	2.266484
O	0.529756	-0.376371	2.571965
C	1.339117	1.965679	0.619846
C	0.732103	0.909512	-0.260842
C	-0.584847	1.019916	-0.701743
C	-1.301659	2.340850	-0.655964
C	-0.790373	3.261371	0.437485
C	0.722358	3.336066	0.388713
N	1.443203	-0.183006	-0.544530
C	1.069965	-1.140519	-1.589754
C	2.242542	-2.108322	-1.650932
C	2.890854	-1.986281	-0.280723
C	2.727556	-0.497528	0.041237
C	3.854384	0.291598	-0.591322
O	3.801535	0.863906	-1.646990
O	4.950952	0.245757	0.156346
H	2.719903	-0.314900	1.113960
H	3.928839	-2.306260	-0.259259
H	2.339538	-2.551971	0.467231
H	1.918273	-3.122706	-1.866421
H	2.939022	-1.807916	-2.431194
H	0.144907	-1.642552	-1.321153
H	0.913761	-0.612223	-2.529314
H	-1.455474	0.562760	1.536577
H	1.104461	4.024715	1.141268
H	1.036594	3.720610	-0.583740
H	-1.228520	4.252014	0.318980
H	-1.102432	2.893965	1.417716
H	-1.182868	2.835334	-1.624802
H	-2.372675	2.171796	-0.544390
H	-3.766273	1.113222	1.419444
H	-5.998318	0.896944	0.409444
H	-6.371850	-0.695931	-1.446047
H	-4.487719	-2.064679	-2.280725
H	-2.260874	-1.843247	-1.281878
H	2.411763	2.020349	0.451085
H	-0.883977	0.366303	-1.507609
H	-1.045325	-2.349486	0.641100
H	5.656141	0.715691	-0.302767
H	1.198100	1.663091	1.656498

(1-2)'*anti* (si-re)₃₀₀

E₀ = -1148.507895
E_{0+ZPE} = -1148.085616
E₂₉₈ = -1148.063595
H₂₉₈ = -1148.062650
G₂₉₈ = -1148.138462

NImag = 1 (-378.1885)

C	-3.766499	0.371917	0.313983
C	-2.533888	0.481027	-0.331240
C	-2.387937	-0.113999	-1.586945
C	-3.434081	-0.813434	-2.164649
C	-4.651220	-0.926456	-1.504648
C	-4.815672	-0.324897	-0.265656
C	-1.466179	1.274283	0.302530
C	-0.649884	2.061724	-0.510970
N	0.033061	3.120151	0.000966
O	0.682991	3.846403	-0.769458
O	0.014267	3.339848	1.225543

C	-1.223491	-1.578866	-0.817393
C	-0.784579	-0.150371	-0.768617
C	0.517967	0.163153	-1.158664
C	1.248455	-0.710414	-2.141822
C	0.854198	-2.174143	-2.064535
C	-0.653674	-2.317545	-2.020576
N	-1.616442	0.775390	-0.288713
C	-1.313509	2.204089	-0.282550
C	-2.560107	2.840514	0.303872
C	-3.090348	1.761602	1.233216
C	-2.824952	0.474012	0.446419
C	-3.991026	0.168450	-0.469211
O	-4.031492	0.369068	-1.653315
O	-5.010576	-0.341191	0.213888
H	-2.665232	-0.368788	1.116404
H	-4.137573	1.881930	1.494912
H	-2.510828	1.724616	2.153180
H	-2.336939	3.769294	0.821489
H	-3.281762	3.056825	-0.482148
H	-0.443660	2.403522	0.343383
H	-1.091857	2.544070	-1.292185
H	0.829957	0.703938	1.196539
H	-0.941821	-3.366109	-1.956900
H	-1.094456	-1.920558	-2.937065
H	1.265894	-2.712100	-2.918248
H	1.280551	-2.626644	-1.168054
H	1.038771	-0.334901	-3.148376
H	2.323783	-0.596556	-2.006323
H	3.687835	-1.537711	0.068467
H	5.882706	-0.670224	-0.568375
H	6.294927	1.766626	-0.634654
H	4.469086	3.332326	-0.049468
H	2.257993	2.464224	0.582175
H	-2.305465	-1.661890	-0.806111
H	0.761958	1.213465	-1.228596
H	2.041075	-2.114065	1.348026
H	-5.742996	-0.489628	-0.394475
H	-0.861462	-2.064606	0.092646

(1-2)'_{anti} (re-si)₆₀

$E_0 = -1148.5088026$
 $E_{0+ZPE} = -1148.086584$
 $E_{298} = -1148.064440$
 $H_{298} = -1148.063495$
 $G_{298} = -1148.139418$
 $N_{\text{Imag}} = 1 (-364.8104)$

C	-3.513433	0.681428	-1.031038
C	-2.466268	0.803602	-0.116506
C	-2.742214	0.616596	1.239822
C	-4.021605	0.298755	1.663321
C	-5.052624	0.167271	0.741308
C	-4.795140	0.365997	-0.607142
C	-1.134079	1.183928	-0.610525
C	-0.350882	2.051418	0.147263
N	0.667861	2.746790	-0.428700
O	1.280384	3.588103	0.248078
O	0.983456	2.521211	-1.611419
C	-0.101755	-0.669417	-1.055756
C	0.360951	-1.055979	0.200928
C	-0.423406	-2.042860	1.011171
C	-1.086353	-3.091238	0.128253
C	-1.922117	-2.438941	-0.953288
C	-1.068564	-1.530317	-1.823198
N	1.457847	-0.515866	0.740716
C	1.876363	-0.704764	2.134561
C	3.273057	-0.104019	2.205647
C	3.327569	0.857155	1.030594
C	2.490140	0.146427	-0.031677
C	3.314681	-0.868888	-0.797697

C	0.139123	-1.966664	-0.016156
C	0.514840	-0.665212	0.621452
C	-0.350766	-0.070249	1.539667
C	-1.343414	-0.904379	2.306504
C	-1.749139	-2.194135	1.609609
C	-0.551136	-2.882725	0.987444
N	1.641204	-0.056868	0.252219
C	2.303683	0.986807	1.044966
C	3.588474	1.286856	0.283036
C	3.302442	0.799136	-1.128716
C	2.449826	-0.447026	-0.883931
C	3.343281	-1.631758	-0.573984
O	3.579736	-2.065105	0.520954
O	3.870430	-2.132541	-1.685617
H	1.833303	-0.694446	-1.743648
H	4.195906	0.587334	-1.708922
H	2.701308	1.523071	-1.674335
H	3.833480	2.344536	0.312466
H	4.424328	0.737436	0.711607
H	1.675294	1.866383	1.138470
H	2.492201	0.605377	2.047150
H	-1.746603	1.727573	1.242126
H	-0.855406	-3.797208	0.479912
H	0.163129	-3.169990	1.761265
H	-2.235676	-2.855344	2.326498
H	-2.479412	-1.984359	0.829151
H	-0.893367	-1.146221	3.273780
H	-2.226875	-0.307519	2.538781
H	-1.453198	-0.029890	-2.121982
H	-3.301089	-1.269159	-3.135383
H	-5.466605	-1.470818	-1.958424
H	-5.762627	-0.393760	0.249996
H	-3.906287	0.850670	1.272690
H	1.011561	-2.466366	-0.425472
H	0.053765	0.761527	2.099034
H	-0.533661	1.933143	-1.570785
H	4.461020	-2.856393	-1.448238
H	-0.534858	-1.772296	-0.853178

(1-2)'_{anti} (re-si)₃₀₀

$E_0 = -1148.5085752$
 $E_{0+ZPE} = -1148.086221$
 $E_{298} = -1148.064135$
 $H_{298} = -1148.063191$
 $G_{298} = -1148.138475$
 $N_{\text{Imag}} = 1 (-385.9484)$

C	2.193162	1.860427	-0.914531
C	2.375343	0.529340	-0.533822
C	3.607043	0.156928	0.006950
C	4.622458	1.088531	0.158876
C	4.428793	2.407123	-0.227449
C	3.208302	2.790367	-0.767629
C	1.276118	-0.427764	-0.751485
C	1.539864	-1.785152	-0.905017
N	0.655537	-2.593840	-1.560493
O	0.960991	-3.784010	-1.739726
O	-0.422715	-2.137519	-1.977063
C	0.146067	0.093394	1.050261
C	-1.031270	-0.606223	0.777026
C	-1.177263	-2.004243	1.291344
C	-0.516335	-2.203736	2.646788
C	0.925642	-1.742731	2.610737
C	0.999423	-0.274397	2.234038
N	-2.006712	-0.107044	0.014509
C	-3.117945	-0.894503	-0.518323
C	-3.970250	0.118388	-1.261407
C	-2.972203	1.176924	-1.695586
C	-1.995145	1.237435	-0.517700
C	-2.447209	2.244944	0.519609

O	3.283509	-2.061021	-0.649617
O	4.116101	-0.267301	-1.669499
H	2.092517	0.853880	-0.753859
H	4.335927	1.071300	0.689093
H	2.842616	1.801439	1.267443
H	3.450990	0.389050	3.157180
H	4.021932	-0.885805	2.090777
H	1.176463	-0.193681	2.793770
H	1.887233	-1.757877	2.400055
H	-1.076606	1.328928	-1.679385
H	-1.704943	-0.900329	-2.446895
H	-0.489599	-2.142099	-2.521682
H	-2.398210	-3.195880	-1.576356
H	-2.722062	-1.866255	-0.484973
H	-0.315685	-3.719910	-0.321870
H	-1.700722	-3.739757	0.751791
H	-1.953734	0.718220	1.971043
H	-4.216303	0.154724	2.716373
H	-6.050186	-0.080606	1.073812
H	-5.592599	0.279022	-1.330941
H	-3.321338	0.848077	-2.081472
H	0.589525	-0.123951	-1.682095
H	0.221124	-2.529994	1.736087
H	-0.506750	2.276831	1.186024
H	4.642886	-0.938771	-2.116793
H	-1.185965	-1.507882	1.582177

O	-3.008638	1.992894	1.550179
O	-2.164918	3.484238	0.128653
H	-1.006423	1.533544	-0.858731
H	-3.422077	2.141458	-1.912583
H	-2.425962	0.850792	-2.577949
H	-4.491860	-0.332811	-2.100761
H	-4.715409	0.547120	-0.593343
H	-2.715164	-1.661346	-1.181820
H	-3.673423	-1.378294	0.279921
H	0.472430	-0.061505	-1.371796
H	2.032232	0.018965	2.043946
H	0.675996	0.330728	3.086769
H	1.404729	-1.898878	3.577135
H	1.473534	-2.343181	1.883442
H	-1.066389	-1.645486	3.407000
H	-0.581705	-3.257143	2.916362
H	3.782685	-0.865133	0.307344
H	5.569647	0.780601	0.577506
H	5.223024	3.130121	-0.111112
H	3.048207	3.813178	-1.076731
H	1.245129	2.166727	-1.335641
H	0.150702	1.150255	0.828466
H	-2.223915	-2.286967	1.339824
H	2.426827	-2.289613	-0.571412
H	-2.500299	4.099172	0.790584
H	-0.709616	-2.671263	0.563047

Other possible conformations

(1-2)' anti-(i) (re-re)₆₀

COOH – NH Interaction

sol-rere-sa-hk-mich-test-smdPCM-NH.log

E₀ = -1148.5091568

E_{0+ZPE} = -1148.086018

E₂₉₈ = -1148.064354

H₂₉₈ = -1148.063410

G₂₉₈ = -1148.136695

NImag = 1 (-408.6458)

C	2.530328	-1.646960	-0.009969
C	2.516250	-0.324368	0.434648
C	3.710378	0.394381	0.434253
C	4.893223	-0.196942	0.013527
C	4.895969	-1.512674	-0.423326
C	3.708983	-2.235496	-0.434975
C	1.282754	0.320871	0.932956
C	0.490176	-0.409394	1.820053
N	-0.437342	0.202663	2.604184
O	-1.093351	-0.481387	3.408421
O	-0.623280	1.427686	2.507219
C	0.343177	0.685102	-0.929274
C	-0.931861	1.059371	-0.501334
C	-1.311095	2.506698	-0.371931
C	-0.526834	3.408988	-1.311865
C	0.956904	3.114874	-1.236855
C	1.220824	1.677623	-1.645059
N	-1.839867	0.139069	-0.141194
C	-3.060699	0.436139	0.623595
C	-3.791032	-0.892864	0.683063
C	-2.670731	-1.916754	0.626341
C	-1.679939	-1.295585	-0.356865
C	-1.982241	-1.722381	-1.789283
O	-1.760122	-2.838358	-2.169672
O	-2.520552	-0.823286	-2.601954
H	-0.667842	-1.623217	-0.150611
H	-2.990754	-2.905362	0.311891
H	-2.185127	-1.997487	1.596468
H	-4.390520	-0.978047	1.584625
H	-4.456954	-1.002862	-0.172791
H	-2.771223	0.791825	1.613748

(1-2)' anti-(i) (si-si)₆₀

COOH – NH Interaction

sol-sisi-aa-hk-mich-test1-conf-smdPCM.log

E₀ = -1148.5000604

E_{0+ZPE} = -1148.077613

E₂₉₈ = -1148.055817

H₂₉₈ = -1148.054873

G₂₉₈ = -1148.129176

NImag = 1 (-411.9596)

C	2.404344	-0.439025	-0.794282
N	1.477572	-0.247627	0.316956
C	1.898899	0.858719	1.189262
C	3.304259	1.179970	0.715386
C	3.257315	0.831479	-0.762864
C	0.319430	-0.909381	0.463491
C	0.027472	-2.088096	-0.397217
C	-0.574900	-3.230640	0.415144
C	-1.822977	-2.772792	1.142344
C	-1.554429	-1.550311	2.004190
C	-0.672674	-0.502416	1.359573
C	3.297689	-1.665515	-0.646600
O	3.347487	-2.245634	0.545168
O	3.961361	-2.074345	-1.558008
C	-1.941836	0.632640	0.133017
C	-2.418580	0.021033	-1.029144
N	-3.575852	-0.707094	-1.028872
O	-4.221159	-0.873809	0.015556
C	-1.183378	1.896237	0.018535
C	-0.413161	2.219301	-1.098315
C	0.253918	3.432948	-1.166995
C	0.159447	4.346432	-0.125920
C	-0.614746	4.040469	0.985524
C	-1.276477	2.825834	1.055788
O	-3.967869	-1.182095	-2.106242
H	1.878919	-0.547062	-1.738405
H	4.233451	0.678326	-1.212871
H	2.741381	1.609332	-1.320852
H	3.558474	2.220864	0.893407
H	4.039886	0.565123	1.233437
H	1.237111	1.709987	1.055564

(1-2)' anti-(ii) (re-re)₆₀

sol-rere-sa-hk-mich-test-t1-smdPCM-

conf1.log

E₀ = -1148.5075479

E_{0+ZPE} = -1148.085326

E₂₉₈ = -1148.063245

H₂₉₈ = -1148.062301

G₂₉₈ = -1148.137460

NImag = 1 (-367.5797)

C	2.524049	-1.655078	0.102128
C	2.512235	-0.307905	0.467769
C	3.705212	0.410447	0.403175
C	4.881849	-0.203351	-0.002992
C	4.881285	-1.542805	-0.360224
C	3.695899	-2.266759	-0.307580
C	1.288338	0.361284	0.947621
C	0.466364	-0.325657	1.832475
N	-0.457829	0.325811	2.597917
O	-1.137230	-0.333891	3.401238
O	-0.604914	1.551875	2.490675
C	0.339813	0.671140	-0.994665
C	-0.926088	1.050492	-0.554020
C	-1.310902	2.500814	-0.474628
C	-0.525330	3.377088	-1.437347
C	0.959010	3.086928	-1.356810
C	1.220865	1.640319	-1.732152
N	-1.799664	0.146682	-0.099673
C	-3.051243	0.475871	0.584512
C	-3.779703	-0.852280	0.706886
C	-2.665310	-1.883935	0.667760
C	-1.676354	-1.276824	-0.329882
C	-2.051047	-1.631068	-1.763836
O	-2.606070	-0.896209	-2.528472
O	-1.740636	-2.873158	-2.136897
H	-0.663712	-1.623716	-0.137839
H	-3.004933	-2.876027	1.630756
H	-2.174190	-1.951658	1.365958
H	-4.363319	-0.907681	1.621197
H	-4.456921	-0.990908	-0.133961
H	-2.814013	0.908024	1.558069

H -3.648342 1.210237 0.138746
H 1.366689 1.377782 1.140590
H 2.266614 1.418801 -1.484278
H 1.053835 1.572449 -2.720716
H 1.515558 3.788748 -1.885611
H 1.311469 3.290190 -0.219114
H -0.872330 3.262133 -2.337208
H -0.734709 4.446598 -1.054219
H 3.714573 1.419328 0.777663
H 5.810922 0.373085 0.026121
H 5.814606 -1.973434 -0.756248
H 3.702146 -3.259647 -0.778908
H 1.612597 -2.218329 -0.032162
H 0.470984 -0.334911 -1.260372
H -2.376617 2.618782 -0.557122
H 0.561268 -1.472023 1.962503
H -2.611811 0.019096 -2.145174
H -1.143325 2.803110 0.662926

H 1.853960 0.546343 2.230556
H -2.643784 0.612585 0.955380
H -0.804063 -4.056182 -0.256940
H 0.168164 -3.598482 1.125657
H -2.207322 -3.576477 1.770266
H -2.603872 -2.546905 0.420059
H -1.050920 -1.863694 2.923747
H -2.495654 -1.100174 2.316524
H -1.879760 2.591986 1.922342
H -0.706411 4.749927 1.795230
H 0.676747 5.292989 -0.184996
H 0.843985 3.669216 -2.040840
H -0.333495 1.528407 -1.924578
H 0.896030 -2.432789 -0.949052
H -0.409072 0.306618 2.027331
H -1.986145 0.134602 -2.005423
H 2.735238 -1.812919 1.149521
H -0.711144 -1.752830 -1.138953

H -3.628765 1.200539 0.017975
H 1.367730 1.427069 1.101223
H 2.266170 1.382480 -1.561550
H 1.058721 1.513234 -2.806696
H 1.516843 3.746978 -2.020639
H 1.314166 3.284138 -0.343176
H -0.870991 3.199911 -2.457681
H -0.733711 4.421828 -1.209770
H 3.713853 1.453524 0.686431
H 5.798084 0.367939 -0.040593
H 5.795286 -2.021092 -0.680891
H 3.686256 -3.309667 -0.589906
H 1.606125 -2.225986 0.128319
H 0.482868 -0.360946 -1.276587
H -2.374087 2.599257 -0.679862
H 0.509656 -1.385186 2.005295
H -1.292182 -3.355038 -1.436772
H -1.159317 2.834274 0.551518

(1-2)' anti-(iii) (re-re)₆₀

sol-rere-sa-hk-mich-test-t1-smdPCM-conf.log

E₀ = -1148.5122692
E_{0+ZPE} = -1148.089866
E₂₉₈ = -1148.067846
H₂₉₈ = -1148.066901
G₂₉₈ = -1148.141912
NImag = 1 (-378.2625)
C 2.539302 -1.656176 0.056915
C 2.523362 -0.315877 0.447162
C 3.712220 0.410002 0.388631
C 4.889624 -0.189255 -0.036412
C 4.893439 -1.521736 -0.418938
C 3.712234 -2.252848 -0.371985
C 1.299082 0.341174 0.944713
C 0.490097 -0.359985 1.832153
N -0.429698 0.279412 2.611024
O -1.098215 -0.389029 3.416625
O -0.585834 1.506184 2.513456
C 0.336141 0.673214 -0.973568
C -0.932607 1.036780 -0.524041
C -1.329916 2.482593 -0.423554
C -0.553914 3.380576 -1.374123
C 0.932802 3.100199 -1.302740
C 1.204845 1.661640 -1.701157
N -1.799411 0.119343 -0.086654
C -3.045068 0.428573 0.618471
C -3.759610 -0.907865 0.734856
C -2.635484 -1.927933 0.673298
C -1.655305 -1.305887 -0.321550
C -1.986644 -1.726329 -1.740589
O -1.678628 -2.801758 -2.184325
O -2.672463 -0.828452 -2.433931
H -0.643521 -1.645718 -0.132915
H -2.956246 -2.920566 0.370941
H -2.137338 -2.000710 1.637610
H -4.332425 -0.976650 1.655192
H -4.446934 -1.043913 -0.098468
H -2.797896 0.849971 1.594332
H -3.636050 1.156895 0.070420
H 1.377409 1.404686 1.114454
H 2.253072 1.410629 -1.539193
H 1.039546 1.549654 -2.776932
H 1.483485 3.774825 -1.957856
H 1.289778 3.284557 -0.287356
H -0.901032 3.218479 -2.396639
H -0.769383 4.419845 -1.128708
H 3.716961 1.447702 0.691280
H 5.802579 0.387647 -0.068916
H 5.807726 -1.988973 -0.754854

(1-2)' anti-(vi) (re-re)₆₀

sol-rere-sa-hk-mich-conf-pyr.log

E₀ = -1148.5124766
E_{0+ZPE} = -1148.090000
E₂₉₈ = -1148.068033
H₂₉₈ = -1148.067089
G₂₉₈ = -1148.141707
NImag = 1 (-361.3293)
C 2.552481 -1.537232 0.535350
C 2.473669 -0.143585 0.563600
C 3.627888 0.594191 0.303188
C 4.831589 -0.041082 0.033024
C 4.897463 -1.425535 0.009250
C 3.751720 -2.171291 0.260836
C 1.224842 0.567404 0.894767
C 0.429803 0.066482 1.918681
N -0.486148 0.854614 2.554026
O -1.097781 0.387563 3.528564
O -0.684998 2.016515 2.168633
C 0.276076 0.409950 -1.063879
C -0.995791 0.857709 -0.719687
C -1.394603 2.289883 -0.932161
C -0.641821 2.940284 -2.082382
C 0.848720 2.691548 -1.967269
C 1.132896 1.201232 -2.012371
N -1.873118 0.049052 -0.120867
C -3.114460 0.495680 0.502237
C -3.488629 -0.679818 1.382748
C -3.056000 -1.883373 0.561759
C -1.781676 -1.399097 -0.154029
C -1.774840 -1.937959 -1.567099
O -2.222906 -1.386926 -2.535025
O -1.256313 -3.161467 -1.600471
H -0.890684 -1.750764 0.357956
H -3.823376 -2.131006 -0.170699
H -2.860040 -2.769531 1.157302
H 1.266274 1.643160 0.812270
H 2.184770 1.004762 -1.806236
H 0.958498 0.834563 -3.028476
H 1.384623 3.192777 -2.772989
H 1.216197 3.117198 -1.030787
H -1.003523 2.538310 -3.030932
H -0.860590 4.007576 -2.087054
H 3.584837 1.674032 0.327047
H 5.716512 0.548178 -0.159493
H 5.832499 -1.922851 -0.204035
H 3.793681 -3.250819 0.241381
H 1.669500 -2.131504 0.723851
H 0.438633 -0.657611 -1.093814
H -2.466105 2.336053 -1.115779

(1-2)' anti-(vi) (si-si)₃₀₀

sol-sisi-aa-hk-mich-conf-pyr.log

E₀ = -1148.5095881
E_{0+ZPE} = -1148.087222
E₂₉₈ = -1148.065222
H₂₉₈ = -1148.064278
G₂₉₈ = -1148.139401
NImag = 1 (-375.4033)
C -3.148540 -1.165308 -0.917841
C -2.847059 -0.323183 0.154597
C -3.860695 0.478764 0.677605
C -5.144335 0.434588 0.152190
C -5.431731 -0.405830 -0.912000
C -4.427359 -1.205161 -1.445740
C -1.506632 -0.280608 0.768405
C -0.831026 -1.480602 0.957766
N 0.199115 -1.595140 1.846826
O 0.698752 -2.716218 2.033447
O 0.611394 -0.600214 2.462399
C 1.329695 1.871100 0.685217
C 0.751260 0.873181 -0.280895
C -0.561966 1.021296 -0.720286
C -1.265417 2.346957 -0.620440
C -0.766875 3.214675 0.519882
C 0.747052 3.263881 0.509226
N 1.465504 -0.207713 -0.608079
C 1.073856 -1.188477 -1.617129
C 1.835216 -2.430289 -1.205251
C 3.149826 -1.885435 -0.670016
C 2.786199 -0.502048 -0.087169
C 3.838072 0.477545 -0.550638
O 3.764134 1.183662 -1.520234
O 4.914342 0.416189 0.224669
H 2.760059 -0.521138 1.001834
H 3.866851 -1.773174 -1.482079
H 3.600720 -2.518086 0.087336
H -1.368065 0.469520 1.532853
H 1.122784 3.903144 1.307304
H 1.093842 3.693066 -0.432930
H -1.186586 4.216364 0.431022
H -1.107393 2.813710 1.477062
H -1.124411 2.881933 -1.564750
H -2.339773 2.183713 -0.536544
H -3.644152 1.131966 1.511232
H -5.917661 1.059041 0.575663
H -6.429148 -0.438974 -1.325621
H -4.642648 -1.859972 -2.277831
H -2.376487 -1.787436 -1.348716
H 2.409439 1.922132 0.593393
H -0.871536 0.417637 -1.559344

H 3.705492 -3.290255 -0.673816
H 1.625962 -2.234416 0.077549
H 0.485234 -0.353356 -1.272495
H -2.394575 2.574557 -0.624830
H 0.537935 -1.421723 1.989862
H -2.853485 -1.197387 -3.306110
H -1.179002 2.802203 0.607000

H 0.507423 -0.927010 2.319694
H -1.333290 -3.503051 -2.498577
H -1.209245 2.834277 -0.006987
H -2.928769 -0.628204 2.314276
H -4.550062 -0.696638 1.615428
H -2.936772 1.406182 1.067596
H -3.876541 0.687980 -0.256046

H -1.087912 -2.401732 0.468792
H 5.589108 1.000780 -0.138769
H 1.121175 1.507077 1.690527
H 1.373896 -0.832350 -2.605746
H 0.002424 -1.340704 -1.613260
H 1.980282 -3.116633 -2.035258
H 1.296654 -2.947548 -0.414557

(1-2)' anti-(v)(re-re)₆₀

sol-rere-sa-hk-mich-test-smdPCM-cycconf-tl.log

E₀ = -1148.513288
E_{0+ZPE} = -1148.091043
E₂₉₈ = -1148.069054
H₂₉₈ = -1148.068110
G₂₉₈ = -1148.142857
NImag = 1 (-372.4372)
C 2.533558 -1.583755 0.330673
C 2.518697 -0.200032 0.516689
C 3.707800 0.507399 0.348120
C 4.882473 -0.149695 0.008666
C 4.884318 -1.523844 -0.173143
C 3.703706 -2.239265 -0.010005
C 1.291366 0.520765 0.910380
C 0.482102 -0.045984 1.890921
N -0.473020 0.694714 2.520727
O -1.166442 0.159940 3.402652
O -0.636846 1.884599 2.208654
C 0.336880 0.598684 -1.009286
C -0.951676 0.963579 -0.617215
C -1.436379 2.377818 -0.726854
C -0.356214 3.347623 -1.166725
C 0.434559 2.763926 -2.320163
C 1.178343 1.520823 -1.858953
N -1.792369 0.072520 -0.091524
C -3.084454 0.424379 0.498952
C -3.778713 -0.910229 0.712061
C -2.628426 -1.893588 0.850233
C -1.606216 -1.362376 -0.155713
C -1.888208 -1.889466 -1.549075
O -2.434144 -1.289264 -2.434309
O -1.469781 -3.145422 -1.673125
H -0.598005 -1.654231 0.117193
H -2.905625 -2.925771 0.656904
H -2.190546 -1.829925 1.844077
H -4.421173 -0.894250 1.587809
H -4.392608 -1.166050 -0.151617
H -2.906446 0.944953 1.441971
H -3.645205 1.081932 -0.159447
H 1.369809 1.597803 0.923136
H -0.822531 4.291380 -1.446054
H 0.313427 3.560815 -0.331764
H 3.716445 1.577426 0.500564
H 5.795689 0.414907 -0.112449
H 5.796985 -2.036551 -0.440179
H 3.695658 -3.310274 -0.152595
H 1.620014 -2.150671 0.445560
H 0.514652 -0.452060 -1.173715
H -2.243541 2.373152 -1.465586
H 0.536797 -1.069104 2.214386
H -1.697491 -3.459009 -2.555514
H -1.873654 2.691263 0.216529
H -0.249488 2.510393 -3.133244
H 1.142830 3.491438 -2.715545
H 2.067005 1.831920 -1.304220
H 1.551354 0.965082 -2.718972

(1-2)' anti-(v)(si-si)₃₀₀

sol-sisi-aa-hk300-cnf-cyc.log

E₀ = -1148.5121134
E_{0+ZPE} = -1148.089628
E₂₉₈ = -1148.067706
H₂₉₈ = -1148.066762
G₂₉₈ = -1148.141380
NImag = 1 (-385.3484)
C -3.087304 -1.274915 -0.822292
C -2.866622 -0.337053 0.188189
C -3.940222 0.437766 0.624022
C -5.203077 0.276142 0.071019
C -5.409900 -0.659073 -0.930911
C -4.345703 -1.435021 -1.375543
C -1.543285 -0.169466 0.822959
C -0.837214 -1.320185 1.168424
N 0.206365 -1.262631 2.039752
O 0.785788 -2.315339 2.359667
O 0.563406 -0.167155 2.505214
C 1.393761 1.959753 0.492520
C 0.727496 0.867397 -0.289319
C -0.597934 0.979395 -0.712370
C -1.302160 2.314328 -0.720710
C -0.411761 3.471934 -0.296990
C 0.436083 3.066888 0.892267
N 1.419916 -0.241013 -0.555351
C 1.025147 -1.215925 -1.577022
C 2.216761 -2.154029 -1.679930
C 2.885339 -2.040624 -0.319712
C 2.704142 -0.559877 0.030388
C 3.830981 0.252461 -0.568425
O 3.803500 0.809678 -1.633341
O 4.900634 0.241148 0.218038
H 2.683902 -0.405956 1.107636
H 3.928683 -2.344035 -0.319318
H 2.355650 -2.625609 0.428988
H 1.911776 -3.171438 -1.909011
H 2.891224 -1.821143 -2.466404
H 0.125219 -1.739986 -1.267128
H 0.817182 -0.698040 -2.512046
H -1.460908 0.659511 1.510502
H -1.703766 2.494776 -1.717858
H -2.171018 2.279335 -0.059636
H -3.789344 1.159911 1.414056
H -6.024005 0.882262 0.426075
H -6.391281 -0.783782 -1.365020
H -4.497276 -2.163945 -2.158584
H -2.265502 -1.876161 -1.186283
H 2.170119 2.378742 -0.152998
H -0.912885 0.287877 -1.478248
H -1.053426 -2.304424 0.796379
H 5.610895 0.721493 -0.222075
H 1.889354 1.549607 1.367435
H 1.011893 3.910539 1.270129
H -0.204237 2.728592 1.708595
H 0.245000 3.760268 -1.120798
H -1.025021 4.341086 -0.061224

(1-2)' anti-(v)(si-re)₆₀

sol-sire-aa-hk-60-cnf-cyc-t2.log

E₀ = -1148.5076707
E_{0+ZPE} = -1148.085460
E₂₉₈ = -1148.063290
H₂₉₈ = -1148.062346
G₂₉₈ = -1148.138880
NImag = 1 (-427.7885)
C -2.837731 -0.603991 -0.580172
N -1.558782 -0.762189 0.078479
C -1.089881 -2.145989 0.034062
C -2.260253 -2.917435 -0.549778
C -2.966008 -1.884098 -1.411585
C -0.865640 0.241739 0.616628
C -1.568386 1.559517 0.765589
C -0.711162 2.643621 1.397127
C 0.090918 2.073294 2.548272
C 1.077451 1.049933 2.012041
C 0.454128 0.063905 1.052851
C -3.982012 -0.510795 0.407334
O -5.077296 -0.038488 -0.176234
O -3.942384 -0.844077 1.561071
C 1.564551 0.230488 -0.757079
C 1.659373 1.547897 -1.201471
N 0.639157 2.095126 -1.919474
O -0.383427 1.425717 -2.147112
C 2.786775 -0.471813 -0.316373
C 2.855512 -1.859216 -0.454830
C 3.987384 -2.560485 -0.074832
C 5.074734 -1.885686 0.463769
C 5.020747 -0.506516 0.606194
C 3.890445 0.195573 0.216469
O 0.752171 3.259124 -2.335823
H -2.848442 0.281167 -1.210803
H -3.998704 -2.133118 -1.638446
H -2.437574 -1.735942 -2.351145
H -1.931675 -3.783042 -1.117915
H -2.917698 -3.265932 0.244502
H -0.210902 -2.223471 -0.603018
H -0.817294 -2.480048 1.033465
H 0.857454 -0.379579 -1.298029
H 1.539953 0.502117 2.832232
H 1.885569 1.593546 1.514936
H 3.877033 1.269188 0.326275
H 5.864312 0.028151 1.018389
H 5.958289 -2.429580 0.764815
H 4.021158 -3.633147 -0.199737
H 2.012281 -2.391299 -0.872602
H -2.434419 1.376399 1.406432
H 0.759975 -0.962643 1.184990
H 2.475842 2.217260 -1.006881
H -5.793894 -0.036825 0.468296
H -1.950655 1.888659 -0.197127
H -0.032107 3.067609 0.656838
H -1.361146 3.452924 1.726727
H 0.626764 2.862288 3.075231
H -0.584914 1.606884 3.269027

(1-2)' anti-(v)(re-si)₆₀

sol-resi-sa-hk-60-cnf-cyc.log

$E_0 = -1148.5092866$
 $E_{0+ZPE} = -1148.087084$
 $E_{298} = -1148.065102$
 $H_{298} = -1148.064158$
 $G_{298} = -1148.138885$
 $N\text{Imag} = 1 (-369.1137)$
C -3.513866 0.638690 -0.939208
C -2.407976 0.816172 -0.107117
C -2.581525 0.664745 1.270646
C -3.818138 0.331339 1.795001
C -4.908967 0.144693 0.954271
C -4.753620 0.304526 -0.414176
C -1.115606 1.201849 -0.698202
C -0.312072 2.101036 0.006041
N 0.710901 2.749785 -0.609794
O 1.355279 3.601574 0.023864
O 1.006603 2.464012 -1.785373
C -0.060151 -0.588629 -1.156066
C 0.285649 -1.015284 0.124993
C -0.543303 -2.024014 0.855883
C -1.705384 -2.574346 0.043276
C -1.299879 -2.773356 -1.403497
C -0.946245 -1.435815 -2.034547
N 1.337199 -0.504870 0.770746
C 1.624737 -0.759384 2.186016
C 3.043161 -0.248409 2.389526
C 3.235363 0.761026 1.269436
C 2.459166 0.135303 0.111824
C 3.300689 -0.893023 -0.619202
O 3.207049 -2.086022 -0.509776
O 4.195149 -0.304364 -1.404179
H 2.158341 0.883360 -0.614885
H 4.276191 0.944485 1.019991
H 2.771582 1.714843 1.511574
H 3.176555 0.189309 3.374757
H 3.754728 -1.066114 2.289105
H 0.907555 -0.217759 2.801849
H 1.537413 -1.817995 2.415071
H -1.129538 1.329253 -1.771299
H -2.029147 -3.512947 0.491326
H -2.553411 -1.892305 0.090732
H -1.744277 0.803629 1.938906
H -3.933225 0.216060 2.863155
H -5.873189 -0.116123 1.365747
H -5.597849 0.174893 -1.075688
H -3.404950 0.782950 -2.004661
H 0.677020 -0.005166 -1.688523
H 0.128223 -2.840981 1.130977
H -0.447929 2.365623 1.037848
H 4.728898 -0.986006 -1.827283
H -0.897085 -1.599599 1.796756
H -0.438185 -3.443112 -1.450477
H -2.103336 -3.248128 -1.965734
H -0.438134 -1.595228 -2.985935
H -1.867799 -0.901663 -2.275666

syn-addition

(1-2)'_{syn} (re-re)₁₈₀

$E_0 = -1148.5080791$
 $E_{0+ZPE} = -1148.085733$
 $E_{298} = -1148.063711$
 $H_{298} = -1148.062767$
 $G_{298} = -1148.137976$
 $N\text{Imag} = 1 (-424.6252)$
C 3.238837 -0.908277 -0.393803
C 1.942708 -0.567411 -0.787732
C 1.160035 -1.540209 -1.411426
C 1.655205 -2.815460 -1.636374

(1-2)'_{syn} (re-re)₃₀₀

$E_0 = -1148.5024339$
 $E_{0+ZPE} = -1148.080080$
 $E_{298} = -1148.058145$
 $H_{298} = -1148.057201$
 $G_{298} = -1148.132417$
 $N\text{Imag} = 1 (-403.2155)$
C 0.528736 2.063392 1.067585
C -0.496225 2.101875 0.122060
C -0.530120 3.164637 -0.783510
C 0.431154 4.161259 -0.748517

(1-2)'_{syn} (si-si)₁₈₀

$E_0 = -1148.5067758$
 $E_{0+ZPE} = -1148.084147$
 $E_{298} = -1148.062179$
 $H_{298} = -1148.061235$
 $G_{298} = -1148.136732$
 $N\text{Imag} = 1 (-422.0564)$
C -3.106198 -0.496204 -0.631168
C -1.773429 -0.260688 -0.972472
C -1.129330 -1.178808 -1.803935
C -1.793094 -2.301147 -2.275599

C	2.942228	-3.143897	-1.235494	C	1.450445	4.110467	0.193551	C	-3.115801	-2.527584	-1.922995
C	3.730475	-2.184559	-0.612992	C	1.492445	3.059490	1.099567	C	-3.768863	-1.619143	-1.100076
C	1.389006	0.787661	-0.623613	C	-1.571935	1.093393	0.064973	C	-1.025976	0.935402	-0.537586
C	2.262483	1.872599	-0.553245	C	-1.957455	0.428675	1.227537	C	-1.716975	2.126374	-0.300642
N	1.806724	3.147149	-0.705869	N	-3.242186	-0.005453	1.409875	N	-1.034367	3.300768	-0.197068
O	2.612032	4.086184	-0.605440	O	-3.527347	-0.553574	2.486286	O	-1.670353	4.351153	-0.008631
O	0.603913	3.355746	-0.942256	O	-4.101129	0.163166	0.532506	O	0.205531	3.307293	-0.288436
C	0.376020	0.809365	1.257312	C	-0.846226	-0.152692	-1.557405	C	-0.282373	-1.924734	1.569384
C	-0.744822	-0.016228	1.109213	C	-0.003421	-1.028256	-0.901112	C	0.512861	-0.744047	1.103471
C	-0.679004	-1.439608	1.569071	C	-0.637224	-2.213245	-0.258570	C	-0.016340	0.542355	1.260965
C	0.133588	-1.578714	2.849406	C	-1.672931	-2.865240	-1.166794	C	-0.985286	0.814356	2.381018
C	1.511757	-0.976553	2.673513	C	-2.722918	-1.857513	-1.587990	C	-1.853641	-0.373474	2.754537
C	1.420143	0.493545	2.296550	C	-2.090534	-0.643120	-2.245097	C	-1.020805	-1.633287	2.869990
N	-1.860010	0.432900	0.524880	N	1.307822	-0.811456	-0.754195	N	1.687155	-0.970558	0.505818
C	-2.060553	1.845388	0.187875	C	2.018020	0.260391	-1.458325	C	2.219178	-2.308560	0.218769
C	-3.393250	1.870583	-0.531298	C	3.437885	0.152880	-0.945693	C	3.579757	-2.040178	-0.924576
C	-4.154037	0.727906	0.115336	C	3.604501	-1.337009	-0.712282	C	4.009336	-0.755211	0.290545
C	-3.071237	-0.338781	0.318231	C	2.234568	-1.766486	-0.170810	C	2.706082	0.051081	0.332049
C	-2.978834	-1.235147	-0.896616	C	2.214091	-1.761500	1.342387	C	2.563733	0.828603	-0.956395
O	-2.160959	-1.153350	-1.772501	O	1.675659	-0.952434	2.046498	O	1.936981	0.475711	-1.920634
O	-3.958665	-2.131686	-0.900233	O	2.899631	-2.795900	1.819547	O	3.280997	1.940523	-0.200209
H	-3.310155	-0.961569	1.175332	H	2.013028	-2.781253	-0.492187	H	2.689875	0.752207	1.162761
H	-4.989314	0.361646	-0.474329	H	4.413658	-1.589624	-0.033598	H	4.809245	-0.228224	-0.221717
H	-4.532303	1.022614	1.092237	H	3.781367	-1.853465	-1.653452	H	4.329962	-0.950359	1.312143
H	-3.895958	2.827014	-0.418031	H	4.157892	0.550794	-1.655279	H	4.268346	-2.861861	-0.219312
H	-3.253435	1.687004	-1.595306	H	3.541975	0.702442	-0.011383	H	3.494510	-1.891933	-1.469412
H	-2.096978	2.423762	1.113488	H	1.964106	0.077063	-2.533810	H	2.330487	-2.870155	1.146141
H	-1.240081	2.226771	-0.412377	H	1.571827	1.224811	-1.247855	H	1.549370	-2.853839	-0.440403
H	0.462768	0.959590	-1.150645	H	-2.390988	1.352862	-0.590588	H	-0.075316	1.046281	-1.031778
H	2.390161	0.859578	1.952108	H	-2.825073	0.157795	-2.332606	H	-1.646012	-2.490562	3.117528
H	1.191343	1.076924	3.192992	H	-1.808352	-0.898399	-3.271505	H	-0.295360	-1.526144	3.679104
H	2.093384	-1.081413	3.589389	H	-3.430228	-2.314691	-2.280273	H	-2.368437	-0.170667	3.693613
H	2.040317	-1.530572	1.898795	H	-3.295545	-1.540843	-0.718288	H	-2.624006	-0.524967	1.999454
H	-0.392647	-1.083065	3.667837	H	-1.173603	-3.283431	-2.043567	H	-0.412215	1.133499	3.256377
H	0.203565	-2.634265	3.109613	H	-2.132335	-3.698342	-0.636223	H	-1.604946	1.670884	2.105502
H	0.155946	-1.288983	-1.723003	H	-1.323320	3.209409	-1.517507	H	-0.101527	-0.997783	-2.085444
H	1.035309	-3.551127	-2.128725	H	0.383002	4.978740	-1.453572	H	-1.278200	-2.995192	-2.924483
H	3.331185	-4.136572	-1.410609	H	2.201827	4.886360	0.224586	H	-3.636446	-3.399891	-2.290748
H	4.735515	-2.429852	-0.301148	H	2.280410	3.013619	1.837871	H	-4.801119	-1.782866	-0.825728
H	3.873280	-0.179806	0.087943	H	0.593488	1.245437	1.767599	H	-3.636192	0.198223	0.003480
H	0.188411	1.866129	1.130192	H	-0.363371	0.678496	-2.092653	H	0.354764	-2.794073	1.694220
H	-1.671745	-1.852630	1.715411	H	0.088149	-2.947311	0.074400	H	0.656758	1.368452	1.069795
H	3.306309	1.811628	-0.311422	H	-1.325002	0.260452	2.078903	H	-2.774267	2.213132	-0.135987
H	-3.895957	-2.652865	-1.708596	H	2.885479	-2.755339	2.782380	H	3.161233	2.411557	-1.752269
H	-0.210992	-2.028648	0.775729	H	-1.139485	-1.831231	0.640817	H	-1.002297	-2.175270	0.786066

(1-2)'_{syn} (si-si)₃₀₀

E₀ = -1148.5013791
E_{0+ZPE} = -1148.079165
E₂₉₈ = -1148.057196
H₂₉₈ = -1148.056252
G₂₉₈ = -1148.131064
NImag = 1 (-381.0101)

C	-2.587146	-1.564899	-0.404948
C	-2.432943	-0.417545	0.373254
C	-3.567719	0.324632	0.698675
C	-4.824967	-0.074108	0.268954
C	-4.965942	-1.217079	-0.503490
C	-3.840865	-1.959951	-0.840058
C	-1.122318	0.018783	0.894174
C	-0.278895	-0.936812	1.452088
N	0.675142	-0.583613	2.366055
O	1.289959	-1.476148	2.963047
O	0.893415	0.616204	2.605286
C	0.954073	2.653827	0.235726
C	0.875498	1.297585	-0.403263
C	-0.338229	0.860621	-0.928498
C	-1.353713	1.859691	-1.417638
C	-1.352437	3.150320	-0.619378

(1-2)'_{syn} (si-re)₆₀

E₀ = -1148.5039153
E_{0+ZPE} = -1148.081615
E₂₉₈ = -1148.059688
H₂₉₈ = -1148.058744
G₂₉₈ = -1148.133243
NImag = 1 (-384.6762)

C	-2.306252	1.841436	-0.483050
C	-2.318482	0.449471	-0.383854
C	-3.502593	-0.175418	0.012733
C	-4.635397	0.570241	0.298277
C	-4.609887	1.953979	0.192020
C	-3.439604	2.587489	-0.202302
C	-1.096618	-0.301486	-0.737579
C	-1.225021	-1.592062	-1.255010
N	-0.251482	-2.130635	-2.045181
O	-0.459643	-3.237679	-2.572766
O	0.812745	-1.519593	-2.231764
C	1.217354	-2.205618	0.920909
C	1.094271	-0.718794	0.841950
C	-0.134382	-0.141940	1.176817
C	-1.016063	-0.804126	2.205056
C	-0.912814	-2.318851	2.215371

(1-2)'_{syn} (re-si)₆₀

E₀ = -1148.5059406
E_{0+ZPE} = -1148.083189
E₂₉₈ = -1148.061349
H₂₉₈ = -1148.060405
G₂₉₈ = -1148.134691
NImag = 1 (-407.6710)

C	3.501326	0.865691	-0.126182
C	2.188072	0.639284	-0.539694
C	1.954085	-0.316260	-1.530844
C	3.005117	-1.032908	-2.079010
C	4.308104	-0.805048	-1.653834
C	4.553126	0.150762	-0.678613
C	1.108161	1.460140	0.033770
C	0.102562	1.926112	-0.811896
N	-0.668331	2.985771	-0.448167
O	-1.501916	3.429566	-1.254300
O	-0.546875	3.482791	0.687415
C	0.336465	0.367757	1.693718
C	-0.451685	-0.637041	1.127238
C	0.128649	-2.003978	0.923301
C	1.065416	-2.390686	2.060178
C	2.141903	-1.342526	2.245534

C	0.062222	3.671201	-0.462841	C	0.536626	-2.758053	2.168091	C	1.528661	0.015102	2.547736
N	1.951369	0.497900	-0.381295	N	2.137542	0.000857	0.421239	N	-1.701437	-0.389796	0.720520
C	3.179316	0.818196	0.351259	C	3.324374	-0.582891	-0.204553	C	-2.476475	0.774558	1.163720
C	4.175988	-0.228963	-0.107141	C	4.192038	0.618179	-0.528638	C	-3.716233	0.725770	0.301374
C	3.714698	-0.536088	-1.522458	C	3.829020	1.605321	0.567648	C	-3.974147	-0.763747	0.174471
C	2.191488	-0.527914	-1.397670	C	2.312966	1.412102	0.702267	C	-2.563918	-1.365159	0.073319
C	1.712158	-1.918290	-1.019036	C	1.607941	2.338289	-0.262684	C	-2.173651	-1.626772	-1.364359
O	2.161407	-2.593254	-0.135096	O	1.195765	2.053711	-1.353899	O	-1.359688	-1.022195	-2.006656
O	0.767770	-2.358708	-1.849836	O	1.535787	3.567537	0.240399	O	-2.869551	-2.647190	-1.855590
H	1.699532	-0.237173	-2.321103	H	1.961146	1.644237	1.705612	H	-2.538390	-2.324790	0.585057
H	4.095171	-1.476037	-1.913511	H	4.100455	2.632944	0.343392	H	-4.595622	-1.032680	-0.674199
H	4.008225	0.260967	-2.204028	H	4.298782	1.326579	1.509022	H	-4.451311	-1.146141	1.074276
H	5.195475	0.145634	-0.071314	H	5.248669	0.365564	-0.533172	H	-4.547600	1.259984	0.752618
H	4.110523	-1.118630	0.512419	H	3.935405	1.020182	-1.506969	H	-3.511545	1.169987	-0.671336
H	3.528437	1.812759	0.076811	H	3.834308	-1.241681	0.498863	H	-2.723890	0.644279	2.220527
H	2.977456	0.803252	1.420392	H	3.029306	-1.158696	-1.078610	H	-1.922862	1.688072	1.062137
H	-1.129784	0.975564	1.395659	H	-0.310548	0.289193	-1.186636	H	1.432385	2.164116	0.786857
H	0.073229	4.597876	0.110184	H	0.611438	-3.844782	2.155984	H	2.286482	0.796234	2.463149
H	0.474945	3.904721	-1.446598	H	1.062862	-2.412748	3.060521	H	1.206984	0.035302	3.593175
H	-1.980080	3.980995	-1.114533	H	-1.405270	-2.713561	3.103951	H	2.815392	-1.625032	3.054625
H	-1.787381	2.890768	0.367489	H	-1.436098	-2.732480	1.352588	H	2.742092	-1.289914	1.337908
H	-1.132799	2.085825	-2.465372	H	-0.729069	-0.418075	3.188248	H	0.490560	-2.506736	2.981267
H	-2.344737	1.408856	-1.417233	H	-2.049924	-0.493019	2.060248	H	1.506567	-3.361473	1.837482
H	-3.464207	1.215027	1.302724	H	-3.547567	-1.250933	0.098317	H	0.944386	-0.501207	-1.868139
H	-5.693054	0.105078	0.536978	H	-5.542117	0.067083	0.601874	H	2.807554	-1.770299	-2.843945
H	-5.943321	-1.527575	-0.843256	H	-5.495643	2.532638	0.410668	H	5.126036	-1.363473	-2.085685
H	-3.941629	-2.849824	-1.444603	H	-3.410369	3.663458	-0.297239	H	5.564067	0.343987	-0.349679
H	-1.719910	-2.145600	-0.681228	H	-1.401041	2.338637	-0.800772	H	3.699721	1.617972	0.624104
H	1.979838	3.010023	0.242777	H	2.255938	-2.516318	0.879327	H	-0.187280	1.252687	2.025759
H	-0.334523	-0.079471	-1.463033	H	-0.170678	0.939483	1.205261	H	-0.654963	-2.749689	0.828834
H	-0.365057	-1.995467	1.294200	H	-2.088522	-2.220030	-1.143440	H	-0.134270	1.511010	-1.772726
H	0.548097	-3.263978	-1.600715	H	1.140239	4.146291	-0.421062	H	-2.616735	-2.774990	-2.776707
H	0.657965	2.546905	1.280096	H	0.723783	-2.630932	0.045059	H	0.681640	-2.009113	-0.018357

Oxazolidinone pathway anti addition

(3-4)*anti* (re-re)₆₀

E ₀	= -1148.0270762
E _{0+ZPE}	= -1147.618684
E ₂₉₈	= -1147.596702
H ₂₉₈	= -1147.595757
G ₂₉₈	= -1147.671036
NImag	= 1 (-286.7505)
C	2.538843 -1.655278 0.197820
C	2.509889 -0.291738 0.501839
C	3.682561 0.448293 0.345712
C	4.853318 -0.155520 -0.090634
C	4.868993 -1.509797 -0.386421
C	3.705212 -2.256351 -0.241277
C	1.304001 0.379766 1.005621
C	0.457565 -0.271463 1.876609
N	-0.469626 0.416286 2.618312
O	-1.173668 -0.217853 3.417682
O	-0.581260 1.643070 2.499074
C	0.297384 0.672383 -1.056950
C	-0.969359 0.995725 -0.590801
C	-1.422234 2.430120 -0.527281
C	-0.653853 3.343372 -1.469843
C	0.839714 3.107120 -1.373935
C	1.156997 1.675800 -1.765947
N	-1.788101 0.060430 -0.106343
C	-3.059140 0.346321 0.547322
C	-3.733598 -1.010766 0.684963
C	-2.576300 -1.996184 0.646520
C	-1.619371 -1.365154 -0.358445
C	-1.971423 -1.783018 -1.811323
O	-2.658746 -1.002804 -2.492171
O	-1.537150 -2.909425 -2.126676
H	-0.596413 -1.666800 -0.164116

(3-4)*anti* (re-re)₁₈₀

E ₀	= -1148.0228559
E _{0+ZPE}	= -1147.614351
E ₂₉₈	= -1147.592442
H ₂₉₈	= -1147.591498
G ₂₉₈	= -1147.666740
NImag	= 1 (-323.6208)
C	-2.251902 2.076009 -0.011387
C	-1.402243 1.264545 -0.769403
C	-0.381048 1.878250 -1.496968
C	-0.211163 3.254151 -1.471766
C	-1.061055 4.046883 -0.714555
C	-2.083493 3.450264 0.013296
C	-1.563271 -0.190633 -0.873937
C	-2.802696 -0.784402 -0.703389
N	-3.029098 -2.065297 -1.136180
O	-4.167980 -2.540421 -0.998629
O	-2.115891 -2.719344 -1.655005
C	-0.211753 -1.109432 0.694905
C	0.663966 -0.076999 1.038212
C	0.345001 0.815211 2.202037
C	-0.461491 0.122830 3.289735
C	-1.646443 -0.617935 2.706169
C	-1.177711 -1.652871 1.702246
N	1.746102 0.211064 0.321931
C	2.680881 1.289656 0.633801
C	3.819480 1.104068 -0.359109
C	3.177248 0.345814 -1.508938
C	2.209001 -0.593804 -0.798579
C	2.925546 -1.906616 -0.374738
O	3.308294 -2.001980 0.803459
O	3.068646 -2.719690 -1.308031
H	1.374574 -0.859050 -1.440866

(3-4)*anti* (re-re)₃₀₀

E ₀	= -1148.018527
E _{0+ZPE}	= -1147.610545
E ₂₉₈	= -1147.588472
H ₂₉₈	= -1147.587528
G ₂₉₈	= -1147.663527
NImag	= 1 (-296.2941)
C	0.331296 2.399480 0.954036
C	-0.333281 2.083824 -0.232466
C	0.122724 2.658359 -1.422220
C	1.209084 3.514940 -1.429747
C	1.867185 3.814658 -0.243548
C	1.421109 3.255808 0.945670
C	-1.520160 1.221122 -0.276774
C	-2.293584 1.021563 0.851259
N	-3.621095 0.678840 0.766780
O	-4.251412 0.529531 1.824152
O	-4.172712 0.548606 -0.332201
C	-0.441167 -0.645241 -1.158954
C	-0.143519 -1.295137 0.034958
C	-1.206109 -2.152476 0.646454
C	-1.973855 -2.946235 -0.402847
C	-2.541891 -2.035222 -1.472626
C	-1.442118 -1.216711 -2.125026
N	0.999459 -1.109411 0.696589
C	1.316116 -1.733413 1.980299
C	2.799501 -1.459327 2.185482
C	3.068434 -0.240591 1.318977
C	2.173259 -0.473468 0.108248
C	2.889659 -1.351035 -0.954270
O	2.608798 -2.560958 -0.998053
O	3.718118 -0.722234 -1.642905
H	1.904935 0.467915 -0.358143

H	-2.869882	-2.998712	0.347427	H	3.889016	-0.201070	-2.120355	H	4.110296	-0.133559	1.031103
H	-2.099348	-2.050734	1.624666	H	2.628371	1.029998	-2.156668	H	2.762384	0.669073	1.835660
H	-4.320114	-1.078071	1.598260	H	4.251729	2.055453	-0.660137	H	3.039634	-1.301864	3.234509
H	-4.397171	-1.180978	-0.160190	H	4.605211	0.500128	0.089096	H	3.382394	-2.305467	1.828534
H	-2.866196	0.807041	1.519280	H	2.189190	2.255270	0.509076	H	0.708904	-1.289689	2.770352
H	-3.662539	1.034895	-0.039088	H	3.032508	1.217611	1.660473	H	1.114401	-2.801762	1.959377
H	1.362487	1.452925	1.098762	H	-0.911613	-0.670142	-1.585513	H	-2.048051	1.199680	-1.217995
H	2.208642	1.452416	-1.578129	H	-2.037926	-2.078179	1.181248	H	-1.876679	-0.418107	-2.730038
H	1.025468	1.563364	-2.847366	H	-0.707991	-2.489959	2.229015	H	-0.894692	-1.851135	-2.831065
H	1.381325	3.799539	-2.018951	H	-2.224743	-1.098437	3.495674	H	-3.061422	-2.621384	-2.231699
H	1.173230	3.300162	-0.351640	H	-2.311712	0.094302	2.214175	H	-3.277772	-1.365879	-1.028066
H	-0.977106	3.160732	-2.496831	H	0.181682	-0.581518	3.821152	H	-1.302505	-3.679888	-0.854196
H	-0.902795	4.379520	-1.240287	H	-0.784402	0.866824	4.018161	H	-2.770674	-3.504850	0.088295
H	3.679131	1.503025	0.582664	H	0.272952	1.267332	-2.101812	H	-0.383990	2.425452	-2.348569
H	5.751712	0.434841	-0.200218	H	0.581890	3.706512	-2.050057	H	1.545867	3.946300	-2.361301
H	5.777353	-1.981502	-0.732293	H	-0.932926	5.119530	-0.694789	H	2.718750	4.479494	-0.246804
H	3.705082	-3.310398	-0.478832	H	-2.753377	4.059096	0.603602	H	1.925534	3.486005	1.873159
H	1.639321	-2.247338	0.287205	H	-3.051764	1.634406	0.564154	H	0.003845	1.977100	1.891977
H	0.494517	-0.359369	-1.301927	H	0.153381	-1.844024	-0.007590	H	0.355398	-0.088402	-1.628220
H	-2.481268	2.476137	-0.772352	H	1.259386	1.218639	2.626760	H	-0.793762	-2.824750	1.391189
H	0.455150	-1.330796	2.054815	H	-3.651892	-0.331429	-0.226996	H	-1.956193	1.145778	1.863081
H	-1.325094	2.777395	0.500787	H	-0.216224	1.669891	1.811792	H	-1.893581	-1.481005	1.175917

(3-4)*anti* (si-si)₆₀

E ₀	= -1148.0212339
E _{0+ZPE}	= -1147.612792
E ₂₉₈	= -1147.590974
H ₂₉₈	= -1147.590029
G ₂₉₈	= -1147.665098
NImag	= 1 (-313.7967)
C	-0.536114 2.279550 -1.073018
C	-1.309428 1.887026 0.020849
C	-1.435704 2.769203 1.097590
C	-0.804600 4.000767 1.087320
C	-0.025770 4.374205 -0.001301
C	0.101969 3.510249 -1.079975
C	-2.034703 0.611815 0.064172
C	-2.403062 -0.027516 -1.105065
N	-3.468352 -0.893064 -1.147516
O	-3.752274 -1.411323 -2.236875
O	-4.133984 -1.128443 -0.132306
C	0.137568 -2.143560 -0.299785
C	0.387049 -0.895975 0.485779
C	-0.563772 -0.517156 1.431414
C	-1.419783 -1.547657 2.120481
C	-1.687482 -2.793242 1.292308
C	-0.435540 -3.252867 0.572438
N	1.450771 -0.149559 0.197682
C	1.900982 0.946822 1.051351
C	3.272789 1.315174 0.505500
C	3.217155 0.840727 -0.938424
C	2.430528 -0.461376 -0.835763
C	3.379664 -1.641321 -0.485367
O	3.373706 -2.062344 0.683420
O	4.075193 -2.024478 -1.446635
H	1.931079 -0.696587 -1.772098
H	4.194385 0.680842 -1.384037
H	2.671897 1.557840 -1.552230
H	3.471243 2.380435 0.599030
H	4.049314 0.776633 1.044618
H	1.211731 1.785503 0.984848
H	1.935628 0.617486 2.089297
H	-2.706586 0.483777 0.899533
H	-0.650112 -4.119777 -0.052327
H	0.320673 -3.564315 1.295483
H	-2.063980 -3.585910 1.940060
H	-2.472566 -2.585551 0.567510
H	-0.908822 -1.839176 3.044887
H	-2.364062 -1.101293 2.436803

(3-4)*anti* (si-si)₁₈₀

E ₀	= -1148.0268314
E _{0+ZPE}	= -1147.618417
E ₂₉₈	= -1147.596555
H ₂₉₈	= -1147.595610
G ₂₉₈	= -1147.670734
NImag	= 1 (-331.6299)
C	1.962539 2.318920 0.326187
C	1.414904 1.409179 -0.582894
C	0.376608 1.845895 -1.407874
C	-0.106788 3.142810 -1.324526
C	0.442798 4.033157 -0.414093
C	1.481868 3.614824 0.408268
C	1.906962 0.035313 -0.738503
C	3.210228 -0.300750 -0.413433
N	3.742330 -1.492505 -0.830687
O	4.922858 -1.745995 -0.545032
O	3.050229 -2.289052 -1.479356
C	-0.872457 0.327844 1.760651
C	-0.583421 -0.605626 0.623755
C	0.631057 -1.291716 0.577828
C	1.452254 -1.491002 1.813825
C	1.274092 -0.388640 2.841227
C	-0.196948 -0.095742 3.055713
N	-1.477578 -0.687300 -0.356017
C	-1.369016 -1.647112 -1.447934
C	-2.692417 -1.528728 -2.187059
C	-3.141794 -0.110840 -1.872278
C	-2.729992 0.057497 -0.413330
C	-3.840853 -0.472613 0.536397
O	-3.637741 -1.544233 1.130430
O	-4.846111 0.263525 0.580125
H	-2.554881 1.102314 -0.169936
H	-4.207325 0.050153 -2.004018
H	-2.606740 0.604405 -2.498329
H	-2.581113 -1.719945 -3.251680
H	-3.408713 -2.243837 -1.787384
H	-0.529872 -1.388880 -2.094328
H	-1.192843 -2.647555 -1.055788
H	1.473436 -0.511892 -1.558309
H	-0.333099 0.689493 3.799207
H	-0.693823 -0.987509 3.443013
H	1.748315 -0.675602 3.780161
H	1.774825 0.517839 2.498313
H	1.193524 -2.455467 2.262714
H	2.505550 -1.571722 1.531180

(3-4)*anti* (si-si)₃₀₀

E ₀	= -1148.0267495
E _{0+ZPE}	= -1147.618001
E ₂₉₈	= -1147.596191
H ₂₉₈	= -1147.595247
G ₂₉₈	= -1147.670139
NImag	= 1 (-310.7915)
C	-3.019683 -1.313253 -0.875636
C	-2.828865 -0.367029 0.134721
C	-3.902072 0.452608 0.485845
C	-5.131625 0.327073 -0.145385
C	-5.307969 -0.617362 -1.144627
C	-4.244592 -1.436241 -1.507513
C	-1.558446 -0.230434 0.862872
C	-0.826807 -1.353748 1.191367
N	0.129287 -1.320314 2.175887
O	0.699577 -2.379143 2.474678
O	0.385858 -0.262570 2.762842
C	1.439978 1.941511 0.606871
C	0.789091 0.901405 -0.262204
C	-0.516241 1.063014 -0.713765
C	-1.210043 2.392136 -0.639303
C	-0.673244 3.278693 0.470434
C	0.840649 3.324413 0.409737
N	1.464237 -0.217359 -0.510149
C	1.061272 -1.170520 -1.539214
C	2.212947 -2.165397 -1.609992
C	2.907364 -2.010739 -0.264753
C	2.793065 -0.513775 0.003589
C	3.942271 0.260323 -0.698864
O	3.666449 0.899133 -1.729590
O	5.048495 0.131558 -0.139617
H	2.833513 -0.296663 1.068472
H	3.943782 -2.335162 -0.270762
H	2.372943 -2.560908 0.509043
H	1.862917 -3.178468 -1.795468
H	2.891611 -1.891037 -2.414815
H	0.127010 -1.651087 -1.259186
H	0.902789 -0.649156 -2.483368
H	-1.495404 0.600328 1.548649
H	1.242231 3.996829 1.167570
H	1.151021 3.719391 -0.560161
H	-1.094386 4.280410 0.381195
H	-0.983301 2.891471 1.443884
H	-1.096551 2.912351 -1.596502
H	-2.284155 2.239594 -0.518983

H -2.037665 2.480847 1.948404
H -0.919552 4.670251 1.927574
H 0.471545 5.333287 -0.011104
H 0.700232 3.795875 -1.933231
H -0.425263 1.625445 -1.924423
H 1.042578 -2.487691 -0.787491
H -0.339318 0.351842 2.033744
H -1.937121 0.115927 -2.061854
H -0.583797 -1.893834 -1.088020

H -0.046771 1.161579 -2.128628
H -0.910813 3.457521 -1.974287
H 0.068551 5.044349 -0.346379
H 1.919304 4.301758 1.118552
H 2.769223 2.016603 0.977205
H -1.944126 0.397419 1.915851
H 0.723716 -2.082553 -0.152457
H 3.875122 0.286053 0.192095
H -0.526326 1.324133 1.469269

H -3.775038 1.183903 1.271649
H -5.950592 0.968712 0.146436
H -6.262905 -0.715147 -1.640340
H -4.370419 -2.171575 -2.289208
H -2.200846 -1.949170 -1.180673
H 2.502375 1.970033 0.381567
H -0.855381 0.404580 -1.499250
H -0.959611 -2.324866 0.752242
H 1.338384 1.631457 1.646249

(3-4)*anti* (si-re)₆₀

E₀ = -1148.0231327
E_{0+ZPE} = -1147.614814
E₂₉₈ = -1147.592829
H₂₉₈ = -1147.591884
G₂₉₈ = -1147.667929
NImag = 1 (-347.0578)
C 2.750103 -1.905271 -0.487348
C 2.756996 -0.519714 -0.310665
C 3.878536 0.064483 0.283425
C 4.950211 -0.715099 0.690857
C 4.928883 -2.090320 0.507404
C 3.823759 -2.683076 -0.089100
C 1.609639 0.263999 -0.790694
C 1.759928 1.593025 -1.133815
N 0.820706 2.228070 -1.906841
O 1.007140 3.420461 -2.191719
O -0.174651 1.614904 -2.310863
C -1.569209 1.575881 0.796893
C -0.947078 0.217094 0.640132
C 0.348224 -0.020007 1.103294
C 0.994143 0.899910 2.101023
C 0.465521 2.322796 2.040276
C -1.048510 2.319992 2.015743
N -1.656386 -0.717389 0.014489
C -1.222164 -2.100807 -0.101347
C -2.396300 -2.811294 -0.756049
C -3.082584 -1.699071 -1.533417
C -2.962872 -0.504502 -0.591967
C -4.142213 -0.481561 0.419311
O -3.916493 -0.856327 1.582666
O -5.218867 -0.094689 -0.075819
H -2.969982 0.432579 -1.142609
H -4.118961 -1.911693 -1.778726
H -2.544730 -1.496159 -2.460183
H -2.072222 -3.638696 -1.383117
H -3.066852 -3.203842 0.005696
H -0.328448 -2.162104 -0.723089
H -0.975992 -2.505648 0.879983
H 0.859771 -0.282275 -1.340248
H -1.440315 3.336757 2.004105
H -1.430242 1.843171 2.921026
H 0.837606 2.891968 2.892785
H 0.836186 2.818254 1.141471
H 0.833001 0.503886 3.109415
H 2.076954 0.894610 1.959132
H 3.925982 1.133311 0.428279
H 5.807058 -0.243727 1.150385
H 5.766938 -2.694670 0.823137
H 3.798131 -3.752065 -0.244313
H 1.892932 -2.374121 -0.949558
H -2.647899 1.474592 0.866708
H 0.657722 -1.052859 1.164851
H 2.569155 2.229223 -0.829593
H -1.363147 2.151201 -0.106921

(3-4)*anti* (si-re)₁₈₀

E₀ = -1148.0236979
E_{0+ZPE} = -1147.615220
E₂₉₈ = -1147.593411
H₂₉₈ = -1147.592467
G₂₉₈ = -1147.667354
NImag = 1 (-309.8510)
C -0.484217 2.206449 -1.229349
C -1.350229 1.741755 -0.239829
C -1.644065 2.581226 0.838777
C -1.077743 3.839876 0.926557
C -0.213096 4.292351 -0.065111
C 0.076431 3.473218 -1.145372
C -1.954394 0.413372 -0.396218
C -3.242720 0.168348 0.032093
N -4.003731 -0.837783 -0.518039
O -5.149287 -1.005580 -0.077717
O -3.564124 -1.526427 -1.445561
C 0.589125 -2.178935 -0.629985
C 0.556563 -0.957844 0.244344
C -0.560403 -0.730915 1.049555
C -1.426431 -1.869536 1.497383
C -1.441384 -3.052228 0.542981
C -0.042619 -3.378538 0.062090
N 1.579216 -0.109593 0.182181
C 1.777516 0.969024 1.146573
C 3.175960 1.489714 0.850967
C 3.389106 1.114566 -0.607373
C 2.731262 -0.257958 -0.699754
C 3.735385 -1.362145 -0.265912
O 3.621519 -1.831638 0.878667
O 4.581650 -1.637179 -1.138967
H 2.404117 -0.475426 -1.713247
H 4.434316 1.075246 -0.899862
H 2.874809 1.820348 -1.259879
H 3.255504 2.558540 1.034867
H 3.906170 0.980111 1.475919
H 1.029502 1.745223 1.003808
H 1.676299 0.581782 2.159818
H -1.631428 -0.146756 -1.259907
H -0.059247 -4.219212 -0.631412
H 0.586382 -3.675134 0.904035
H -1.886905 -3.915782 1.038089
H -2.068626 -2.818137 -0.316968
H -1.079348 -2.202783 2.481485
H -2.445922 -1.504412 1.654906
H -2.304680 2.242285 1.623446
H -1.308664 4.472324 1.771838
H 0.226945 5.276572 0.005459
H 0.741350 3.817479 -1.924428
H -0.256378 1.572666 -2.074803
H 1.608967 -2.417226 -0.910778
H -0.501122 0.093227 1.746350
H -3.759930 0.726493 0.790638
H 0.047133 -1.960001 -1.554257

(3-4)*anti* (si-re)₃₀₀

E₀ = -1148.0243126
E_{0+ZPE} = -1147.615553
E₂₉₈ = -1147.593790
H₂₉₈ = -1147.592846
G₂₉₈ = -1147.667708
NImag = 1 (-312.9718)
C -3.747937 0.353030 0.328439
C -2.527780 0.512280 -0.331557
C -2.373086 -0.073207 -1.591255
C -3.398752 -0.809408 -2.158932
C -4.603874 -0.970255 -1.486083
C -4.776517 -0.380692 -0.242252
C -1.487961 1.339089 0.290676
C -0.673483 2.132582 -0.496658
N 0.016616 3.181851 0.046253
O 0.663367 3.922337 -0.708840
O -0.003675 3.372048 1.271336
C 0.186684 -1.987621 -0.043475
C 0.561353 -0.682813 0.594939
C -0.273879 -0.117685 1.553465
C -1.279497 -0.944101 2.305253
C -1.704116 -2.214416 1.583447
C -0.513731 -2.904957 0.949332
N 1.667039 -0.066178 0.184641
C 2.344670 0.963853 0.970316
C 3.639809 1.231893 0.212097
C 3.350251 0.724367 -1.192872
C 2.491001 -0.507440 -0.933036
C 3.386660 -1.740672 -0.631606
O 3.517177 -2.085935 0.555148
O 3.902286 -2.244566 -1.648602
H 1.863338 -0.746351 -1.787678
H 4.244114 0.478172 -1.758637
H 2.779255 1.463658 -1.754606
H 3.909320 2.285059 0.235727
H 4.455659 0.661745 0.650697
H 1.736045 1.859013 1.058835
H 2.523489 0.588721 1.977679
H -1.730488 1.730451 1.266491
H -0.826647 -3.813630 0.435379
H 0.198602 -3.206408 1.719853
H -2.204454 -2.882713 2.285043
H -2.428319 -1.976466 0.804850
H -0.844713 -1.212465 3.273821
H -2.157398 -0.338297 2.542052
H -1.444565 0.041707 -2.131166
H -3.257861 -1.260009 -3.130967
H -5.402552 -1.544974 -1.932248
H -5.713536 -0.489390 0.284846
H -3.893434 0.820301 1.292020
H 1.074366 -2.479133 -0.427548
H 0.116778 0.729906 2.098381
H -0.543911 2.026520 -1.557483
H -0.470797 -1.799157 -0.895363

(3-4)*anti* (re-si)₆₀

E₀ = -1148.0204726
E_{0+ZPE} = -1147.611826

(3-4)*anti* (re-si)₁₈₀

E₀ = -1148.0203706
E_{0+ZPE} = -1147.612009

(3-4)*anti* (re-si)₃₀₀

E₀ = -1148.0228163
E_{0+ZPE} = -1147.614551

$E_{298} = -1147.589950$
 $H_{298} = -1147.589005$
 $G_{298} = -1147.663788$
 $N\text{Imag} = 1 (-298.3973)$
C -3.523246 0.686011 -0.951994
C -2.451327 0.829207 -0.068563
C -2.678682 0.606024 1.292231
C -3.932106 0.234179 1.747786
C -4.987398 0.083830 0.856254
C -4.778987 0.316879 -0.495325
C -1.155399 1.268974 -0.595161
C -0.341193 2.098671 0.149709
N 0.656058 2.820789 -0.454635
O 1.303046 3.623224 0.232717
O 0.893304 2.663964 -1.658979
C -0.066837 -0.674673 -1.128137
C 0.392966 -1.068019 0.122254
C -0.381476 -2.087777 0.907628
C -1.053046 -3.109271 0.001368
C -1.901193 -2.424877 -1.050557
C -1.053133 -1.497723 -1.906424
N 1.473123 -0.518681 0.682883
C 1.904635 -0.797744 2.050781
C 3.260716 -0.111021 2.186818
C 3.313521 0.858207 1.015439
C 2.539087 0.127462 -0.073415
C 3.437808 -0.891178 -0.827364
O 3.315977 -2.095671 -0.541029
O 4.221819 -0.365084 -1.641209
H 2.142833 0.824305 -0.803159
H 4.324581 1.094964 0.697287
H 2.806498 1.791124 1.258666
H 3.367940 0.382483 3.150190
H 4.056201 -0.847894 2.099601
H 1.171408 -0.403813 2.754802
H 1.996085 -1.867941 2.221565
H -1.110323 1.397131 -1.665716
H -1.696940 -0.842651 -2.498115
H -0.497394 -2.093775 -2.637947
H -2.393585 -3.162035 -1.685492
H -2.689140 -1.858602 -0.553963
H -0.286204 -3.720674 -0.478199
H -1.660073 -3.780327 0.609254
H -1.871151 0.718684 2.000591
H -4.087221 0.061028 2.803115
H -5.964389 -0.206680 1.214516
H -5.594680 0.213737 -1.196423
H -3.370252 0.877691 -2.004482
H 0.604507 -0.086074 -1.735249
H 0.276362 -2.599584 1.603497
H -0.433001 2.279515 1.204555
H -1.137741 -1.579845 1.511402

$E_{298} = -1147.589942$
 $H_{298} = -1147.588997$
 $G_{298} = -1147.665264$
 $N\text{Imag} = 1 (-290.6555)$
C -0.216575 2.272344 -1.309594
C 0.572632 1.954896 -0.204471
C 0.376472 2.663804 0.983882
C -0.584645 3.654869 1.061287
C -1.363060 3.967200 -0.048463
C -1.171992 3.275659 -1.234290
C 1.617956 0.935580 -0.352805
C 2.841968 1.097372 0.259007
N 3.969048 0.464473 -0.214484
O 5.034549 0.646048 0.389117
O 3.916731 -0.239252 -1.229575
C 0.525956 -0.784629 0.785783
C -0.163221 -1.392138 -0.261134
C 0.528916 -2.466847 -1.052137
C 1.388943 -3.350073 -0.158845
C 2.377081 -2.515174 0.628667
C 1.656219 -1.481975 1.479198
N -1.395998 -1.031309 -0.620970
C -2.128823 -1.601614 -1.749953
C -3.548552 -1.076075 -1.591936
C -3.378763 0.185153 -0.762290
C -2.253567 -0.181326 0.197335
C -2.808635 -0.897715 1.459262
O -2.762870 -2.139346 1.490534
O -3.284634 -0.118175 2.308359
H -1.717840 0.704596 0.518770
H -4.278875 0.480092 -0.230535
H -3.068407 1.017655 -1.393486
H -4.022277 -0.896754 -2.554471
H -4.149723 -1.801162 -1.048073
H -1.678523 -1.274249 -2.688471
H -2.109706 -2.688170 -1.726650
H 1.624874 0.399974 -1.289104
H 2.371587 -0.736772 1.840108
H 1.257262 -1.966656 2.376564
H 2.992464 -3.149991 1.266869
H 3.046952 -2.015497 -0.069911
H 0.741174 -3.906537 0.521802
H 1.907990 -4.083416 -0.776324
H 0.963834 2.424272 1.858581
H -0.733222 4.184173 1.991429
H -2.113310 4.741938 0.015667
H -1.769605 3.512907 -2.102847
H -0.070900 1.735587 -2.236633
H -0.036153 -0.114911 1.418852
H -0.192109 -3.077420 -1.584635
H 3.027924 1.720545 1.114327
H 1.155194 -1.992416 -1.812151

$E_{298} = -1147.592485$
 $H_{298} = -1147.591541$
 $G_{298} = -1147.667729$
 $N\text{Imag} = 1 (-301.0305)$
C -2.205274 -1.843169 -0.929547
C -2.377743 -0.504696 -0.567943
C -3.603915 -0.119807 -0.020106
C -4.621449 -1.044579 0.155997
C -4.437133 -2.369705 -0.212472
C -3.222852 -2.765573 -0.758340
C -1.283912 0.442119 -0.814022
C -1.520098 1.797313 -0.934366
N -0.619543 2.623625 -1.559516
O -0.915949 3.822591 -1.681102
O 0.445414 2.175567 -2.003105
C -0.104739 -0.171711 1.108371
C 1.057576 0.536158 0.818629
C 1.214141 1.929801 1.352843
C 0.525952 2.129637 2.693878
C -0.916742 1.671655 2.633545
C -0.985636 0.200141 2.265245
N 2.012656 0.054743 0.025187
C 3.130797 0.841217 -0.474951
C 3.966327 -0.155608 -1.260688
C 2.948965 -1.189177 -1.713201
C 1.999934 -1.292287 -0.520973
C 2.465178 -2.384516 0.478581
O 3.148348 -2.027726 1.453070
O 2.118816 -3.538923 0.155664
H 0.999654 -1.556692 -0.851743
H 3.387713 -2.151301 -1.963345
H 2.407203 -0.825994 -2.586841
H 4.491499 0.319249 -2.086255
H 4.703144 -0.618067 -0.607061
H 2.746735 1.643377 -1.110289
H 3.698883 1.287794 0.337992
H -0.447079 0.060872 -1.377677
H -2.016213 -0.088307 2.049399
H -0.693537 -0.400145 3.133880
H -1.414752 1.839130 3.589018
H -1.448334 2.267604 1.889807
H 1.058735 1.565346 3.462158
H 0.589130 3.181839 2.971302
H -3.772940 0.906737 0.268800
H -5.562387 -0.726688 0.581618
H -5.232028 -3.088341 -0.074995
H -3.066863 -3.794380 -1.048992
H -1.260789 -2.161302 -1.348814
H -0.125090 -1.218643 0.845454
H 2.266321 2.184842 1.438193
H -2.399202 2.308661 -0.590256
H 0.789105 2.620483 0.619852

Oxazolidinone Pathway *syn*-addition

(3-4)_{syn} (re-re)₁₈₀

$E_0 = -1148.0257813$
 $E_{0+ZPE} = -1147.616939$
 $E_{298} = -1147.595257$
 $H_{298} = -1147.594313$
 $G_{298} = -1147.668525$
 $N\text{Imag} = 1 (-349.7389)$
C 3.309025 -0.646983 -0.464580
C 1.973511 -0.410457 -0.803392
C 1.235738 -1.445842 -1.383365
C 1.821217 -2.680516 -1.619351
C 3.146477 -2.906945 -1.274335
C 3.886986 -1.884574 -0.694633
C 1.329856 0.896081 -0.623270

(3-4)_{syn} (re-re)₃₀₀

$E_0 = -1148.0181618$
 $E_{0+ZPE} = -1147.609761$
 $E_{298} = -1147.588045$
 $H_{298} = -1147.587101$
 $G_{298} = -1147.661816$
 $N\text{Imag} = 1 (-340.0828)$
C 0.913444 1.911806 0.962323
C -0.174606 2.134671 0.115859
C -0.150796 3.242159 -0.735081
C 0.928058 4.111471 -0.740121
C 2.004527 3.886008 0.108106
C 1.990646 2.784358 0.954109
C -1.371421 1.280836 0.126634

(3-4)_{syn} (si-si)₆₀

$E_0 = -1148.0031643$
 $E_{0+ZPE} = -1147.594299$
 $E_{298} = -1147.572891$
 $H_{298} = -1147.571947$
 $G_{298} = -1147.644789$
 $N\text{Imag} = 1 (-314.2345)$
C 0.195898 2.061446 -1.257813
C -0.375459 1.955614 0.011418
C 0.111314 2.772105 1.032996
C 1.109767 3.699908 0.785718
C 1.652132 3.812506 -0.485606
C 1.199234 2.981880 -1.501233
C -1.549295 1.122002 0.290638

C 2.098432 2.039710 -0.479651
 N 1.543322 3.285051 -0.584613
 O 2.268113 4.273917 -0.391990
 O 0.343525 3.431795 -0.869037
 C 0.265591 0.720627 1.361935
 C -0.818575 -0.133046 1.140501
 C -0.705065 -1.583196 1.506426
 C 0.161348 -1.796079 2.738585
 C 1.512370 -1.133931 2.564293
 C 1.354494 0.360876 2.334352
 N -1.950310 0.295755 0.585156
 C -2.195613 1.702809 0.290532
 C -3.489169 1.698369 -0.501862
 C -4.212939 0.474237 0.030580
 C -3.089658 -0.542011 0.225906
 C -2.880054 -1.404491 -1.044994
 O -1.908613 -1.138424 -1.775534
 O -3.750596 -2.280768 -1.204307
 H -3.334929 -1.220693 1.038033
 H -4.980868 0.092077 -0.635543
 H -4.677803 0.701272 0.990764
 H -4.048875 2.621481 -0.370277
 H -3.275487 1.579353 -1.562627
 H -2.305394 2.250111 1.231204
 H -1.365535 2.147363 -0.252369
 H 0.367634 1.005332 -1.097631
 H 2.300834 0.792960 1.996132
 H 1.143199 0.846478 3.293047
 H 2.141225 -1.306359 3.438388
 H 2.018949 -1.591020 1.714653
 H -0.345309 -1.385462 3.615211
 H 0.275402 -2.866003 2.912060
 H 0.193375 -1.281427 -1.634766
 H 1.236656 -3.468083 -2.073422
 H 3.601129 -3.869979 -1.457856
 H 4.920252 -2.050013 -0.424568
 H 3.907744 0.132311 -0.018005
 H 0.059979 1.778238 1.286879
 H -1.688710 -2.012827 1.667408
 H 3.137418 2.058693 -0.210573
 H -0.275238 -2.115433 0.654919

(3-4)_{syn} (si-si)₁₈₀

E₀ = -1148.0214368
 E_{0+ZPE} = -1147.612168
 E₂₉₈ = -1147.590723
 H₂₉₈ = -1147.589779
 G₂₉₈ = -1147.662828
 NImag = 1 (-353.4562)
 C -2.643602 -1.532125 -0.700298
 C -1.478653 -0.823629 -1.006932
 C -0.454542 -1.490381 -1.684157
 C -0.593596 -2.822915 -2.043381
 C -1.755031 -3.516747 -1.733346
 C -2.779354 -2.863744 -1.059578
 C -1.291662 0.605340 -0.691764
 C -2.410487 1.411820 -0.515533
 N -2.308321 2.774247 -0.479227
 O -3.349876 3.441680 -0.345004
 O -1.202540 3.321571 -0.573836
 C 0.165828 -1.617129 1.810578
 C 0.667581 -0.342764 1.194460
 C -0.167145 0.778819 1.185184
 C -1.215437 0.945977 2.246595
 C -1.805657 -0.366240 2.728128
 C -0.708550 -1.365486 3.032022
 N 1.881164 -0.347424 0.645518
 C 2.721776 -1.542098 0.545742
 C 4.021931 -1.033856 -0.050869

C -1.745295 0.612444 1.279791
 N -3.056160 0.294078 1.526414
 O -3.326336 -0.289159 2.586876
 O -3.948783 0.602080 0.722834
 C -0.805658 -0.043121 -1.640855
 C -0.140985 -1.062610 -0.957393
 C -0.973229 -2.142544 -0.348550
 C -2.109867 -2.571681 -1.267087
 C -2.963574 -1.385712 -1.670156
 C -2.120781 -0.307007 -2.328190
 N 1.179045 -1.065090 -0.777863
 C 2.064999 -0.138274 -1.479558
 C 3.440735 -0.451595 -0.925479
 C 3.345156 -1.929885 -0.594293
 C 1.932765 -2.074417 -0.036998
 C 1.878487 -1.937266 1.509483
 O 1.132135 -1.070920 1.997241
 O 2.597042 -2.761657 2.105652
 H 1.548015 -3.067018 -0.261354
 H 4.080702 -2.271939 0.126330
 H 3.451805 -2.523716 -1.503027
 H 4.228945 -0.215226 -1.636480
 H 3.618100 0.127461 -0.019667
 H 2.010934 -0.336082 -2.553786
 H 1.777250 0.893782 -1.310724
 H -2.185359 1.619900 -0.497170
 H -2.694266 0.618790 -2.407068
 H -1.906562 -0.603802 -3.361412
 H -3.753086 -1.700670 -2.353955
 H -3.453999 -0.973570 -0.789153
 H -1.694650 -3.054196 -2.155544
 H -2.714044 -3.320815 -0.755716
 H -0.990550 3.424316 -1.392243
 H 0.926201 4.966721 -1.400909
 H 2.846458 4.563601 0.109743
 H 2.828888 2.598559 1.610855
 H 0.940079 1.025473 1.582516
 H -0.194102 0.697859 -2.134687
 H -0.373622 -2.999213 -0.061907
 H -1.065333 0.295356 2.048614
 H -1.380081 -1.729078 0.580783

(3-4)_{syn} (si-si)₃₀₀

E₀ = -1148.0167429
 E_{0+ZPE} = -1147.607740
 E₂₉₈ = -1147.586264
 H₂₉₈ = -1147.585320
 G₂₉₈ = -1147.658285
 NImag = 1 (-340.4886)
 C -2.493722 -1.545946 -0.314464
 C -2.380068 -0.364536 0.421123
 C -3.536094 0.360834 0.712040
 C -4.781290 -0.088617 0.295987
 C -4.886799 -1.267807 -0.426553
 C -3.738215 -1.988866 -0.732229
 C -1.088901 0.126869 0.935617
 C -0.209812 -0.757202 1.540508
 N 0.719910 -0.309170 2.440631
 O 1.382548 -1.136655 3.081219
 O 0.871155 0.909478 2.632194
 C 1.181486 2.632460 0.008639
 C 0.948711 1.244809 -0.524490
 C -0.304268 0.884955 -1.001417
 C -1.286792 1.927921 -1.455404
 C -1.137344 3.249410 -0.722587
 C 0.318438 3.671167 -0.693174
 N 1.940302 0.346266 -0.457123
 C 3.191969 0.600864 0.251340
 C 4.052111 -0.601774 -0.080249

C -2.500746 0.931038 -0.693857
 N -3.819494 0.688227 -0.391439
 O -4.615762 0.568537 -1.333390
 O -4.199070 0.614679 0.782035
 C -1.063478 -2.075398 -0.954477
 C -0.066603 -1.400086 -0.065825
 C -0.562448 -0.805282 1.090474
 C -1.714959 -1.445241 1.830133
 C -2.663276 -2.258510 0.960369
 C -1.931419 -3.020425 -0.126883
 N 1.236517 -1.402565 -0.385969
 C 1.755188 -1.944996 -1.643476
 C 3.245103 -2.114480 -1.402329
 C 3.319265 -2.327992 0.100140
 C 2.288827 -1.335441 0.638815
 C 2.973641 0.033328 0.868063
 O 3.384353 0.634118 -0.139923
 O 3.122272 0.345068 2.067872
 H 1.862422 -1.661499 1.582666
 H 4.310636 -2.151620 0.510883
 H 3.020200 -3.345997 0.355969
 H 3.649647 -2.946050 -1.975682
 H 3.774427 -1.203254 -1.662850
 H 1.302697 -2.914308 -1.850583
 H 1.530487 -1.280845 -2.476084
 H -1.923848 1.168292 1.301811
 H -2.643641 -3.521813 -0.782591
 H -1.301077 -3.798489 0.309613
 H -3.228775 -2.947060 1.589500
 H -3.393999 -1.598183 0.500297
 H -1.278245 -2.105005 2.588029
 H -2.279021 -0.695987 2.385502
 H -0.314611 2.691411 2.023540
 H 1.466871 4.330005 1.587463
 H 2.435970 4.529997 -0.680386
 H 1.635657 3.047957 -2.487422
 H -0.147762 1.427914 -2.062611
 H -0.595038 -2.609603 -1.772653
 H 0.156032 -0.303369 1.725931
 H -2.323557 1.043068 -1.747351
 H -1.705094 -1.306273 -1.397461

(3-4)_{syn} (si-re)₆₀

E₀ = -1148.0205551
 E_{0+ZPE} = -1147.611731
 E₂₉₈ = -1147.590099
 H₂₉₈ = -1147.589155
 G₂₉₈ = -1147.662709
 NImag = 1 (-344.8445)
 C -2.233871 1.758860 -0.504187
 C -2.249112 0.365115 -0.405145
 C -3.434836 -0.262240 -0.014421
 C -4.569313 0.482574 0.269213
 C -4.542961 1.866624 0.164723
 C -3.370555 2.500564 -0.225147
 C -1.023653 -0.375575 -0.757463
 C -1.128386 -1.679121 -1.233682
 N -0.144495 -2.246666 -1.992339
 O -0.334069 -3.394200 -2.439709
 O 0.903254 -1.630683 -2.236227
 C 1.456528 -2.102527 0.961388
 C 1.181959 -0.631253 0.881193
 C -0.081644 -0.167476 1.247594
 C -0.927639 -0.931406 2.228767
 C -0.680358 -2.430631 2.212088
 C 0.805192 -2.729633 2.187032
 N 2.138262 0.179381 0.435868
 C 3.322901 -0.289031 -0.272380
 C 4.011913 0.993098 -0.701175

C 4.075519 0.399077 0.450084
 C 2.629127 0.856271 0.282793
 C 2.412510 1.390733 -1.154617
 O 1.737096 0.701266 -1.942195
 O 2.987586 2.471072 -1.374252
 H 2.377053 1.655457 0.975869
 H 4.757553 1.036154 -0.103883
 H 4.358619 0.420378 1.503540
 H 4.870419 -1.637012 0.263425
 H 3.975037 -1.050479 -1.138169
 H 2.905175 -1.954602 1.538833
 H 2.240508 -2.307646 -0.058347
 H -0.420289 1.045918 -1.152975
 H -1.128302 -2.314188 3.366819
 H -0.087106 -0.990367 3.848479
 H -2.421965 -0.195825 3.611339
 H -2.460798 -0.777242 1.959438
 H -0.779039 1.484118 3.094555
 H -2.007601 1.593151 1.863152
 H 0.448479 -0.937082 -1.912393
 H 0.207813 -3.219286 -2.572827
 H -1.864438 -4.554228 -2.015644
 H -3.690103 -3.392158 -0.815400
 H -3.456076 -1.049173 -0.178139
 H 0.994260 -2.263026 2.083931
 H 0.267720 1.708413 0.846484
 H -3.409969 1.055325 -0.352101
 H -0.408322 -2.154612 1.051613

(3-4)_{syn} (si-re)₃₀₀

E₀ = -1148.0156059
 E_{0+ZPE} = -1147.606520
 E₂₉₈ = -1147.585046
 H₂₉₈ = -1147.584102
 G₂₉₈ = -1147.656939
 NImag = 1 (-376.4372)
 C -3.100092 -0.419256 -0.836168
 C -1.785578 0.027291 -0.979975
 C -0.949084 -0.619184 -1.891853
 C -1.428456 -1.685166 -2.638282
 C -2.740851 -2.118971 -2.496007
 C -3.577449 -1.480120 -1.591733
 C -1.340284 1.191467 -0.196629
 C -0.619399 2.196356 -0.822752
 N -0.470649 3.411966 -0.213700
 O 0.107844 4.320874 -0.826990
 O -0.918612 3.591646 0.930691
 C -0.646199 -1.958648 1.477467
 C 0.284058 -0.817051 1.176292
 C -0.117455 0.479461 1.508380
 C -1.060694 0.702238 2.664680
 C -2.089754 -0.401855 2.818016
 C -1.417667 -1.758771 2.775219
 N 1.435734 -1.094050 0.560741
 C 1.830547 -2.443337 0.149869
 C 3.273327 -2.296916 -0.303198
 C 3.758722 -1.103877 0.502321
 C 2.557151 -0.161625 0.446073
 C 2.631945 0.661375 -0.863277
 O 2.045260 0.209473 -1.866235
 O 3.350996 1.672494 -0.783098
 H 2.541589 0.525916 1.286535
 H 4.655292 -0.640509 0.100488
 H 3.955822 -1.395221 1.535242
 H 3.843814 -3.204383 -0.118718
 H 3.314719 -2.068705 -1.365028
 H 1.776497 -3.122608 1.000985
 H 1.173346 -2.821130 -0.630304
 H -2.027967 1.519675 0.568849

C 3.594116 -0.948763 -1.486246
 C 2.082591 -0.767792 -1.419404
 C 1.349369 -2.090297 -1.052949
 O 0.249914 -2.259104 -1.625025
 O 1.929627 -2.873327 -0.285211
 H 1.666392 -0.430311 -2.366464
 H 3.862925 -1.957470 -1.785728
 H 4.018699 -0.245431 -2.205072
 H 5.112707 -0.368427 -0.013990
 H 3.824613 -1.429853 0.585378
 H 3.663406 1.510923 -0.124498
 H 2.999159 0.731809 1.315048
 H -1.114310 1.118115 1.363553
 H 0.435137 4.629205 -0.186003
 H 0.673890 3.811187 -1.716791
 H -1.748474 4.013699 -1.203599
 H -1.504832 3.153049 0.301470
 H -1.149072 2.096697 -2.528703
 H -2.302676 1.547173 -1.350439
 H -3.458953 1.278626 1.278753
 H -5.666118 0.483819 0.535741
 H -5.854098 -1.619491 -0.756115
 H -3.811709 -2.901271 -1.307280
 H -1.597170 -2.084929 -0.596514
 H 2.229776 2.900674 -0.097561
 H -0.384718 -0.093243 -1.460366
 H -0.204775 -1.820858 1.395254
 H 0.969849 2.627359 1.077441

(3-4)_{syn} (re-si)₆₀

E₀ = -1148.0219491
 E_{0+ZPE} = -1147.613068
 E₂₉₈ = -1147.591426
 H₂₉₈ = -1147.590482
 G₂₉₈ = -1147.664415
 NImag = 1 (-349.8379)
 C 3.440813 0.962604 -0.129915
 C 2.126256 0.719523 -0.531624
 C 1.888568 -0.236939 -1.522532
 C 2.946321 -0.932005 -2.086096
 C 4.252353 -0.684956 -1.679164
 C 4.496661 0.267273 -0.699870
 C 1.046977 1.525142 0.051423
 C 0.008728 1.964686 -0.750360
 N -0.782661 3.002425 -0.347285
 O -1.659213 3.418429 -1.119490
 O -0.631098 3.503599 0.780321
 C 0.280116 0.278935 1.759307
 C -0.468068 -0.715005 1.129531
 C 0.155228 -2.057170 0.877713
 C 1.120971 -2.451038 1.985517
 C 2.162485 -1.372866 2.199092
 C 1.504298 -0.053029 2.570127
 N -1.718606 -0.506394 0.716226
 C -2.526462 0.629477 1.152176
 C -3.728982 0.584418 0.235181
 C -3.938016 -0.906858 0.042753
 C -2.517178 -1.469935 -0.041122
 C -2.067428 -1.700571 -1.508100
 O -1.190379 -0.960074 -1.984844
 O -2.667442 -2.641545 -0.062249
 H -2.484786 -2.444790 0.440844
 H -4.512560 -1.161477 -0.842479
 H -4.452972 -1.323449 0.908958
 H -4.590490 1.089231 0.665953
 H -3.488822 1.065215 -0.711543
 H -2.820943 0.474614 2.195505
 H -1.986275 1.565783 1.100771
 H 1.344439 2.192782 0.846266

C 3.632324 1.963878 0.405613
 C 2.166438 1.619850 0.677669
 C 1.248333 2.497897 -0.202306
 O 0.929078 2.071325 -1.327273
 O 0.950131 3.591490 0.316161
 H 1.894227 1.804245 1.715227
 H 3.757794 3.008078 0.131967
 H 4.231794 1.772499 1.296686
 H 5.086234 0.861848 -0.808659
 H 3.605794 1.333766 -1.651002
 H 3.967807 -0.864251 0.395936
 H 3.027316 -0.925515 -1.104237
 H -0.223059 0.230690 -1.164872
 H 0.982136 -3.805080 2.171388
 H 1.278386 -2.343658 3.092845
 H -1.150972 -2.891968 3.080798
 H -1.142743 -2.872957 1.328897
 H -0.720889 -0.546011 3.233039
 H -1.982492 -0.718544 2.050364
 H -3.481783 -1.338176 0.067551
 H -5.477180 -0.020963 0.569867
 H -5.429155 2.445276 0.383285
 H -3.339188 3.577262 -0.313622
 H -1.317422 2.248057 -0.808619
 H 2.526413 -2.290543 0.963959
 H -0.214322 0.905283 1.274837
 H -1.979089 -2.319886 -1.096176
 H 1.057314 -2.579317 0.065987

(3-4)_{syn} (re-si)₁₈₀

E₀ = -1148.0209693
 E_{0+ZPE} = -1147.612587
 E₂₉₈ = -1147.590664
 H₂₉₈ = -1147.589720
 G₂₉₈ = -1147.665899
 NImag = 1 (-342.8930)
 N 1.537915 -0.871009 -0.746956
 C 2.071763 0.283338 -1.467423
 C 3.485698 0.431436 -0.938724
 C 3.865586 -0.991001 -0.567566
 C 2.576002 -1.554936 0.017418
 C 2.472005 -1.349747 1.554416
 O 1.503721 -0.704525 1.992674
 C 0.259078 -1.230907 -0.807302
 C -0.721360 -0.426029 -1.393454
 C -1.189343 -3.237311 -1.091052
 O 3.393947 -1.892992 2.191351
 C -1.350841 -0.727559 0.454566
 H 2.528934 -2.627850 -0.151771
 H 4.677332 -1.059658 0.149254
 H 4.147081 -1.549055 -1.461335
 H 4.149672 0.880698 -1.673421
 H 3.485938 1.064270 -0.052039
 H 2.062309 0.067629 -2.539008
 H 1.474865 1.171526 -1.294882
 H -0.860955 0.039417 1.126556
 C -0.159558 -2.542029 -0.210127
 C -1.993586 -1.016327 -1.927733
 H -2.806652 -0.294756 -1.803604
 H -1.879017 -1.149067 -3.008897
 C -2.395081 -2.344702 -1.302979
 H -3.132654 -2.836944 -1.937731
 H -2.865481 -2.175442 -0.336349
 H -0.734019 -3.495085 -2.050739
 H -1.485640 -4.174577 -0.620098
 C -0.613639 1.976611 0.196306
 C 0.552565 2.223304 0.921793
 C 1.243460 3.415775 0.758353
 C 0.790579 4.370636 -0.140329

H	-2.150455	-2.559483	2.876212	H	2.232079	0.758703	2.492785	C	-0.364812	4.127311	-0.874994
H	-0.731574	-1.851459	3.620238	H	1.219936	-0.083934	3.627489	C	-1.063644	2.944308	-0.705063
H	-2.634901	-0.274980	3.753766	H	2.864069	-1.664404	2.981496	H	0.921270	1.455524	1.589770
H	-2.824921	-0.340419	2.014411	H	2.740747	-1.258162	1.282777	H	2.142315	3.594647	1.331569
H	-0.475999	0.774229	3.588493	H	0.564191	-2.620753	2.910196	H	1.331568	5.297002	-0.270936
H	-1.547317	1.670487	2.549224	H	1.594580	-3.397210	1.724004	H	-0.722305	4.863697	-1.580795
H	0.085574	-0.306538	-1.985669	H	0.870519	-0.450486	-1.826821	H	-1.956717	2.767636	-1.287792
H	-0.770283	-2.181366	-3.338003	H	2.749235	-1.673365	-2.847672	H	-0.378843	0.441274	-1.937787
H	-3.107673	-2.947694	-3.084866	H	5.072809	-1.228878	-2.125148	H	0.696770	-3.189228	-0.055335
H	-4.601509	-1.804956	-1.474071	H	5.508902	0.472195	-0.381423	H	-0.585793	-2.344200	0.773584
H	-3.757806	0.078713	-0.137178	H	3.636305	1.712058	0.624272	C	-2.734025	0.764329	0.483357
H	-0.103854	-2.897222	1.522555	H	-0.257734	1.149494	2.106101	H	-3.335849	1.529466	0.028625
H	0.609257	1.265942	1.370956	H	-0.612713	-2.817443	0.774435	N	-3.468881	-0.186150	1.144946
H	-0.091875	2.088756	-1.751903	H	-0.277100	1.519328	-1.684620	O	-2.910585	-1.118899	1.734540
H	-1.346009	-2.048808	0.642901	H	0.678678	-2.020667	-0.078857	O	-4.704890	-0.071899	1.146493

Optimized Geometries in solven phase with **enaine-DBU (lowest energy)** carboxylate Pathway

(3-4)DBU-anti (re-re)₆₀

E ₀	= -1610.5785535		
E _{0+ZPE}	= -1609.901588		
E ₂₉₈	= -1609.868146		
H ₂₉₈	= -1609.867201		
G ₂₉₈	= -1609.971049		
NImag	= 1 (-315.4675)		
N	-5.757593	-0.037396	0.781615
C	-6.152658	-1.245690	1.499694
C	-4.944349	-1.983455	2.028951
C	-3.943287	-2.181030	0.916710
N	-3.687942	-0.912466	0.270528
C	-4.557630	0.061683	0.227942
C	-4.158011	1.306074	-0.500327
C	-4.924341	1.532874	-1.804092
C	-6.320199	2.201280	-1.618100
C	-7.248429	1.248017	-0.770806
C	-6.758208	1.017160	0.649758
O	-1.314090	-0.502414	-0.844113
C	-0.430439	-1.290330	-0.402415
O	-0.582297	-2.150924	0.469739
C	0.935808	-1.129767	-1.093339
N	2.022680	-1.765456	-0.363737
C	2.379246	-3.057799	-0.938647
C	1.386536	-3.258256	-2.073364
C	0.968647	-1.843749	-2.441402
C	2.516852	-1.292060	0.781214
C	2.271346	0.015561	1.183700
C	2.646811	0.494350	2.555722
C	3.812268	-0.272964	3.152321
C	3.559144	-1.761772	3.031914
C	3.429220	-2.184909	1.577367
H	1.122725	-0.069066	-1.214527
H	0.011051	-1.791121	-2.951765
H	1.725517	-1.382704	-3.074140
H	1.830442	-3.798603	-2.905692
H	0.527145	-3.824745	-1.720258
H	3.409266	-3.014567	-1.300157
H	2.311988	-3.852407	-0.199926
H	2.641043	-2.012036	3.567867
H	4.361435	-2.334737	3.496196
H	1.436580	0.529005	0.732012
H	3.052588	-3.204485	1.532275
H	-2.739360	-0.761094	-0.163574
H	-6.736196	-1.883288	0.833844
H	-6.798584	-0.942277	2.319304
H	-7.591202	0.710761	1.273964
H	-6.370931	1.943633	1.075641
H	-8.215816	1.746551	-0.704831

(3-4)DBU-anti (re-re)₁₈₀

E ₀	= -1610.5755987		
E _{0+ZPE}	= -1609.898545		
E ₂₉₈	= -1609.865139		
H ₂₉₈	= -1609.864195		
G ₂₉₈	= -1609.966997		
NImag	= 1 (-351.9992)		
N	-5.184031	0.089958	0.764276
C	-5.700550	-0.911277	1.692038
C	-4.621662	-1.899086	2.073235
C	-3.980352	-2.457497	0.825675
N	-3.595035	-1.368583	-0.044520
C	-4.166378	-0.192473	-0.034728
C	-3.646331	0.832843	-0.989447
C	-4.628770	1.174711	-2.111020
C	-5.730486	2.103985	-1.706422
C	-6.613604	1.660008	-0.567166
C	-5.861872	1.382405	0.724822
O	-1.362789	-1.626362	-1.479773
C	-0.439185	-2.032062	-0.721867
O	-0.568743	-2.663710	0.330812
C	0.974331	-1.693649	-1.234302
N	1.996080	-1.805674	-0.205917
C	2.748993	-3.053705	-0.321823
C	2.075716	-3.795940	-1.466537
C	1.437375	-2.691184	-2.291861
C	2.133276	-0.924927	0.783282
C	1.396680	0.259124	0.837085
C	1.269174	1.020376	2.121448
C	2.468106	0.874473	3.039282
C	2.857171	-0.583213	3.172426
C	3.186342	-1.191119	1.817331
H	0.943850	-0.685501	-1.635509
H	0.614060	-3.032959	-2.912556
H	2.176637	-2.222137	-2.940878
H	2.785254	-4.394853	-2.031913
H	1.308093	-4.460695	-1.076116
H	3.795730	-2.838248	-0.538430
H	2.704110	-3.624097	0.602432
H	2.035218	-1.140758	3.626443
H	3.718243	-0.698798	3.830244
H	0.523676	0.322923	0.204293
H	3.350368	-2.258839	1.925220
H	-2.743550	-1.503517	-0.640997
H	-6.550845	-1.420100	1.235232
H	-6.061664	-0.386075	2.571640
H	-3.383144	1.734144	-0.435546
H	-2.727508	0.436328	-1.411364
H	-5.273800	3.089023	-1.417075

(3-4)DBU-anti (re-re)₃₀₀

E ₀	= -1610.5695515		
E _{0+ZPE}	= -1609.892685		
E ₂₉₈	= -1609.860182		
H ₂₉₈	= -1609.859238		
G ₂₉₈	= -1609.959718		
NImag	= 1 (-321.3954)		
N	5.785588	-0.810674	-0.771089
C	6.137275	-2.161536	-0.342417
C	4.899452	-2.979482	-0.054392
C	3.990659	-2.215137	0.877720
N	3.774040	-0.886140	0.350772
C	4.631319	-0.265439	-0.415491
C	4.269302	1.112536	-0.871290
C	5.132403	2.213167	-0.252646
C	6.500568	2.370083	-0.892547
C	7.373548	1.128105	-0.840912
C	6.780427	-0.079206	-1.549243
O	1.499881	0.370245	0.868381
C	0.563023	-0.398226	1.225111
O	0.627234	-1.623404	1.361549
C	-0.747982	0.342890	1.546210
N	-1.905690	-0.539469	1.596139
C	-2.283855	-0.858847	2.972978
C	-1.215029	-0.192920	3.824905
C	-0.710173	0.941037	2.949365
C	-2.415729	-1.133701	0.516306
C	-2.081798	-0.761496	-0.784212
C	-2.202496	-1.746819	-1.917884
C	-3.291837	-2.789291	-1.734786
C	-3.310856	-3.313973	-0.313388
C	-3.472920	-2.175464	0.685863
H	-0.886288	1.119937	0.802571
H	0.284825	1.286818	3.214776
H	-1.388655	1.791633	2.998448
H	-1.612229	0.147916	4.777906
H	-0.411567	-0.898424	4.026553
H	-3.277292	-0.463198	3.187470
H	-2.303906	-1.932965	3.135885
H	-2.384406	-3.850655	-0.097368
H	-4.126799	-4.023541	-0.178230
H	-1.269521	-0.059133	-0.900879
H	-3.496393	-2.565129	1.697313
H	2.860320	-0.407936	0.570645
H	6.779014	-2.102630	0.537980
H	6.712807	-2.619365	-1.142340
H	4.333436	1.153928	-1.959090
H	3.229004	1.269356	-0.602172
H	6.368518	2.659291	-1.938252

H	-7.426240	0.281886	-1.246835	H	-6.353048	2.350081	-2.576444	H	7.024359	3.194889	-0.408917
H	-6.238097	3.088831	-1.157074	H	-4.052129	1.623217	-2.918636	H	4.586721	3.149871	-0.358742
H	-6.772629	2.255855	-2.597856	H	-5.057011	0.254814	-2.513056	H	5.232187	2.036600	0.819402
C	3.719971	1.053812	-0.221131	C	2.503135	1.638639	-0.526555	C	-3.733492	0.758609	-1.171075
H	4.534316	0.757782	0.422011	H	1.901059	1.220609	-1.316076	H	-3.532737	0.539178	-2.209075
C	3.208756	2.418999	-0.021666	C	3.910772	1.217895	-0.538588	C	-3.040159	1.935431	-0.628727
C	2.073509	2.898197	-0.679626	C	4.880855	1.777660	0.297305	C	-3.341870	2.484335	0.618701
C	3.895447	3.281933	0.832720	C	4.311731	0.240665	-1.451400	C	-2.073020	2.565888	-1.416020
C	1.647579	4.201895	-0.494553	C	6.201761	1.368313	0.223786	C	-2.687824	3.621866	1.065453
H	1.510939	2.244027	-1.330455	H	4.607425	2.539844	1.011526	H	-4.091467	2.028781	1.247885
C	3.470702	4.590310	1.015328	C	5.633718	-0.171318	-1.524205	C	-1.422045	3.703032	-0.970655
H	4.778357	2.927912	1.346108	H	3.578295	-0.188848	-2.118244	H	-1.834756	2.156209	-2.388003
C	2.345338	5.055199	0.352646	C	6.585024	0.389621	-0.684674	C	-1.723937	4.234164	0.276961
H	0.765465	4.553626	-1.010070	H	6.935835	1.816016	0.878248	H	-2.934849	4.033335	2.033598
H	4.021077	5.244309	1.676326	H	5.921399	-0.925182	-2.242999	H	-0.680103	4.176822	-1.597153
H	2.010833	6.072536	0.495191	H	7.616417	0.072945	-0.740484	H	-1.216620	5.120878	0.628472
C	3.693091	0.488486	-1.481678	C	2.146082	2.910247	-0.105174	C	-5.002993	0.426778	-0.728355
H	3.108071	0.853566	-2.305505	H	2.766790	3.575840	0.464788	H	-5.422988	0.714839	0.217194
N	4.449003	-0.613181	-1.784088	N	0.890768	3.396432	-0.355580	N	-5.880407	-0.275488	-1.516121
O	5.159151	-1.140600	-0.917777	O	0.056264	2.690509	-0.938629	O	-5.559678	-0.636633	-2.654895
O	4.413880	-1.055737	-2.942195	O	0.616132	4.548634	0.015135	O	-7.007475	-0.516622	-1.059052
H	4.406360	-2.193059	1.095840	H	4.124296	-0.771721	1.440095	H	-4.436098	-1.677106	0.516057
H	3.950118	0.011252	4.195655	H	2.241538	1.300620	4.016738	H	-3.134224	-3.607276	-2.438767
H	4.737261	-0.018008	2.630080	H	3.311999	1.437012	2.637672	H	-4.258832	-2.349450	-1.974369
H	2.869940	1.561799	2.521160	H	1.100398	2.075891	1.893354	H	-2.347053	-1.216380	-2.860262
H	1.780022	0.399784	3.218090	H	0.367017	0.683216	2.642083	H	-1.236129	-2.254226	-2.012850
H	-2.988622	-2.552570	1.277201	H	-3.867021	-1.400308	2.680766	H	3.015076	-2.681388	0.979668
H	-4.322169	-2.891888	0.180762	H	-3.077296	-3.018390	1.049019	H	4.431479	-2.143157	1.873177
H	-4.488927	-1.413141	2.837964	H	-4.670204	-3.117354	0.297816	H	4.375062	-3.193016	-0.985326
H	-5.256629	-2.942903	2.433520	H	-5.055462	-2.698888	2.668109	H	5.188868	-3.928441	0.389865
H	-4.289863	2.161958	0.162293	H	-7.356210	2.429490	-0.354139	H	8.326281	1.351578	-1.321495
H	-3.096160	1.219871	-0.710644	H	-7.166057	0.763948	-0.856758	H	7.599607	0.857945	0.192411
H	-4.340161	2.229227	-2.404251	H	-5.141918	2.176606	0.924890	H	6.353017	0.212949	-2.509369
H	-4.963453	0.601122	-2.370229	H	-6.558514	1.373694	1.556743	H	7.568155	-0.793925	-1.763066

(3-4)DBU-anti (si-si)₆₀

$E_0 = -1610.5719208$
 $E_{0+ZPE} = -1609.894553$
 $E_{298} = -1609.861364$
 $H_{298} = -1609.860420$
 $G_{298} = -1609.963376$
 $N\text{Imag} = 1 (-337.2864)$

N	6.174931	0.425978	-0.462095
C	6.549935	-0.001052	-1.807061
C	5.325920	-0.283515	-2.647252
C	4.402953	-1.218941	-1.904069
N	4.170495	-0.704722	-0.572686
C	5.014267	0.063911	0.064011
C	4.629033	0.513689	1.437440
C	5.479652	-0.102251	2.549373
C	6.841157	0.546152	2.728571
C	7.733266	0.502896	1.500097
C	7.152891	1.209850	0.285914
O	1.838338	-1.205450	0.599924
C	0.876541	-1.202983	-0.217887
O	0.952264	-1.127123	-1.447617
C	-0.502526	-1.347603	0.452891
N	-1.621036	-0.998534	-0.411605
C	-2.247546	-2.184016	-0.994070
C	-1.381311	-3.338747	-0.516836
C	-0.779726	-2.813648	0.777180
C	-1.934980	0.241996	-0.777911
C	-1.087067	1.381822	-0.316930
C	-0.932604	2.437511	-1.404544
C	-2.284769	2.924751	-1.885556
C	-3.142487	1.771034	-2.376371
C	-3.086522	0.541711	-1.505750
H	-0.508245	-0.734867	1.350295
H	0.121236	-3.336725	1.084606

(3-4)DBU-anti (si-si)₁₈₀

$E_0 = -1610.5767092$
 $E_{0+ZPE} = -1609.899693$
 $E_{298} = -1609.866228$
 $H_{298} = -1609.865283$
 $G_{298} = -1609.970212$
 $N\text{Imag} = 1 (-361.8048)$

N	6.279350	-0.673384	-0.780928
C	6.474953	-2.119220	-0.732121
C	5.148566	-2.843896	-0.718629
C	4.270994	-2.275392	0.369942
N	4.219928	-0.835607	0.239613
C	5.171426	-0.124519	-0.305462
C	4.980466	1.357787	-0.349686
C	5.924885	2.120647	0.580961
C	7.329179	2.302328	0.031388
C	8.066142	1.011188	-0.280803
C	7.372701	0.135115	-1.311831
O	2.019424	0.444303	1.037234
C	1.010223	-0.311806	0.993766
O	0.996369	-1.509125	0.693084
C	-0.304160	0.391006	1.385977
N	-1.494356	-0.400515	1.109219
C	-1.990334	-1.068904	2.308285
C	-0.970727	-0.724620	3.382271
C	-0.380374	0.589792	2.897318
C	-2.017287	-0.590688	-0.098170
C	-1.349701	0.069427	-1.266932
C	-1.554329	-0.690547	-2.569023
C	-3.015874	-1.022346	-2.791068
C	-3.553472	-1.852320	-1.639960
C	-3.200347	-1.308224	-0.288586
H	-0.346744	1.341481	0.860950
H	0.592902	0.816141	3.322391

(3-4)DBU-anti (si-si)₃₀₀

$E_0 = -1610.5784044$
 $E_{0+ZPE} = -1609.900719$
 $E_{298} = -1609.867586$
 $H_{298} = -1609.866642$
 $G_{298} = -1609.968582$
 $N\text{Imag} = 1 (-340.0630)$

N	6.479740	-0.988668	-0.028452
C	6.616337	-2.092449	0.916909
C	5.268123	-2.690183	1.247724
C	4.318237	-1.596303	1.671157
N	4.336490	-0.536307	0.686911
C	5.355585	-0.290126	-0.092954
C	5.219068	0.841212	-1.061755
C	6.111658	2.041084	-0.740867
C	7.562455	1.872920	-1.158195
C	8.275042	0.688219	-0.528327
C	7.641232	-0.656880	-0.847234
O	2.131895	0.902467	0.354641
C	1.090796	0.264113	0.672315
O	1.040244	-0.881497	1.132386
C	-0.210630	1.061033	0.464690
N	-1.420236	0.277936	0.651180
C	-1.939724	0.404057	2.011512
C	-0.989121	1.379974	2.692816
C	-0.359665	2.139498	1.534570
C	-1.897798	-0.601131	-0.226083
C	-1.120013	-0.846590	-1.489051
C	-1.444792	-2.190693	-2.122071
C	-2.942710	-2.394006	-2.236114
C	-3.578426	-2.371015	-0.857458
C	-3.136600	-1.201789	-0.025427
H	-0.195564	1.491715	-0.533842
H	0.593942	2.596901	1.780583

H	-1.505357	-2.877735	1.587217	H	-1.052693	1.416684	3.125361	H	-1.032963	2.912759	1.168320
H	-1.961146	-4.247941	-0.377909	H	-1.427653	-0.651101	4.365759	H	-1.509389	2.029523	3.392667
H	-0.594414	-3.543084	-1.239843	H	-0.198203	-1.489738	3.424692	H	-0.225873	0.834925	3.244931
H	-3.269935	-2.283956	-0.637208	H	-2.979502	-0.691184	2.565648	H	-2.958851	0.781450	1.990207
H	-2.271911	-2.093029	-2.078972	H	-2.074076	-2.140340	2.135203	H	-1.951231	-0.573617	2.493160
H	-2.809071	1.480011	-3.378543	H	-3.173309	-2.875672	-1.718379	H	-3.326795	-3.298224	-0.332114
H	-4.176152	2.098734	-2.495640	H	-4.640879	-1.935656	-1.713641	H	-4.666419	-2.371160	-0.939044
H	-0.112092	1.046257	0.018558	H	-0.287240	0.184828	-1.077860	H	-0.057552	-0.796042	-1.267770
H	-3.654706	-0.295654	-1.885051	H	-3.535226	-1.922934	0.534586	H	-3.546712	-1.165521	0.972648
H	-1.592752	1.828196	0.548760	H	-1.765632	1.077455	-1.355615	H	-1.343275	-0.040552	-2.186832
H	3.245987	-0.918367	-0.119082	H	3.350065	-0.343093	0.563000	H	3.457029	0.029873	0.561319
H	7.187951	-0.883456	-1.738326	H	7.065182	-2.371913	0.150030	H	7.114623	-1.733722	1.818812
H	7.135574	0.798068	-2.253083	H	7.050623	-2.400932	-1.609499	H	7.258598	-2.838733	0.457635
H	7.949311	1.432380	-0.416355	H	5.108202	1.703635	-1.375741	H	8.361283	-1.449061	-0.670754
H	6.713172	2.165436	0.574495	H	3.949825	1.552098	-0.067811	H	7.369365	-0.707651	-1.902311
H	8.679155	0.989685	1.738738	H	7.271619	2.898743	-0.882591	H	5.434767	0.457461	-2.066213
H	7.970509	-0.528260	1.231205	H	7.915057	2.884857	0.742671	H	4.176786	1.145967	-1.046095
H	6.697781	1.590282	3.017872	H	5.486726	3.102825	0.752928	H	5.694912	2.900900	-1.263601
H	7.355194	0.064114	3.560400	H	5.954964	1.624318	1.552362	H	6.044890	2.270081	0.323789
C	-4.507440	0.968586	0.190173	C	-4.784058	0.158821	0.183321	C	-4.430043	0.515612	-0.690986
H	-5.095426	1.045286	-0.574969	H	-4.658246	-0.134615	1.211858	H	-4.235530	0.253933	-1.720005
C	-4.887161	-0.419687	0.490977	C	-4.271691	1.499418	-0.135203	C	-5.688746	0.001678	-0.126301
C	-5.822529	-1.052352	-0.332160	C	-3.566433	2.196084	0.847768	C	-6.601414	-0.635549	-0.966909
C	-4.386501	-1.121474	1.588723	C	-4.489485	2.129534	-1.363325	C	-6.022104	0.157431	1.221263
C	-6.237853	-2.347439	-0.075721	C	-3.086025	3.475455	0.613267	C	-7.817167	-1.094803	-0.479971
H	-6.226724	-0.516674	-1.180193	H	-3.406921	1.731441	1.809977	H	-6.362306	-0.757611	-2.013995
C	-4.797237	-2.421293	1.841720	C	-4.011459	3.407985	-1.597768	C	-7.232646	-0.303779	1.707872
H	-3.673711	-0.658315	2.254127	H	-5.036368	1.622292	-2.143952	H	-5.323756	0.631349	1.896587
C	-5.719748	-3.041470	1.010700	C	-3.305056	4.086719	-0.612496	C	-8.137144	-0.931432	0.858816
H	-6.966428	-2.815590	-0.721848	H	-2.547270	3.996612	1.391708	H	-8.512722	-1.579867	-1.149582
H	-4.396890	-2.950375	2.694619	H	-4.192581	3.878084	-2.553718	H	-7.471562	-0.176904	2.754031
H	-6.039014	-4.053652	1.212698	H	-2.935111	5.084649	-0.798123	H	-9.081429	-1.291151	1.241026
C	-4.043822	1.800887	1.197338	C	-5.920635	-0.334529	-0.443021	C	-3.949562	1.742734	-0.268509
H	-3.592537	1.468987	2.113272	H	-6.349207	0.046949	-1.350691	H	-4.271371	2.252102	0.620587
N	-4.181398	3.163258	1.125587	N	-6.561515	-1.434256	0.058346	N	-3.030182	2.442906	-1.003242
O	-4.723040	3.695439	0.148567	O	-6.114703	-2.010028	1.061307	O	-2.568897	1.965724	-2.048517
O	-3.763809	3.841359	2.076441	O	-7.589042	-1.834446	-0.511153	O	-2.694806	3.569523	-0.606908
H	-0.345283	3.267197	-1.011719	H	-3.586368	-0.096880	-2.878675	H	-0.968359	-2.244801	-3.100782
H	-0.366790	2.012818	-2.236159	H	-3.145951	-1.562233	-3.729204	H	-1.016600	-2.993031	-1.517112
H	-2.798648	3.437608	-1.074415	H	-1.161303	-0.093515	-3.391718	H	-3.367599	-1.603455	-2.858723
H	-2.161350	3.653048	-2.687751	H	-0.970905	-1.612905	-2.539856	H	-3.166346	-3.339052	-2.731378
H	4.806140	0.649190	-2.864030	H	4.657214	-2.728976	-1.684447	H	3.291405	-1.943308	1.743044
H	5.630616	-0.722704	-3.593760	H	5.317805	-3.905027	-0.554814	H	4.605218	-1.192558	2.643185
H	3.433190	-1.305308	-2.385700	H	3.248254	-2.635666	0.309223	H	4.870562	-3.205647	0.374049
H	4.836923	-2.217585	-1.836856	H	4.661016	-2.535855	1.354991	H	5.382195	-3.422765	2.042755
H	4.919290	-0.002147	3.477965	H	9.052478	1.259714	-0.673497	H	8.335028	-8.005558	0.555315
H	5.589420	-1.173133	2.371424	H	8.228801	0.429736	0.628504	H	9.300774	0.661773	-0.897155
H	4.685429	1.601776	1.482270	H	7.006928	0.740315	-2.142213	H	7.603954	1.765941	-2.245067
H	3.588009	0.237872	1.578016	H	8.084982	-0.569691	-1.728402	H	8.107359	2.786400	-0.918478

(3-4)DBU-anti (si-re)₆₀

E_0	= -1610.5747416		
E_{0+ZPE}	= -1609.897845		
E_{298}	= -1609.864429		
H_{298}	= -1609.863484		
G_{298}	= -1609.967326		
NImag	= 1 (-345.2359)		
N	-6.484303	-0.496091	0.834827
C	-6.663371	-1.908035	1.158554
C	-5.329636	-2.594345	1.343645
C	-4.444037	-2.310182	0.154685
N	-4.406979	-0.884230	-0.083805
C	-5.373248	-0.071104	0.250971
C	-5.194596	1.377330	-0.072485
C	-6.126891	1.872076	-1.179489
C	-7.542581	2.168705	-0.716104
C	-8.274976	0.987549	-0.102226
C	-7.596157	0.403539	1.126498
O	-2.196803	0.155503	-1.115613

(3-4)DBU-anti (si-re)₁₈₀

E_0	= -1610.57384		
E_{0+ZPE}	= -1609.896772		
E_{298}	= -1609.863402		
H_{298}	= -1609.862458		
G_{298}	= -1609.967056		
NImag	= 1 (-339.5862)		
N	6.379422	0.700361	-0.397325
C	6.638728	0.672428	-1.833627
C	5.345491	0.693022	-2.615619
C	4.427396	-0.391215	-2.106013
N	4.313882	-0.284152	-0.667988
C	5.239722	0.236255	0.093366
C	4.981634	0.266818	1.565596
C	5.875066	-0.687602	2.359824
C	7.276700	-0.161351	2.614717
C	8.078195	0.153552	1.363441
C	7.441928	1.204486	0.467557
O	2.033112	-1.049406	0.477092

(3-4)DBU-anti (si-re)₃₀₀

E_0	= -1610.5749458		
E_{0+ZPE}	= -1609.896934		
E_{298}	= -1609.863962		
H_{298}	= -1609.863018		
G_{298}	= -1609.964731		
NImag	= 1 (-334.7702)		
N	6.299806	-0.740119	0.527474
C	6.616906	-0.297007	1.882455
C	5.358110	-0.036634	2.677257
C	4.440780	0.871340	1.894531
N	4.264129	0.338172	0.561772
C	5.148876	-0.411423	-0.040671
C	4.821495	-0.879153	-1.423213
C	5.694631	-0.251073	-2.510272
C	7.075462	-0.869471	-2.638443
C	7.925051	-0.795613	-1.381340
C	7.322354	-1.505272	-0.179626
O	1.963487	0.814608	-0.690151

C	-1.170093	-0.519723	-0.826058	C	1.058537	-0.929855	-0.315499	C	1.018812	0.993895	0.127178
O	-1.140522	-1.584662	-0.201170	O	1.103975	-0.561103	-1.493194	O	1.092878	0.965021	1.359620
C	0.139306	0.093866	-1.354830	C	-0.294046	-1.337355	0.298395	C	-0.331349	1.300249	-0.547899
N	1.338269	-0.566878	-0.868940	N	-1.448411	-0.852404	-0.446034	N	-1.469181	1.259637	0.358790
C	1.915821	-1.457149	-1.865419	C	-1.993604	-1.882165	-1.329131	C	-1.766856	2.586884	0.899492
C	0.904548	-1.452575	-2.999303	C	-1.048513	-3.061615	-1.162296	C	-0.769882	3.511625	0.211874
C	0.248193	-0.087538	-2.867667	C	-0.466488	-2.852513	0.226879	C	-0.367363	2.744221	-1.038645
C	1.885094	-0.363596	0.326644	C	-1.873593	0.407872	-0.445733	C	-2.035943	0.145452	0.808898
C	1.150247	0.488527	1.317832	C	-1.078835	1.433153	0.309960	C	-1.406795	-1.174496	0.479072
C	1.421360	0.069192	2.754546	C	-1.060456	2.766801	-0.424383	C	-1.588389	-2.168438	1.618208
C	2.911127	0.002822	3.021970	C	-2.469855	3.243992	-0.707951	C	-3.051868	-2.313296	1.984651
C	3.574883	-0.997284	2.090598	C	-3.239497	2.221393	-1.528111	C	-3.651520	-0.975248	2.389447
C	3.144413	-0.862792	0.656546	C	-3.055878	0.802737	-1.076485	C	-3.237554	0.176609	1.514655
H	0.157889	1.147144	-1.084493	H	-0.324931	-0.980702	1.324134	H	-0.471044	0.595475	-1.362982
H	-0.721024	-0.018337	-3.352265	H	0.472455	-3.374177	0.389963	H	0.587165	3.054848	-1.453063
H	0.894509	0.685642	-3.281888	H	-1.174604	-3.175938	0.988983	H	-1.129615	2.840655	-1.809864
H	1.376985	-1.609538	-3.965792	H	-1.567366	-4.011229	-1.266859	H	-1.209143	4.480439	-0.011459
H	0.168895	-2.240865	-2.849457	H	-0.259033	-3.020060	-1.909536	H	0.098264	3.671480	0.848002
H	2.881855	-1.074729	-2.199153	H	-3.004935	-2.141600	-1.026185	H	-2.793657	2.874798	0.690711
H	2.076216	-2.447733	-1.441291	H	-2.028424	-1.509950	-2.351906	H	-1.641459	2.569400	1.981494
H	3.339988	-2.011346	2.431044	H	-2.931504	2.290157	-2.576524	H	-3.347614	-0.743592	3.415512
H	4.661111	-0.915122	2.158683	H	-4.306444	2.462144	-1.517259	H	-4.740250	-1.047527	2.420915
H	0.083736	0.462143	1.119166	H	-0.063123	1.090500	0.474074	H	-0.349641	-1.047824	0.271063
H	3.567297	-1.597117	-0.013137	H	-3.538744	0.066809	-1.703605	H	-3.562817	1.145698	1.865234
H	1.472514	1.521951	1.176732	H	-1.530735	1.563729	1.297041	H	-1.865950	-1.572044	-0.428968
H	-3.527620	-0.479596	-0.500623	H	3.413101	-0.593235	-0.223123	H	3.352789	0.530299	0.073547
H	-7.240967	-2.387707	0.366920	H	7.226012	-0.214680	-2.075581	H	7.237065	0.599084	1.830336
H	-7.246165	-1.961635	2.073917	H	7.239539	1.545170	-2.074543	H	7.204347	-1.080357	2.353517
H	-8.311930	-0.187455	1.688421	H	5.110746	1.286956	1.928219	H	8.100966	-1.699082	0.551477
H	-7.256500	1.199911	1.789848	H	3.938639	0.000618	1.709808	H	6.917485	-2.475155	-0.471590
H	-5.344584	1.964185	0.834200	H	7.204355	0.746649	3.218647	H	8.889209	-1.262161	-1.584421
H	-4.160106	1.508942	-0.375740	H	7.823692	-0.888081	3.215687	H	8.129577	0.242970	-1.114456
H	-9.270169	1.314600	0.200337	H	5.388348	-0.865474	3.317736	H	6.965685	-1.918945	-2.923394
H	-8.417615	0.195747	-0.840107	H	5.915560	-1.652942	1.852575	H	7.606074	-0.382318	-3.456754
C	4.414849	0.795200	-0.227359	C	-4.538955	0.595282	0.608027	C	-4.703889	0.298241	-0.164835
H	3.865315	0.689362	-1.149633	H	-3.841139	0.889453	1.377235	H	-5.353656	0.693294	0.601148
C	5.675577	0.042884	-0.150318	C	-4.789065	-0.849840	0.502019	C	-4.961900	-1.100649	-0.531968
C	6.606456	0.220393	0.875610	C	-5.638913	-1.396264	-0.463676	C	-4.274116	-1.755708	-1.557450
C	5.976203	-0.866835	-1.166590	C	-4.195477	-1.705650	1.428744	C	-5.981936	-1.790912	0.125689
C	7.796746	-0.490614	0.880526	C	-5.875887	-2.758456	-0.503417	C	-4.581049	-3.063407	-1.892400
H	6.411569	0.918868	1.675609	H	-6.106035	-0.755767	-1.198059	H	-3.492769	-1.244084	-2.099730
C	7.167673	-1.571407	-1.166101	C	-4.439659	-3.071508	1.393234	C	-6.291645	-3.099424	-0.211575
H	5.265667	-1.016777	-1.967924	H	-3.547405	-1.295606	2.190511	H	-6.545542	-1.290860	0.900318
C	8.083423	-1.388094	-0.138200	C	-5.275804	-3.603872	0.424214	C	-5.587414	-3.743950	-1.217730
H	8.504100	-0.339321	1.683064	H	-6.531046	-3.165300	-1.260342	H	-4.035179	-3.553608	-2.685789
H	7.382300	-2.263022	-1.967944	H	-3.975972	-3.717869	2.124615	H	-7.086743	-3.612969	0.309595
H	9.013310	-1.937909	-0.132873	H	-5.465061	-4.667054	0.392082	H	-5.825488	-4.764076	-1.482105
C	4.272547	2.018247	0.404885	C	-5.559752	1.494843	0.356616	C	-4.310406	1.204820	-1.139889
H	4.877561	2.378223	1.215132	H	-6.414607	1.298806	-0.263920	H	-3.889232	0.942339	-2.092275
N	3.305502	2.904599	0.007092	N	-5.569435	2.746974	0.921376	N	-4.489604	2.545804	-0.964537
O	2.522260	2.611760	-0.906994	O	-4.680268	3.091978	1.709837	O	-4.931052	2.981006	0.111813
O	3.249011	4.004915	0.577758	O	-6.510361	3.503657	0.642922	O	-4.197463	3.313851	-1.894835
H	0.938422	0.777887	3.426951	H	-2.984437	3.412840	0.237348	H	-1.171368	-3.130444	1.320903
H	0.966808	-0.906058	2.940728	H	-2.451375	4.196688	-1.237859	H	-1.016017	-1.827650	2.483296
H	3.342479	0.993849	2.873345	H	-0.520484	3.496523	0.178829	H	-3.590737	-2.720214	1.129331
H	3.104430	-0.274227	4.058602	H	-0.505091	2.651758	-1.357589	H	-3.171218	-3.026797	2.800354
H	-5.485789	-3.664293	1.455253	H	4.864191	1.664159	-2.503165	H	5.619756	0.417198	3.629719
H	-4.851867	-2.229477	2.252348	H	5.558457	0.546138	-3.671323	H	4.852502	-0.979295	2.884471
H	-4.819594	-2.816535	-0.735770	H	3.422544	-0.306938	-2.509703	H	4.856904	1.877763	1.829915
H	-3.418653	-2.630311	0.316045	H	4.813728	-1.377757	-2.366459	H	3.452482	0.944956	2.339331
H	-5.693013	2.784626	-1.585971	H	8.192663	1.617115	-0.198423	H	5.773158	0.823271	-2.337460
H	-6.136269	1.147342	-1.995217	H	7.060973	2.033879	1.064637	H	5.168290	-0.370653	-3.456398
H	-8.119721	2.546065	-1.560557	H	9.057116	0.529291	1.662415	H	4.903890	-1.965960	-1.458980
H	-7.507647	2.976361	0.019271	H	8.255777	-0.751733	0.780087	H	3.779926	-0.628671	-1.601268

(3-4)DBU-anti (re-si)₆₀

$E_0 = -1610.5732478$
 $E_{0+ZPE} = -1609.895740$
 $E_{298} = -1609.862535$

(3-4)DBU-anti (re-si)₃₀₀

$E_0 = -1610.5739661$
 $E_{0+ZPE} = -1609.896626$
 $E_{298} = -1609.863231$

$H_{298} = -1609.861591$
 $G_{298} = -1609.963957$
 $N_{\text{Imag}} = 1 (-321.6881)$

N	6.001766	-0.943875	-0.699308
C	6.295851	-2.193803	-0.005427
C	5.023937	-2.864288	0.460270
C	4.190007	-1.879709	1.243259
N	4.040625	-0.661560	0.477879
C	4.898370	-0.262601	-0.422927
C	4.600608	1.020204	-1.131853
C	5.563860	2.156123	-0.783725
C	6.901215	2.085704	-1.500569
C	7.699826	0.820320	-1.239206
C	6.989878	-0.457847	-1.656837
O	1.825402	0.743570	0.813526
C	0.853381	0.024481	1.176920
O	0.884835	-1.186335	1.420411
C	-0.464448	0.807354	1.333381
N	-1.602912	-0.065729	1.577725
C	-1.858704	-0.204692	3.011632
C	-0.857946	0.730197	3.680545
C	-0.447894	1.690188	2.575168
C	-2.166668	-0.833127	0.642171
C	-2.037555	-0.554787	-0.714673
C	-2.357316	-1.582389	-1.764148
C	-3.322352	-2.663322	-1.304696
C	-2.972111	-3.137542	0.089815
C	-3.021333	-1.985677	1.083095
H	-0.596163	1.400621	0.435407
H	0.525263	2.145137	2.732706
H	-1.181486	2.486062	2.457271
H	-1.290037	1.233232	4.542115
H	0.005385	0.163338	4.023914
H	-2.889151	0.077313	3.227712
H	-1.714301	-1.230698	3.341067
H	-1.970976	-3.573349	0.096478
H	-3.659906	-3.917371	0.416156
H	-1.267728	0.147180	-0.999703
H	-2.699944	-2.335439	2.059408
H	3.157658	-0.100744	0.620062
H	6.959210	-1.990387	0.836707
H	6.828752	-2.837023	-0.700219
H	7.715714	-1.257546	-1.762500
H	6.519480	-0.329995	-2.632539
H	4.609199	0.841882	-2.207633
H	3.587696	1.302956	-0.860455
H	5.071189	3.089492	-1.052237
H	5.712027	2.189234	0.296771
C	-3.552340	1.087703	-0.983338
H	-3.033485	1.208079	-1.922177
C	-4.846032	0.399323	-1.067727
C	-5.330080	0.024870	-2.322510
C	-5.643845	0.153270	0.052569
C	-6.566311	-0.588536	-2.455037
H	-4.734671	0.227579	-3.201349
C	-6.876381	-0.463477	-0.079184
H	-5.298673	0.441059	1.034911
C	-7.341816	-0.841039	-1.332904
H	-6.923165	-0.867949	-3.435882
H	-7.477023	-0.650362	0.799432
H	-8.304171	-1.321692	-1.433129
C	-3.367714	2.100142	-0.057450
H	-3.995982	2.285611	0.793805
N	-2.351617	3.004155	-0.207933
O	-1.527469	2.865858	-1.123788
O	-2.275116	3.949189	0.590516
H	-4.052897	-1.644510	1.198979
H	-3.303171	-3.494801	-2.009589
H	-4.341112	-2.276661	-1.299401
H	-2.747351	-1.088381	-2.656824

$H_{298} = -1609.862287$
 $G_{298} = -1609.966252$
 $N_{\text{Imag}} = 1 (-333.6441)$

N	-5.729169	0.017747	0.883108
C	-6.060171	-1.067021	1.802353
C	-4.809247	-1.746964	2.308962
C	-3.931910	-2.127783	1.141555
N	-3.731215	-0.970238	0.297804
C	-4.591009	0.009368	0.204909
C	-4.255629	1.130081	-0.727346
C	-5.146751	1.182878	-1.969568
C	-6.514106	1.800750	-1.732907
C	-7.358602	1.100327	-0.681994
C	-6.726452	1.067499	0.700499
O	-1.436743	-0.727368	-1.023419
C	-0.540126	-1.478764	-0.546351
O	-0.673963	-2.292022	0.372351
C	0.820778	-1.335051	-1.251154
N	1.922996	-1.915551	-0.506110
C	2.392447	-3.161181	-1.099908
C	1.368569	-3.467040	-2.179443
C	0.853599	-2.094385	-2.576867
C	2.496330	-1.321690	0.539416
C	2.154381	-0.035551	0.952649
C	2.506668	0.460425	2.326816
C	3.744919	-0.193559	2.914117
C	3.686660	-1.694853	2.723447
C	3.604866	-2.044017	1.246096
H	0.986404	-0.274782	-1.418890
H	-0.121031	-2.114774	-3.056204
H	1.555614	-1.610258	-3.255135
H	1.807659	-4.014780	-3.009511
H	0.560011	-4.067140	-1.766105
H	3.391042	-3.005853	-1.514441
H	2.445431	-3.956630	-0.360802
H	2.815490	-2.100227	3.242495
H	4.565029	-2.176061	3.152875
H	1.248922	0.387868	0.544060
H	3.496036	-3.117281	1.123932
H	-2.822515	-0.894436	-0.229127
H	-6.713041	-1.779924	1.296502
H	-6.617986	-0.635400	2.629003
H	-7.491976	0.879132	1.446064
H	-6.284489	2.035177	0.941064
H	-4.317903	2.075096	-0.187142
H	-3.219911	0.993658	-1.023980
H	-4.621345	1.773689	-2.718790
H	-5.248679	0.180671	-2.388186
C	3.482773	1.130067	-0.496444
H	3.036216	0.570022	-1.302986
C	2.865157	2.432430	-0.210634
C	1.678180	2.769860	-0.864805
C	3.430692	3.367427	0.659190
C	1.078163	4.001236	-0.665790
H	1.225879	2.056535	-1.539740
C	2.826210	4.598176	0.864406
H	4.350661	3.142380	1.177649
C	1.649635	4.921361	0.203503
H	0.165095	4.243202	-1.190423
H	3.279347	5.307996	1.541320
H	1.182701	5.882605	0.362307
C	4.838960	0.925094	-0.315480
H	5.484063	1.524349	0.298664
N	5.486546	-0.099412	-0.956117
O	4.860241	-0.879906	-1.686868
O	6.711782	-0.210128	-0.794407
H	4.543822	-1.773401	0.757593
H	3.830005	0.058685	3.971382
H	4.639491	0.191843	2.422705
H	2.625166	1.545118	2.306285

H -1.419017 -2.050450 -2.079179
H 4.460264 -3.219257 -0.402062
H 5.272219 -3.726237 1.074449
H 3.188713 -2.250330 1.443690
H 4.661891 -1.650193 2.199756
H 7.973411 0.747132 -0.184880
H 8.632723 0.873977 -1.801164
H 6.726576 2.170451 -2.576161
H 7.500278 2.951587 -1.217263

H 1.656042 0.274524 2.991351
H -4.267035 -1.073049 2.971720
H -5.083776 -2.628820 2.882256
H -2.948374 -2.468883 1.450637
H -4.393808 -2.925104 0.557362
H -7.590589 0.079195 -0.990416
H -8.310699 1.624311 -0.594323
H -6.380602 2.843211 -1.432554
H -7.060925 1.820380 -2.675893

(3-4)DBU1-anti (re-re)₆₀

E₀ = -1610.5778275
E_{0+ZPE} = -1609.900592
E₂₉₈ = -1609.867193
H₂₉₈ = -1609.866249
G₂₉₈ = -1609.970511
NImag = 1 (-325.8187)
N -5.675683 0.177406 0.754439
C -6.269339 -1.016800 1.347152
C -5.201934 -1.946260 1.875769
C -4.178629 -2.203615 0.796981
N -3.728623 -0.943593 0.245981
C -4.452535 0.146900 0.246196
C -3.859295 1.366168 -0.379015
C -4.572964 1.798819 -1.661737
C -5.862120 2.570431 -1.443335
C -6.930196 1.812786 -0.674947
C -6.498294 1.383670 0.717665
O -1.175460 -1.184877 -0.421713
C -0.534986 -0.434767 -1.199945
O -0.972607 0.554131 -1.806187
C 0.939905 -0.781510 -1.476637
N 1.528614 -1.650622 -0.467161
C 1.581409 -3.039350 -0.910225
C 0.915857 -3.030688 -2.278108
C 1.091933 -1.598329 -2.756152
C 1.831622 -1.244153 0.765347
C 1.937488 0.109722 1.068064
C 2.070925 0.583712 2.485995
C 2.712382 -0.446124 3.397555
C 2.020738 -1.782977 3.223996
C 2.150284 -2.291878 1.796839
H 1.485340 0.152394 -1.545250
H 0.373520 -1.301086 -3.515215
H 2.095711 -1.458227 -3.154405
H 1.366041 -3.758319 -2.948704
H -0.141599 -3.267524 -2.179796
H 2.625776 -3.354719 -0.966692
H 1.066400 -3.697243 -0.214994
H 0.963895 -1.672732 3.477317
H 2.431929 -2.528777 3.903876
H 1.464606 0.808901 0.395795
H 1.483542 -3.139854 1.655299
H -2.741132 -0.912529 -0.107396
H -6.887941 -1.518725 0.601778
H -6.919445 -0.692730 2.154603
H -7.374615 1.159856 1.317101
H -5.971214 2.196191 1.218884
H -3.868113 2.178083 0.349539
H -2.822479 1.139090 -0.620022
H -7.804458 2.454625 -0.562505
H -7.256592 0.933483 -1.233305
C 3.946874 0.494155 0.120020
H 4.423772 0.034311 0.971697
C 3.879284 1.964070 0.140122
C 3.196721 2.696195 -0.834474
C 4.542118 2.660271 1.151211
C 3.185247 4.079598 -0.799146

(3-4)DBU1-anti (si-si)₃₀₀

E₀ = -1610.5772056
E_{0+ZPE} = -1609.899565
E₂₉₈ = -1609.866328
H₂₉₈ = -1609.865384
G₂₉₈ = -1609.967816
NImag = 1 (-342.8028)
N -6.054226 -1.319258 -0.032365
C -6.192158 -2.448665 -0.946146
C -4.847657 -3.069714 -1.244041
C -3.883874 -1.998565 -1.692803
N -3.908862 -0.895038 -0.756816
C -4.934122 -0.612387 0.005934
C -4.816302 0.575031 0.904326
C -5.748379 1.723795 0.512013
C -7.188689 1.561225 0.964361
C -7.889144 0.329519 0.418241
C -7.209898 -0.977765 0.792193
O -1.479281 0.154835 -0.639644
C -1.197613 1.327286 -0.281653
O -1.986604 2.185916 0.135169
C 0.272276 1.769953 -0.405613
N 1.224072 0.675389 -0.511843
C 1.553628 0.374507 -1.903457
C 0.758538 1.392038 -2.710903
C 0.496155 2.515843 -1.719175
C 1.601444 -0.094286 0.505411
C 0.972672 0.141406 1.850827
C 1.048427 -1.079932 2.752603
C 2.454478 -1.644084 2.789857
C 2.878294 -2.076676 1.397588
C 2.622211 -1.028488 0.352234
H 0.516795 2.392267 0.451199
H -0.354882 3.137829 -1.982649
H 1.373044 3.153359 -1.618546
H 1.303258 1.724665 -3.591137
H -0.180879 0.953516 -3.039821
H 2.623498 0.475323 -2.066460
H 1.272819 -0.653060 -2.134140
H 2.337161 -2.989579 1.127931
H 3.933621 -2.352519 1.389007
H -0.065984 0.432001 1.717865
H 2.885874 -1.308977 -0.656549
H 1.479816 0.984350 2.318614
H -3.017036 -0.352360 -0.650169
H -6.676230 -2.111128 -1.863757
H -6.846623 -3.175712 -0.474225
H -7.909197 -1.798869 0.673949
H -6.913944 -0.964936 1.841565
H -5.010272 0.265236 1.931994
H -3.789083 0.928777 0.844359
H -5.341100 2.630461 0.956833
H -5.704236 1.869867 -0.568607
C 4.363070 0.379503 0.483894
H 4.249027 0.418037 1.556675
C 5.376331 -0.562872 -0.019943
C 6.224440 -1.198549 0.886604
C 5.542801 -0.822143 -1.382190

(3-4)DBU1-anti (si-si)₁₈₀

E₀ = -1610.5764967
E_{0+ZPE} = -1609.899203
E₂₉₈ = -1609.865898
H₂₉₈ = -1609.864953
G₂₉₈ = -1609.967714
NImag = 1 (-360.8896)
N -5.963027 1.106258 -0.504376
C -6.094582 2.496065 -0.077627
C -4.742842 3.163444 0.023018
C -3.818702 2.311473 0.858503
N -3.836389 0.951064 0.365934
C -4.854144 0.422505 -0.264809
C -4.737209 -1.006751 -0.682222
C -5.668722 -1.941530 0.092700
C -7.110448 -1.938946 -0.384854
C -7.800938 -0.587950 -0.317979
C -7.123363 0.492965 -1.144533
O -1.443164 -0.121199 0.771885
C -1.081396 -1.311261 0.600394
O -1.783238 -2.260207 0.223883
C 0.387428 -1.654478 0.919448
N 1.257605 -0.489840 1.008239
C 1.500713 -0.097775 2.392303
C 0.639857 -1.045458 3.212434
C 0.502709 -2.264618 2.314154
C 1.691952 0.211648 -0.033442
C 1.293414 -0.246945 -1.403954
C 1.249453 0.884487 -2.420093
C 2.514483 1.716288 -2.373709
C 2.713292 2.300968 -0.988351
C 2.564581 1.293385 0.111922
H 0.746041 -2.341494 0.185292
H -0.353869 -2.888559 2.552914
H 1.398754 -2.882242 2.370037
H 1.092332 -1.273299 4.174226
H -0.336510 -0.601204 3.393480
H 2.557507 -0.213286 2.631656
H 1.234340 0.947058 2.541298
H 1.996200 3.112172 -0.826417
H 3.701139 2.761866 -0.916856
H 0.328600 -0.743132 -1.371820
H 2.665432 1.707721 1.104598
H 2.021954 -1.000124 -1.718960
H -2.960299 0.392320 0.493600
H -6.616532 2.528920 0.879783
H -6.712782 3.006656 -0.810620
H -4.936752 -1.082369 -1.751846
H -3.707023 -1.316445 -0.512555
H -7.137250 -2.292113 -1.418933
H -7.679480 -2.660888 0.201524
H -5.267651 -2.948922 -0.009223
H -5.619403 -1.701171 1.156124
C 4.555851 0.353370 0.301398
H 4.375143 0.342895 1.363045
C 4.496639 -0.967744 -0.340532
C 4.090699 -2.065080 0.420783
C 4.868030 -1.185978 -1.669812

H	2.660549	2.182603	-1.619833	C	7.217978	-2.061636	0.446190	C	4.053011	-3.339375	-0.125140
C	4.533988	4.047516	1.184421	H	6.113621	-1.002529	1.943864	H	3.818008	-1.915573	1.455654
H	5.088074	2.108890	1.909161	C	6.530965	-1.685753	-1.821420	C	4.833187	-2.458481	-2.214839
C	3.854862	4.762312	0.209980	H	4.885997	-0.354494	-2.102078	H	5.186647	-2.537968	-2.285248
H	2.648708	4.628253	-1.559818	C	7.374412	-2.309099	-0.908743	C	4.423485	-3.541225	-1.446378
H	5.059050	4.567159	1.972967	H	7.868729	-2.539313	1.164445	H	3.740881	-4.175066	0.484744
H	3.843682	5.842371	0.234909	H	6.642871	-1.877164	-2.878993	H	5.126984	-2.606432	-3.244116
C	4.073308	-0.168442	-1.087719	H	8.144726	-2.983250	-1.253875	H	4.397969	-4.533014	-1.873948
H	3.879869	0.267977	-2.050056	C	4.143948	1.564570	-0.197038	C	5.455691	1.314956	-0.138611
N	4.480502	-1.473789	-1.143229	H	4.458836	1.757094	-1.205753	H	5.959191	1.311280	-1.087141
O	4.722322	-2.097811	-0.100608	N	3.529948	2.631088	0.403738	N	5.732520	2.407063	0.637045
O	4.611984	-2.008357	-2.255171	O	3.109271	2.539116	1.564572	O	5.156140	2.559294	1.724349
H	2.635306	1.517117	2.506395	O	3.430932	3.689601	-0.235266	O	6.565717	3.231042	0.227525
H	1.078533	0.836014	2.874290	H	0.712694	-0.802598	3.751509	H	3.368313	1.089169	-2.634016
H	3.773385	-0.551684	3.160138	H	0.361066	-1.846989	2.388868	H	2.473685	2.516288	-3.113151
H	2.653021	-0.113646	4.434020	H	3.138571	-0.882924	3.171605	H	1.096655	0.460825	-1.412403
H	3.160507	-2.656222	1.614904	H	2.512238	-2.490536	3.474255	H	0.386525	1.520077	-2.210753
H	-3.878150	2.425975	-2.218268	H	-2.865072	-2.372984	-1.735708	H	-4.321780	3.296083	-0.972864
H	-4.756806	0.921436	-2.284307	H	-4.145484	-1.635115	-2.687179	H	-4.857539	4.147732	0.469593
H	-5.632491	3.492664	-0.903515	H	-4.464311	-3.561519	-0.350844	H	-2.793939	2.668064	0.809028
H	-6.263329	2.872205	-2.411247	H	-4.960288	-3.825292	-2.017395	H	-4.123987	3.321610	1.905418
H	-3.308354	-2.722802	1.188178	H	-7.978163	0.386662	-0.668260	H	-8.818996	-0.696110	-0.693178
H	-4.601365	-2.817323	0.000632	H	-8.904583	0.296700	0.814311	H	-7.883742	-0.246452	0.715537
H	-4.718302	-1.495525	2.741774	H	-7.211507	1.520359	2.056340	H	-6.834328	0.101022	-2.120143
H	-5.658987	-2.879006	2.196060	H	-7.751836	2.450076	0.678396	H	-7.821802	1.303093	-1.326417

(3-4)DBU2-anti (re-re)₆₀

$E_0 = -1610.5785737$
 $E_{0+ZPE} = -1609.901283$
 $E_{298} = -1609.867939$
 $H_{298} = -1609.866995$
 $G_{298} = -1609.970096$
 $N\text{Imag} = 1 (-318.6306)$

N	-5.957905	-0.238140	0.608574
C	-6.103377	-0.614353	2.011360
C	-4.915803	-1.425289	2.476824
C	-3.638918	-0.692685	2.142349
N	-3.658572	-0.303696	0.749429
C	-4.755422	-0.115866	0.065368
C	-4.608642	0.263622	-1.374228
C	-5.044518	1.694466	-1.692568
C	-6.547599	1.880565	-1.804287
C	-7.332074	1.504156	-0.559099
C	-7.175915	0.050034	-0.141918
O	-1.341992	-0.087394	-0.507430
C	-0.517638	-0.984283	-0.169541
O	-0.683158	-1.847487	0.696640
C	0.784382	-0.955685	-0.989971
N	1.854941	-1.743335	-0.396437
C	1.997362	-3.041229	-1.047904
C	0.870718	-3.081077	-2.067872
C	0.592980	-1.614281	-2.353177
C	2.518007	-1.378862	0.701924
C	2.475341	-0.068244	1.165652
C	3.052021	0.306586	2.499804
C	4.177759	-0.612740	2.935477
C	3.735019	-2.055762	2.809472
C	3.389901	-2.406814	1.370890
H	1.083291	0.080424	-1.097343
H	-0.399127	-1.428987	-2.755302
H	1.330643	-1.222185	-3.051711
H	1.151664	-3.640631	-2.956533
H	-0.008461	-3.552813	-1.632916
H	2.979541	-3.094447	-1.523380
H	1.922775	-3.855762	-0.332294
H	2.860245	-2.216234	3.443257
H	4.509202	-2.736376	3.162969
H	1.662037	0.553858	0.825495
H	2.878656	-3.366878	1.351400

(3-4)DBU2-anti (si-si)₃₀₀

$E_0 = -1610.5782112$
 $E_{0+ZPE} = -1609.900668$
 $E_{298} = -1609.867495$
 $H_{298} = -1609.866551$
 $G_{298} = -1609.968957$
 $N\text{Imag} = 1 (-336.1154)$

N	-6.603872	0.771808	0.479264
C	-6.629545	2.222135	0.644025
C	-5.311705	2.729167	1.182829
C	-4.179907	2.192780	0.340120
N	-4.314537	0.758344	0.216734
C	-5.458380	0.131914	0.293733
C	-5.435741	-1.356076	0.142689
C	-6.077382	-1.855914	-1.152500
C	-7.595230	-1.891211	-1.124432
C	-8.259591	-0.551034	-0.860706
C	-7.887580	0.076821	0.473584
O	-2.122819	-0.695507	-0.116096
C	-1.099825	-0.153862	0.386719
O	-1.056971	0.927778	0.982647
C	0.183122	-0.989985	0.231406
N	1.403896	-0.270222	0.553715
C	1.828976	-0.511834	1.931138
C	0.781670	-1.466268	2.487869
C	0.204113	-2.130081	1.246747
C	1.966521	0.650193	-0.226175
C	1.277330	1.021095	-1.510320
C	1.678435	2.401129	-2.005798
C	3.185679	2.556857	-2.023039
C	3.742206	2.397032	-0.619453
C	3.211442	1.184024	0.089895
H	0.231352	-1.364053	-0.788647
H	-0.784854	-2.552578	1.399540
H	0.865557	-2.916179	0.886214
H	1.213093	-2.178046	3.187431
H	0.007902	-0.906817	3.009560
H	2.823364	-0.951548	1.946622
H	1.866746	0.431653	2.475455
H	3.495139	3.288493	-0.033725
H	4.832221	2.359321	-0.644067
H	0.201525	0.985972	-1.363759
H	3.563278	1.048843	1.101555

(3-4)DBU2-anti (re-si)₃₀₀

$E_0 = -1610.5737969$
 $E_{0+ZPE} = -1609.896610$
 $E_{298} = -1609.863174$
 $H_{298} = -1609.862230$
 $G_{298} = -1609.966475$
 $N\text{Imag} = 1 (-331.8091)$

N	-6.097687	-0.182716	0.701517
C	-6.164146	-0.308404	2.154052
C	-4.887937	-0.905055	2.700679
C	-3.702358	-0.127178	2.182230
N	-3.800800	-0.000307	0.744826
C	-4.929704	-0.050281	0.089865
C	-4.864316	0.071569	-1.399596
C	-5.455044	1.374293	-1.941368
C	-6.971685	1.388137	-2.019967
C	-7.681113	1.170436	-0.694473
C	-7.360856	-0.158787	-0.029117
O	-1.519124	0.046226	-0.601536
C	-0.731650	-0.845287	-0.173621
O	-0.914821	-1.585558	0.796113
C	0.549934	-0.986252	-1.015137
N	1.571233	-1.797897	-0.379273
C	1.683319	-3.116512	-0.990779
C	0.514433	-3.178989	-1.959076
C	0.282802	-1.723257	-2.326545
C	2.382771	-1.348690	0.576822
C	2.403885	-0.015400	0.980714
C	3.024904	0.394548	2.286121
C	4.146098	-0.522701	2.740359
C	3.720813	-1.970825	2.616584
C	3.367275	-2.308099	1.176665
H	0.919894	0.015980	-1.212963
H	-0.714039	-1.520568	-2.707370
H	1.005152	-1.403907	-3.077050
H	0.735453	-3.806308	-2.818971
H	-0.363238	-3.585594	-1.459483
H	2.644459	-3.187864	-1.504856
H	1.631273	-3.906065	-0.244910
H	2.856105	-2.157085	3.257083
H	4.513475	-2.639395	2.951663
H	1.582825	0.608652	0.661387
H	2.987804	-3.323620	1.116876

H	-2.731687	-0.226822	0.250590	H	1.523803	0.267809	-2.257624	H	-2.898600	0.028302	0.200105
H	-2.760490	-1.315634	2.285828	H	-3.435462	0.189238	0.096785	H	-2.763085	-0.631793	2.390227
H	-3.528340	0.195254	2.766234	H	-3.207321	2.383652	0.784681	H	-3.664446	0.865417	2.632856
H	-4.921088	-2.397851	1.985409	H	-4.190892	2.645216	-0.652580	H	-4.807739	-1.946366	2.389890
H	-4.988323	-1.592688	3.548419	H	-5.187116	2.403737	2.215261	H	-4.912436	-0.881538	3.787227
H	-7.016751	-1.195621	2.101836	H	-5.311359	3.816247	1.173508	H	-7.012277	-0.945639	2.387753
H	-6.220515	0.286504	2.615730	H	-7.435859	2.457480	1.333174	H	-6.353860	0.672589	2.592311
H	-7.229523	-0.604207	-1.013017	H	-6.862947	2.688515	-0.314193	H	-7.371832	-0.964986	-0.763896
H	-7.996936	-0.229391	0.510119	H	-7.899102	-0.674228	1.264751	H	-8.126887	-0.391957	0.703142
H	-3.559780	0.136257	-1.626106	H	-8.627053	0.824772	0.740621	H	-3.815659	0.002157	-1.674187
H	-5.176761	-0.440435	-1.983434	H	-4.393548	-1.659662	0.175200	H	-5.374022	-0.781976	-1.847706
H	-7.057671	2.146284	0.280025	H	-5.932900	-1.807026	1.002129	H	-7.455605	1.980182	0.001880
H	-8.391517	1.676673	-0.750427	H	-8.033734	0.155741	-1.661313	H	-8.757341	1.197353	-0.867220
H	-6.757062	2.920097	-2.057643	H	-9.340766	-0.692047	-0.864002	H	-7.294948	2.338191	-2.445826
H	-6.914057	1.280038	-2.640668	H	-7.957187	-2.287983	-2.073229	H	-7.293783	0.611725	-2.718522
H	-4.630427	2.376973	-0.949248	H	-7.915654	-2.596432	-0.353327	H	-5.097308	2.213606	-1.343339
H	-4.587105	1.965851	-2.643199	H	-5.725480	-1.251712	-1.989861	H	-5.051797	1.519578	-2.942605
C	3.867420	0.867764	-0.353679	H	-5.706454	-2.864757	-1.327811	C	3.784788	0.778654	-0.657327
H	4.707719	0.463675	0.189222	C	4.472551	-0.530848	-0.644709	H	3.107492	0.352691	-1.380724
C	3.531238	2.271218	-0.066516	H	4.326338	-0.196293	-1.660369	C	3.558462	2.193169	-0.330163
C	2.400858	2.893773	-0.601515	C	5.723291	-0.097902	-0.000336	C	2.403588	2.817135	-0.807181
C	4.382614	3.022662	0.743830	C	6.694654	0.546821	-0.765801	C	4.465614	2.955238	0.409205
C	2.137134	4.226428	-0.338107	C	5.989603	-0.337225	1.349681	C	2.163867	4.158337	-0.563263
H	1.715412	2.329732	-1.217773	C	7.903845	0.931139	-0.203499	H	1.688476	2.240422	-1.377683
C	4.120386	4.360155	1.004863	H	6.505987	0.734032	-1.813563	C	4.223272	4.297198	0.658843
H	5.265350	2.557895	1.160082	C	7.193676	0.049415	1.911582	H	5.370499	2.506112	0.790104
C	2.996517	4.966737	0.465646	H	5.242728	-0.815839	1.967327	C	3.073822	4.904883	0.174022
H	1.255755	4.689482	-0.757986	C	8.157701	0.684436	1.136716	H	1.267195	4.621265	-0.949261
H	4.795960	4.926007	1.630132	H	8.645851	1.423822	-0.815217	H	4.937810	4.869943	1.232308
H	2.787784	6.006800	0.670333	H	7.381115	-0.141193	2.958512	H	2.888858	5.951493	0.367786
C	3.649173	0.357586	-1.619631	H	9.096647	0.986077	1.577726	C	5.059378	0.239417	-0.651112
H	3.025166	0.814037	-2.365478	C	3.935181	-1.763589	-0.320209	H	5.909606	0.657480	-0.146182
N	4.240946	-0.807403	-2.028116	H	4.203952	-2.337156	0.547221	N	5.343016	-0.908905	-1.343367
O	4.973729	-1.439662	-1.255436	N	3.023044	-2.383879	-1.132530	O	4.450871	-1.509230	-1.959367
O	4.036023	-1.202735	-3.186196	O	2.621125	-1.827634	-2.162843	O	6.515228	-1.316271	-1.347716
H	4.297703	-2.524799	0.780323	O	2.633918	-3.519549	-0.820480	H	4.272380	-2.282203	0.565081
H	4.466131	-0.386867	3.962177	H	1.259017	2.555934	-2.999522	H	4.422344	-0.288624	3.768678
H	5.061257	-0.447529	2.314749	H	1.243299	3.163726	-1.356085	H	5.033747	-0.358612	2.127671
H	3.394136	1.342073	2.470161	H	3.617914	1.805101	-2.687291	H	3.381784	1.423434	2.214701
H	2.258936	0.283017	3.254555	H	3.468447	3.530335	-2.423741	H	2.243399	0.411187	3.053536

(3-4)DBU6-anti (re-re)₆₀

$E_0 = -1610.5785206$
 $E_{0+ZPE} = -1609.900558$
 $E_{298} = -1609.867500$
 $H_{298} = -1609.866556$
 $G_{298} = -1609.967905$
 $N_{\text{Imag}} = 1 (-323.4316)$

N	-5.402185	0.986607	-0.284597
C	-5.953069	1.281008	-1.603987
C	-4.853331	1.385206	-2.635931
C	-3.977950	0.157361	-2.570668
N	-3.571672	-0.070250	-1.201270
C	-4.250161	0.343226	-0.164065
C	-3.688587	0.037310	1.187274
C	-4.504047	-0.994861	1.967381
C	-5.752269	-0.435153	2.627385
C	-6.752601	0.195314	1.673447
C	-6.199859	1.366839	0.877291
O	-1.195428	-1.193499	-0.784019
C	-0.361958	-0.764299	-1.623438
O	-0.605360	-0.044304	-2.602447
C	1.108066	-1.192916	-1.463785
N	1.416270	-1.736119	-0.148173
C	1.455124	-3.194689	-0.160428
C	1.078961	-3.575833	-1.584014
C	1.455853	-2.348204	-2.397360
C	1.495790	-0.993316	0.956076

(3-4)DBU6-anti (re-re)₁₈₀

$E_0 = -1610.5743363$
 $E_{0+ZPE} = -1609.896787$
 $E_{298} = -1609.863509$
 $H_{298} = -1609.862565$
 $G_{298} = -1609.966385$
 $N_{\text{Imag}} = 1 (-351.0302)$

N	-5.722474	-0.331137	0.406641
C	-6.467195	0.618524	1.227378
C	-5.535385	1.404259	2.121056
C	-4.429056	2.012112	1.292877
N	-3.837327	0.991790	0.455377
C	-4.460897	-0.092846	0.079522
C	-3.698487	-1.067562	-0.759799
C	-4.196241	-1.164700	-2.202378
C	-5.447530	-2.007177	-2.378325
C	-6.653638	-1.531867	-1.586562
C	-6.437297	-1.506170	-0.081618
O	-1.276791	1.350863	-0.195902
C	-0.635081	1.719255	0.820855
O	-1.099965	1.969665	1.940539
C	0.888152	1.915135	0.678146
N	1.421489	1.456005	-0.593763
C	1.577622	2.561563	-1.539123
C	1.097958	3.788196	-0.774760
C	1.256242	3.394298	0.684492
C	1.648697	0.178518	-0.886440

(3-4)DBU6-anti (re-re)₃₀₀

$E_0 = -1610.5695014$
 $E_{0+ZPE} = -1609.892402$
 $E_{298} = -1609.858984$
 $H_{298} = -1609.858040$
 $G_{298} = -1609.961771$
 $N_{\text{Imag}} = 1 (-329.7996)$

N	-5.507873	-0.050602	-0.949502
C	-6.049861	-1.280954	-1.518771
C	-4.944128	-2.253109	-1.858992
C	-4.039701	-2.431475	-0.663465
N	-3.623465	-1.132327	-0.182218
C	-4.333058	-0.045809	-0.337084
C	-3.778393	1.221925	0.228251
C	-4.555548	1.738004	1.440576
C	-5.838881	2.471735	1.092593
C	-6.849693	1.651801	0.309098
C	-6.337581	1.147438	-1.030842
O	-1.217287	-0.878335	0.935217
C	-0.419450	-1.747557	0.497359
O	-0.700982	-2.701424	-0.241297
C	1.050323	-1.662536	0.949479
N	1.423071	-0.350567	1.463080
C	1.448092	-0.328987	2.925590
C	0.976650	-1.715581	3.336126
C	1.316140	-2.583266	2.136492
C	1.519153	0.732805	0.691149

C	1.633258	0.388776	0.883836	C	1.529861	-0.844036	0.058437	C	1.550513	0.672347	-0.700600
C	1.506314	1.250711	2.106011	C	1.398389	-2.270891	-0.380704	C	1.100798	1.847105	-1.529950
C	1.882217	0.524474	3.383947	C	2.118634	-2.573784	-1.680124	C	1.306832	3.200177	-0.871416
C	1.154039	-0.802429	3.451413	C	1.771056	-1.538765	-2.729481	C	0.928255	3.158284	0.595526
C	1.527718	-1.701396	2.283005	C	2.142294	-0.138174	-2.267142	C	1.704804	2.071432	1.328343
H	1.724119	-0.326485	-1.675545	H	1.360196	1.393050	1.504496	H	1.673010	-1.938757	0.105842
H	0.929627	-2.274677	-3.344932	H	0.625036	3.961579	1.361481	H	0.731194	-3.496919	2.079360
H	2.527185	-2.343573	-2.592110	H	2.291580	3.513334	1.002742	H	2.370253	-2.856655	2.150127
H	1.596705	-4.474537	-1.909515	H	1.664877	4.676386	-1.041882	H	1.456469	-2.049506	4.252879
H	0.008192	-3.758553	-1.651039	H	0.050172	3.979721	-0.998043	H	-0.098498	-1.706369	3.501771
H	2.463653	-3.525683	0.098171	H	2.623220	2.651235	-1.833256	H	2.459942	-0.125302	3.277912
H	0.763900	-3.615983	0.565042	H	0.985149	2.394269	-2.435906	H	0.791013	0.442621	3.317888
H	0.077253	-0.618731	3.440159	H	0.699508	-1.576053	-2.937431	H	-0.141733	2.966821	0.703452
H	1.374100	-1.324308	4.382440	H	2.282064	-1.747582	-3.669090	H	1.127548	4.118609	1.070548
H	1.364403	0.868857	-0.044524	H	0.981191	-0.613774	0.959746	H	1.345393	-0.285478	-1.155984
H	0.843574	-2.546534	2.248006	H	1.768441	0.592677	-2.977725	H	1.433878	2.058589	2.378227
H	-2.636503	-0.524131	-1.041508	H	-2.826547	1.111689	0.196863	H	-2.676159	-1.053197	0.267210
H	-3.067532	0.269467	-3.152899	H	-3.629794	2.412984	1.910114	H	-3.136154	-2.983897	-0.903978
H	-4.513011	-0.718350	-2.940473	H	-4.813526	2.817572	0.665558	H	-4.558237	-2.964233	0.135066
H	-4.254724	2.275428	-2.444511	H	-5.109849	0.744752	2.876664	H	-4.367005	-1.874497	-2.702097
H	-5.293254	1.486000	-3.624826	H	-6.095328	2.181914	2.634379	H	-5.377956	-3.205396	-2.153205
H	-6.493003	2.220745	-1.530361	H	-7.175220	0.051231	1.824964	H	-6.604282	-1.010584	-2.413693
H	-6.669423	0.504304	-1.876012	H	-7.036881	1.285209	0.578092	H	-6.753547	-1.723562	-0.812157
H	-5.614442	2.023656	1.521827	H	-5.919014	-2.408831	0.244325	H	-5.790560	1.934424	-1.551143
H	-7.020748	1.960876	0.488934	H	-7.397846	-1.496993	0.422776	H	-7.178856	0.880858	-1.8661929
H	-2.678865	-0.331854	1.032463	H	-2.660468	-0.748296	-0.749980	H	-2.749621	1.017885	0.509657
H	-3.610914	0.962810	1.758836	H	-3.738689	-2.047757	-0.283525	H	-3.758641	1.980850	-0.554730
H	-7.149471	-0.549527	0.980977	H	-6.967170	-0.539867	-1.917727	H	-7.197257	0.801883	0.899529
H	-7.599260	0.565155	2.252456	H	-7.487637	-2.205507	-1.785141	H	-7.723824	2.272790	0.111324
H	-6.244804	-1.231781	3.185445	H	-5.705363	-2.040063	-3.437174	H	-6.303892	2.826992	2.012524
H	-5.451802	0.316262	3.362066	H	-5.221926	-3.035135	-2.083699	H	-5.586877	3.362106	0.511009
H	-4.759980	-1.826750	1.309276	H	-4.354004	-0.161548	-2.601318	H	-4.763483	0.907376	2.117162
H	-3.854217	-1.404789	2.739343	H	-3.393276	-1.604921	-2.792149	H	-3.899071	2.417668	1.982324
C	3.824244	0.548934	0.333110	C	3.456108	-0.781111	1.164738	C	3.798079	0.582672	-1.021355
H	4.082788	0.232215	1.356093	H	2.966858	-0.094091	1.835447	H	3.553506	0.943043	-2.009410
C	3.865723	1.882432	-0.037416	C	4.456936	-0.163197	0.283220	C	3.953661	-0.873914	-0.902233
C	3.428022	2.347004	-1.280060	C	5.319733	-0.900204	-0.532812	C	4.472051	-1.491312	0.237272
C	4.383782	2.804577	0.872156	C	4.582432	1.227149	0.288360	C	3.615673	-1.674304	-1.996680
C	3.516844	3.689972	-1.602761	C	6.269249	-0.265224	-1.316016	C	4.638605	-2.866892	0.279409
H	3.000409	1.657547	-1.994368	H	5.255299	-1.977597	-0.559880	H	4.751128	-0.903279	1.098707
C	4.476278	4.150446	0.547297	C	5.531454	1.863817	-0.496899	C	3.783483	-3.047177	-1.954786
H	4.730601	2.460371	1.836443	H	3.935301	1.811116	0.926624	H	3.217006	-1.208854	-2.887597
C	4.043045	4.598160	-0.691150	C	6.378633	1.119711	-1.304931	C	4.293206	-3.650883	-0.812200
H	3.169435	4.031195	-2.567359	H	6.928098	-0.854774	-1.937372	H	5.042662	-3.327968	1.169298
H	4.886665	4.847186	1.264008	H	5.614046	2.941010	-0.470173	H	3.517610	-3.647019	-2.813190
H	4.110178	5.646044	-0.945514	H	7.121719	1.611789	-1.915616	H	4.424610	-4.722587	-1.075540
C	4.138728	-0.504823	-0.606931	C	3.636889	-2.066605	1.654522	C	4.571091	1.436747	-0.252271
H	4.174363	-0.338178	-1.667668	H	4.313459	-2.798476	1.254960	H	5.036861	1.177667	0.679661
N	4.447004	-1.786044	-0.235387	N	2.883598	-2.519502	2.704143	N	4.865891	2.711766	-0.664512
O	4.424751	-2.113099	0.959157	O	2.019162	-1.790166	3.209290	O	4.445883	3.141619	-1.745826
O	4.759340	-2.602521	-1.117743	O	3.089845	-3.667418	3.129490	O	5.581439	3.409286	0.069655
H	2.525242	-2.114884	2.426832	H	3.231029	-0.026638	-2.254841	H	2.777707	2.298555	1.281618
H	1.638101	1.141513	4.248895	H	1.857079	-3.573604	-2.026828	H	0.716315	3.953463	-1.394181
H	2.959966	0.350359	3.414301	H	3.196463	-2.569272	-1.511744	H	2.350131	3.495365	-0.970581
H	2.113899	2.148311	1.983623	H	1.773770	-2.921971	0.412134	H	1.592784	1.827367	-2.503851
H	0.474195	1.607886	2.188129	H	0.335772	-2.513765	-0.483927	H	0.034153	1.709757	-1.739461

(3-4)DBU6-anti (si-si)₆₀

$E_0 = -1610.571551$
 $E_{0+ZPE} = -1609.894067$
 $E_{298} = -1609.860805$
 $H_{298} = -1609.859861$
 $G_{298} = -1609.963322$
 $N\text{Imag} = 1 (-343.5992)$

N	-5.986424	0.379660	-0.272474
C	-6.704975	-0.310401	-1.339809
C	-5.758340	-0.758633	-2.429282
C	-4.607357	-1.521148	-1.819608
N	-4.028957	-0.737422	-0.749987

(3-4)DBU6-anti (si-si)₁₈₀

$E_0 = -1610.5769283$
 $E_{0+ZPE} = -1609.899615$
 $E_{298} = -1609.866333$
 $H_{298} = -1609.865389$
 $G_{298} = -1609.968210$
 $N\text{Imag} = 1 (-366.4766)$

N	-6.031022	0.165232	-0.524916
C	-6.846430	-1.022557	-0.286635
C	-6.006944	-2.277819	-0.352235
C	-4.801698	-2.131689	0.545281
N	-4.132042	-0.884532	0.249018

(3-4)DBU6-anti (si-si)₃₀₀

$E_0 = -1610.577716$
 $E_{0+ZPE} = -1609.900256$
 $E_{298} = -1609.867029$
 $H_{298} = -1609.866084$
 $G_{298} = -1609.968635$
 $N\text{Imag} = 1 (-345.6221)$

N	6.019548	0.547867	0.244740
C	6.939921	-0.582347	0.169006
C	6.233550	-1.876640	0.499793
C	4.989669	-2.007973	-0.345639
N	4.211096	-0.792396	-0.248713

C	-4.702700	0.139031	-0.052695	C	-4.734245	0.159937	-0.254536	C	4.722176	0.375444	0.037511
C	-3.974632	0.853638	1.040383	C	-3.903491	1.378373	-0.500796	C	3.784446	1.539347	0.099192
C	-4.423234	0.442193	2.443607	C	-4.239217	2.547641	0.426476	C	3.969023	2.539726	-1.043054
C	-5.720580	1.087936	2.899260	C	-5.475610	3.331038	0.021340	C	5.141558	3.488250	-0.860785
C	-6.921371	0.807594	2.011379	C	-6.756551	2.516755	-0.040348	C	6.494732	2.812745	-0.717557
C	-6.757275	1.282936	0.576244	C	-6.709999	1.357642	-1.023149	C	6.593637	1.870217	0.471800
O	-1.417046	-1.007680	-0.257768	O	-1.496721	-0.781797	0.670162	O	1.571694	-0.945249	-0.543762
C	-0.800863	-1.401489	-1.281284	C	-0.978852	-1.906241	0.450795	C	1.122097	-2.036927	-0.104842
O	-1.293801	-1.671167	-2.385157	O	-1.564792	-2.933519	0.082769	O	1.786091	-2.986993	0.329318
C	0.718584	-1.619915	-1.155535	C	0.538412	-2.054588	0.679821	C	-0.404425	-2.240694	-0.134218
N	1.330530	-0.942857	-0.020083	N	1.228647	-0.799433	0.943564	N	-1.167475	-1.030775	-0.396331
C	1.506329	-1.844349	1.117552	C	1.447557	-0.595632	2.372624	C	-1.486328	-0.891049	-1.815937
C	0.895638	-3.158642	0.655286	C	0.771967	-1.787495	3.032518	C	-0.903768	-2.141652	-2.461661
C	1.013057	-3.088055	-0.859399	C	0.810527	-2.854348	1.950243	C	-0.803811	-3.129320	-1.308910
C	1.541212	0.369145	0.053266	C	1.542622	0.107382	0.023718	C	-1.385907	-0.066848	0.493572
C	1.105825	1.244813	-1.075614	C	1.168635	-0.174224	-1.400509	C	-0.773689	-2.054612	1.059826
C	0.555977	2.574242	-0.574159	C	0.942301	1.093310	-2.211007	C	-0.625936	1.131318	2.570209
C	1.562851	3.281123	0.310988	C	2.094953	2.063202	-2.051308	C	-1.918163	1.921927	2.520243
C	1.988775	2.401158	1.473940	C	2.281557	2.433721	-0.591496	C	-2.297740	2.209959	1.078333
C	2.241435	0.961431	1.104729	C	2.275454	1.255405	0.335061	C	-2.238498	0.993638	0.198775
H	1.181115	-1.301836	-2.085509	H	0.959283	-2.544867	-0.193681	H	-0.709739	-2.675705	0.814129
H	0.329467	-3.750889	-1.382469	H	0.081025	-3.646640	2.087813	H	-0.082874	-3.924207	-1.476307
H	2.028287	-3.327091	-1.174189	H	1.800737	-3.306183	1.895005	H	-1.773925	-3.577759	-1.100511
H	1.411358	-4.015253	1.082204	H	1.279358	-2.085062	3.946516	H	-1.526484	-2.503532	-3.276125
H	-0.151296	-3.209855	0.946181	H	-0.259026	-1.543942	3.282219	H	0.085000	-1.928943	-2.862817
H	2.562607	-1.960496	1.348299	H	2.515147	-0.578058	2.588798	H	-2.562620	-0.830191	-1.953536
H	1.008715	-1.432121	1.994388	H	1.025242	0.356963	2.687949	H	-1.043292	0.025856	-2.204468
H	1.202699	2.413485	2.237076	H	1.491918	3.127468	-0.285972	H	-1.622776	2.973440	0.677768
H	2.871392	2.824031	1.955830	H	3.219414	2.980177	-0.461628	H	-3.294513	2.650470	1.027852
H	0.373447	0.751519	-1.705381	H	0.279190	-0.794641	-1.440029	H	0.199632	-0.679347	1.771145
H	2.491223	0.326289	1.942693	H	2.351979	1.517931	1.380520	H	-2.464873	1.167563	-0.842360
H	1.991108	1.432517	-1.696298	H	1.980912	-0.757769	-1.844246	H	-1.402213	-0.872825	2.446777
H	-3.002353	-0.848987	-0.560651	H	-3.095131	-0.841416	0.404832	H	3.168364	-0.868032	-0.365199
H	-3.812753	-1.716776	-2.533728	H	-4.074121	-2.923456	0.391135	H	4.349377	-2.820431	-0.013752
H	-4.947446	-2.478801	-1.422738	H	-5.098807	-2.142665	1.594918	H	5.249701	-2.188252	-1.389632
H	-5.379623	0.109256	-2.968195	H	-5.682596	-2.450037	-1.378136	H	5.964907	-1.889105	1.555625
H	-6.294651	-1.383296	-3.139122	H	-6.607410	-3.130667	-0.045756	H	6.904965	-2.711770	0.317609
H	-7.439646	0.383278	-1.739499	H	-7.620700	-1.046552	-1.048749	H	7.743340	-0.398874	0.876814
H	-7.243511	-1.160219	-0.917716	H	-7.336278	-0.932211	0.684021	H	7.377568	-0.622628	-0.829634
H	-6.309900	2.277271	0.552020	H	-6.251611	1.671981	-1.961539	H	6.134204	2.320093	1.352782
H	-7.732093	1.367213	0.107153	H	-7.721435	1.043613	-1.258888	H	7.637306	1.700660	0.715894
H	-2.919217	0.632192	0.913749	H	-2.866557	1.086628	-0.361969	H	2.777126	1.134272	0.072887
H	-4.100408	1.928616	0.909319	H	-4.018768	1.681850	-1.542017	H	3.907834	2.043674	1.058137
H	-7.158209	-0.258086	2.007357	H	-7.020320	2.134837	0.947656	H	6.752337	2.266803	-1.627060
H	-7.789210	1.319088	2.428462	H	-7.571306	3.172394	-0.348736	H	7.256303	3.582559	-0.589424
H	-5.942177	0.758220	3.914492	H	-5.612561	4.159320	0.716918	H	5.173098	4.177565	-1.074861
H	-5.572968	2.169579	2.951475	H	-5.300416	3.778324	-0.960338	H	4.962170	4.097796	0.028442
H	-4.498688	-0.645042	2.496728	H	-4.337639	2.182761	1.449953	H	4.056044	2.001624	-1.988167
H	-3.629729	0.727185	3.133234	H	-3.382407	3.220050	0.422647	H	3.053291	3.125878	-1.109730
C	4.317261	0.945569	0.246547	C	4.366102	0.539622	0.388031	C	-4.192634	-0.055166	0.517382
H	4.518010	1.681705	1.010873	H	4.179473	0.266913	1.413226	H	-4.076694	-0.072310	1.582945
C	4.676180	-0.437038	0.596009	C	4.479409	-0.598039	-0.536119	C	-5.034527	0.945589	-0.159889
C	5.077746	-0.715553	1.904899	C	4.229664	-1.882378	-0.049917	C	-5.742354	1.870912	0.606993
C	4.675868	-1.477282	-0.334624	C	4.862502	-0.460897	-1.872983	C	-5.178988	0.983358	-1.548831
C	5.459569	-1.993011	2.276887	C	4.351430	-2.994401	-0.869504	C	-6.578185	2.802171	0.006702
H	5.093948	0.083349	2.633680	H	3.950751	-2.007907	0.986176	H	-5.648794	1.849716	1.683677
C	5.052009	-2.758192	0.039342	C	4.986108	-1.570886	-2.691683	C	-6.009723	1.914034	-2.147841
H	4.384318	-1.293724	-1.357713	H	5.064011	0.517812	-2.281882	H	-4.627583	0.287866	-2.165898
C	5.441404	-3.023322	1.344972	C	4.729218	-2.842948	-2.195444	C	-6.714586	2.827785	-1.372483
H	5.772957	-2.185425	3.292940	H	4.157330	-3.979227	-0.469322	H	-7.122252	3.506319	0.619619
H	5.044803	-3.551701	-0.694271	H	5.284649	-1.442872	-3.722287	H	-6.106725	1.929872	-3.223928
H	5.736997	-4.022124	1.631920	H	4.827329	-3.707017	-2.836426	H	-7.362436	3.553408	-1.842521
C	4.458696	1.390414	-1.1059204	C	5.136809	1.679438	0.204276	C	-4.188647	-1.359030	0.051689
H	4.472926	0.758083	-1.926967	H	5.649847	1.947134	-0.700140	H	-4.546881	-1.663846	-0.914035
N	4.665003	2.713832	-1.351347	N	5.251640	2.604419	1.205803	N	-3.754339	-2.395994	0.833555
O	4.714178	3.562042	-0.451443	O	4.639810	2.444464	2.272254	O	-3.304219	-2.179614	1.966615
O	4.818754	3.030193	-2.540514	O	5.974008	3.595993	1.018463	O	-3.846227	-3.549267	0.386473
H	0.296616	3.195713	-1.430953	H	3.006373	1.604337	-2.436290	H	-0.318528	0.951826	3.600068
H	-0.368768	2.393168	-0.022299	H	1.921848	2.962582	-2.642544	H	0.170734	1.711145	2.098487
H	2.438223	3.554037	-0.275476	H	0.802966	0.823061	-3.257495	H	-2.708893	1.350032	3.010783

H 1.142148 4.211183 0.694946

H 0.016166 1.568184 -1.880794

H -1.819109 2.857772 3.070357

(3-4)DBU6-anti (si-re)₆₀

E₀ = -1610.5741068
E_{0+ZPE} = -1609.896936
E₂₉₈ = -1609.863617
H₂₉₈ = -1609.862673
G₂₉₈ = -1609.966528
NImag = 1 (-357.0693)

N	6.074250	0.476756	0.379933
C	6.983676	-0.657578	0.248039
C	6.239190	-1.964008	0.400541
C	5.056675	-1.985877	-0.536601
N	4.288175	-2.771297	-0.369997
C	4.792346	0.351420	0.068602
C	3.865773	1.519276	0.186988
C	4.160596	2.641724	-0.809996
C	5.316663	3.543542	-0.413832
C	6.649991	2.836943	-0.240010
C	6.640349	1.748098	0.820552
O	1.660800	-0.898655	-0.804006
C	1.218825	-2.022867	-0.450493
O	1.888546	-2.991598	-0.067079
C	-0.303683	-2.249833	-0.513972
N	-1.082880	-1.049293	-0.771304
C	-1.515360	-0.965695	-2.159329
C	-0.828951	-2.141004	-2.835190
C	-0.665298	-3.139781	-1.701071
C	-1.409062	-0.145495	0.148110
C	-0.806146	-0.269730	1.516020
C	-0.628860	-1.079743	2.194491
C	-1.926449	1.861191	2.183631
C	-2.395394	2.096111	0.757559
C	-2.333161	0.868188	-0.107599
H	-0.615944	-2.702295	0.424015
H	0.094302	-3.893681	-1.884311
H	-1.609354	-3.646421	-1.502370
H	-1.412172	-2.528104	-3.666892
H	0.145227	-1.839337	-3.215674
H	-2.600248	-1.057238	-2.221700
H	-1.235131	-0.003431	-2.586464
H	-1.776640	2.877111	0.302766
H	-3.411041	2.495798	0.755225
H	0.149126	-0.781549	1.457692
H	-2.601233	1.028824	-1.141466
H	-1.463404	-0.898190	2.119123
H	3.254179	-0.822057	-0.551328
H	4.382914	-2.813211	-0.332679
H	5.387481	-2.064087	-1.573225
H	5.896984	-2.072937	1.429237
H	6.910097	-2.791065	0.183033
H	7.742543	-0.561237	1.019364
H	7.484052	-0.605751	-0.720156
H	6.114098	2.090148	1.712552
H	7.658538	1.527858	1.123803
H	2.860225	1.140914	0.027739
H	3.909174	1.905062	1.206071
H	6.987920	2.409603	-1.185930
H	7.398248	3.572990	0.054903
H	5.424137	4.329297	-1.162010
H	5.063782	4.044338	0.524134
H	4.331084	2.214142	-1.799345
H	3.258170	3.246407	-0.890812
C	-4.246485	-0.258918	0.294692
H	-3.880331	-1.066589	-0.319394
C	-5.122837	0.706771	-0.386025
C	-5.823212	1.707164	0.291562
C	-5.296993	0.596024	-1.767268
C	-6.666533	2.567614	-0.394485

(3-4)DBU6-anti (si-re)₁₈₀

E₀ = -1610.5737477
E_{0+ZPE} = -1609.896245
E₂₉₈ = -1609.863053
H₂₉₈ = -1609.862109
G₂₉₈ = -1609.964843
NImag = 1 (-343.5265)

N	-6.040492	0.419479	-0.244736
C	-6.842311	-0.565933	-0.964211
C	-5.978626	-1.400434	-1.881486
C	-4.811475	-1.961978	-1.106192
N	-4.150527	-0.889385	-0.394648
C	-4.753608	0.206488	-0.015532
C	-3.937493	1.218778	0.722966
C	-4.323391	1.359845	2.196460
C	-5.562999	2.202578	2.441034
C	-6.824921	1.695430	1.764232
C	-6.724954	1.610264	0.249766
O	-1.508478	-1.091371	-0.027850
C	-0.987748	-1.776289	-0.945018
O	-1.576050	-2.324244	-1.887446
C	0.535009	-2.004167	-0.886535
N	1.242908	-1.085899	-0.003749
C	1.506784	-1.689957	1.301020
C	0.841333	-3.055388	1.228710
C	0.835372	-3.363373	-0.259917
C	1.483192	0.193726	-0.274968
C	0.959630	0.765144	-1.561063
C	0.498730	2.205278	-1.383518
C	1.600745	3.055633	-0.786052
C	2.054840	2.497299	0.552203
C	2.246407	1.009228	0.564808
H	0.923348	-1.939398	-1.899107
H	0.102745	-4.111049	-0.549977
H	1.818507	-3.704685	-0.581589
H	1.378817	-3.797019	1.814368
H	-0.178682	-2.998427	1.602559
H	2.578008	-1.782408	1.461862
H	1.096356	-1.060186	2.088999
H	1.320656	2.756775	1.322255
H	2.986908	2.978410	0.861717
H	0.143757	0.164417	-1.947981
H	2.507477	0.599098	1.530310
H	1.758757	0.725841	-2.306462
H	-3.115877	-0.972162	-0.242548
H	-4.065341	-2.417956	-1.750691
H	-5.149517	-2.714906	-0.392672
H	-5.612105	-0.785025	-2.702495
H	-6.574299	-2.203889	-2.307013
H	-7.589586	-0.024261	-1.537432
H	-7.366551	-1.196382	-0.244535
H	-6.240325	2.501035	-0.151951
H	-7.721422	1.576417	-0.178226
H	-2.900554	0.906224	0.644413
H	-4.025115	2.182603	0.220540
H	-7.107605	0.716967	2.157078
H	-7.643879	2.375284	2.000269
H	-5.737024	2.271368	3.515046
H	-5.367780	3.220426	2.094418
H	-4.442705	0.368994	2.637338
H	-3.480281	1.822237	2.708100
C	4.321693	0.757091	-0.280457
H	3.990842	0.737217	-1.307738
C	4.642918	-0.553268	0.302557
C	5.103232	-0.702334	1.613985
C	4.534393	-1.689408	-0.498137
C	5.433407	-1.951787	2.106960

(3-4)DBU6-anti (si-re)₃₀₀

E₀ = -1610.5746715
E_{0+ZPE} = -1609.896740
E₂₉₈ = -1609.863654
H₂₉₈ = -1609.862710
G₂₉₈ = -1609.965228
NImag = 1 (-342.8168)

N	5.901033	-0.692350	-0.449480
C	6.691365	0.073457	-1.408634
C	5.798512	0.791055	-2.394302
C	4.749708	1.579394	-1.648154
N	4.093537	0.715752	-0.691020
C	4.659009	-0.335693	-0.158615
C	3.854609	-1.121656	0.827051
C	4.372691	-1.017821	2.262826
C	5.574946	-1.896579	2.561282
C	6.794978	-1.626178	1.697617
C	6.554902	-1.818910	0.208935
O	1.529640	1.169993	-0.086694
C	0.930751	1.720934	-1.046025
O	1.433109	2.100404	-2.112562
C	-0.579058	1.985857	-0.889423
N	-1.200251	1.295932	0.232544
C	-1.230926	2.142125	1.426539
C	-0.637666	3.469174	0.969808
C	-0.827048	3.449674	-0.539389
C	-1.511211	0.004443	0.246534
C	-1.095913	-0.854757	-0.909594
C	-0.756176	-2.267485	-0.453359
C	-1.901122	-2.877002	0.330704
C	-2.250117	-2.028528	1.543894
C	-2.271648	-0.547978	1.276888
H	-1.064841	1.709401	-1.820984
H	-0.151880	4.112092	-1.073237
H	-1.850502	3.718153	-0.798370
H	-1.129183	4.313606	1.446029
H	0.422139	3.512141	1.212471
H	-2.244843	2.260003	1.798330
H	-0.643831	1.672094	2.214792
H	-1.516879	-2.217466	2.334767
H	-3.208916	-2.346325	1.957514
H	-0.241577	-0.418381	-1.416550
H	-2.400725	0.064985	2.157563
H	-1.910878	-0.892428	-1.635797
H	3.089834	0.914427	-0.457150
H	3.976966	1.966752	-3.205956
H	5.201452	2.422890	-1.124137
H	5.316479	0.066246	-3.049621
H	6.400561	1.451104	-3.013593
H	7.343445	-0.624907	-1.925951
H	7.322137	0.781582	-0.869293
H	5.979510	-2.728045	0.030871
H	7.505060	-1.944990	-0.299759
H	2.838390	-0.742407	0.776864
H	3.828309	-2.165990	1.513694
H	7.174220	-0.617145	1.869112
H	7.589226	-2.312669	1.992039
H	5.846850	-1.777851	3.610371
H	5.284464	-2.942653	2.434959
H	4.595918	0.024814	2.493882
H	3.555657	-1.307610	2.922319
C	-4.341163	-0.035606	0.632170
H	-4.566753	-0.197293	1.675162
C	-4.732522	-1.133982	-0.261312
C	-4.571796	-1.075806	-1.648374
C	-5.346041	-2.261494	0.287837
C	-4.990492	-2.121593	-2.453064

H -5.720027 1.817274 1.360594
 C -6.145561 1.449351 -2.451484
 H -4.764853 -0.176220 -2.305573
 C -6.832430 -2.443176 -1.766540
 H -7.199458 3.335581 0.147417
 H -6.272643 1.338056 -3.518659
 H -7.493931 3.112428 -2.297256
 C -4.440312 -0.572345 1.629179
 H -4.974542 0.027939 2.340895
 N -3.944204 -1.736778 2.154307
 O -3.293768 -2.518403 1.446280
 O -4.177261 -1.987613 3.346732
 H -0.281629 0.919859 3.214925
 H 0.149155 1.647247 1.679330
 H -2.681588 1.300738 2.736134
 H -1.805327 2.817004 2.693890

H 5.191480 0.160184 2.258524
 C 4.873126 -2.941981 -0.005661
 H 4.193272 -1.588198 -1.518830
 C 5.318925 -3.079039 1.299716
 H 5.782753 -2.049505 3.124843
 H 4.789362 -3.809441 -0.644448
 H 5.581210 -4.053172 1.686357
 C 5.037142 1.881109 0.091540
 H 5.551233 2.003701 1.026874
 N 5.161214 2.963716 -0.745085
 O 4.674447 2.943572 -1.882328
 O 5.802668 3.942545 -0.337566
 H 2.445921 3.082124 -1.473070
 H 1.262031 4.084016 -0.656751
 H 0.187162 2.599332 -2.350778
 H -0.380489 2.220660 -0.735813

H -4.115870 -0.209463 -2.104417
 C -5.768553 -3.307455 -0.518159
 H -5.505122 -2.310405 1.355659
 C -5.586243 -3.244652 -1.891775
 H -4.853740 -2.060001 -3.523195
 H -6.243666 -4.169323 -0.072080
 H -5.912870 -4.058745 -2.522523
 C -4.449171 1.278183 0.195918
 H -4.521986 1.584207 -0.831102
 N -4.521823 2.307265 1.088491
 O -4.404408 2.086301 2.305369
 O -4.697160 3.458838 0.660217
 H -0.523128 -2.876326 -1.326736
 H 0.145202 -2.237979 0.162129
 H -2.767387 -2.966837 -0.323680
 H -1.645782 -3.886452 0.654290

(3-4)DBU6-anti (re-si)₆₀

E₀ = -1610.5721705
 E_{0,ZPE} = -1609.894852
 E₂₉₈ = -1609.861513
 H₂₉₈ = -1609.860569
 G₂₉₈ = -1609.963849
 NImag = 1 (-324.4205)
 N 5.649420 -0.426437 -0.750123
 C 6.504512 0.742734 -0.929643
 C 5.674825 1.986369 -1.152936
 C 4.644219 2.113999 -0.057607
 N 3.931346 0.863288 0.082639
 C 4.422929 -0.295427 -0.265907
 C 3.552093 -1.495812 -0.073652
 C 4.042628 -2.440436 1.025020
 C 5.181096 -3.353708 0.604357
 C 6.434611 -2.636898 0.132533
 C 6.215145 -1.732874 -1.070136
 O 1.387283 1.035009 0.843326
 C 0.836000 1.963033 0.194688
 O 1.396895 2.759226 -0.570101
 C -0.683372 2.163602 0.361988
 N -1.307427 1.129633 1.175878
 C -1.398452 1.551004 2.574901
 C -0.873144 2.981627 2.587571
 C -0.993401 3.434628 1.141669
 C -1.525102 -0.118178 0.757850
 C -1.582457 -0.444217 -0.594007
 C -1.450952 -1.866553 -1.064116
 C -1.832257 -2.907721 -0.023554
 C -1.275462 -2.540042 1.336066
 C -1.789009 -1.179973 1.785034
 H -1.111006 2.203328 -0.634227
 H -0.313793 4.239645 0.879699
 H -2.008531 3.757697 0.916881
 H -1.430070 3.609226 3.278879
 H 0.170615 2.989662 2.896466
 H -2.434347 1.492897 2.908041
 H -0.800812 0.909833 3.218175
 H -0.184304 -2.516795 1.299489
 H -1.551478 -3.287358 2.079798
 H -1.201379 0.289449 -1.289116
 H -1.325891 -0.911344 2.729322
 H 2.927223 0.916043 0.392608
 H 3.900337 2.872930 -0.283725
 H 5.118127 2.368561 0.891363
 H 5.177308 1.925813 -2.120294
 H 6.324562 2.857764 -1.166161
 H 7.141470 0.553576 -1.788999
 H 7.147707 0.855694 -0.055439
 H 5.585686 -2.229581 -1.809483
 H 7.166220 -1.532925 -1.552758

(3-4)DBU6-anti (re-si)₁₈₀

E₀ = -1610.5713338
 E_{0,ZPE} = -1609.894422
 E₂₉₈ = -1609.860886
 H₂₉₈ = -1609.859941
 G₂₉₈ = -1609.964706
 NImag = 1 (-328.9950)
 N -5.482813 0.096976 -1.131567
 C -5.915205 -0.991762 -2.003340
 C -4.732011 -1.789043 -2.502084
 C -3.866609 -2.195410 -1.334502
 N -3.561095 -1.026988 -0.538427
 C -4.336958 0.022347 -0.470817
 C -3.896767 1.146595 0.410445
 C -4.767019 1.319347 1.656639
 C -6.074344 2.051346 1.408098
 C -6.992990 1.391102 0.394134
 C -6.383244 1.237282 -0.989992
 O -1.231642 -0.960800 0.754658
 C -0.388473 -1.714790 0.203338
 O -0.587589 -2.462113 -0.764474
 C 1.026871 -1.768517 0.807897
 N 1.348956 -0.610304 1.632968
 C 1.246996 -0.919578 3.059904
 C 0.708831 -2.340371 3.103701
 C 1.159837 -2.935605 1.781845
 C 1.542557 0.609870 1.132110
 C 1.694013 0.853170 -0.233714
 C 1.366882 2.199374 -0.809703
 C 1.519453 3.360136 0.160331
 C 0.962093 3.006309 1.523415
 C 1.651875 1.768807 2.080744
 H 1.733451 -1.869052 -0.007882
 H 0.572654 -3.793377 1.466148
 H 2.203301 -3.241592 1.837886
 H 1.080603 -2.886058 3.967391
 H -0.377548 -2.321033 3.156017
 H 2.230114 -0.845470 3.527131
 H 0.578321 -0.229837 3.566836
 H -0.111587 2.816235 1.455452
 H 1.095195 3.832580 2.221608
 H 1.488681 0.029423 -0.901721
 H 1.236489 1.519986 3.050655
 H -2.642145 -1.009026 -0.027637
 H -2.917207 -2.621048 -1.646018
 H -4.378560 -2.932161 -0.713528
 H -4.149448 -1.186185 -3.198150
 H -5.086922 -2.666403 -3.036765
 H -6.450734 -0.547699 -2.837945
 H -6.613885 -1.630118 -1.460653
 H -5.863399 2.150649 -1.281826
 H -7.172284 1.080037 -1.718072

(3-4)DBU6-anti (re-si)₃₀₀

E₀ = -1610.5736467
 E_{0,ZPE} = -1609.896848
 E₂₉₈ = -1609.863305
 H₂₉₈ = -1609.862361
 G₂₉₈ = -1609.967047
 NImag = 1 (-334.8414)
 N -5.513375 0.888618 0.086365
 C -6.237458 1.192638 -1.143675
 C -5.277975 1.394128 -2.294048
 C -4.344173 0.211530 -2.389534
 N -3.770566 -0.056052 -1.088856
 C -4.332364 0.289465 0.038749
 C -3.600733 -0.042551 1.299154
 C -4.282933 -1.132468 2.127265
 C -5.454765 -0.643619 2.960599
 C -6.584581 -0.012048 2.165154
 C -6.165849 1.203650 1.353144
 O -1.359106 -1.166723 -1.009017
 C -0.593287 -0.635368 -1.853812
 O -0.909239 0.193675 -2.718502
 C 0.885260 -1.067361 -1.854561
 N 1.292550 -1.771047 -0.650974
 C 1.459545 -3.200698 -0.880483
 C 0.938833 -3.416099 -2.291410
 C 1.176982 -2.075345 -2.965177
 C 1.581713 -1.161898 0.496936
 C 1.638192 0.225381 0.619044
 C 1.563112 0.891842 1.963552
 C 2.110860 0.041797 3.095969
 C 1.564608 -1.367665 3.005580
 C 1.943402 -2.009590 1.679825
 H 1.478922 -0.168405 -1.994380
 H 0.552812 -1.906406 -3.838149
 H 2.219033 -1.986896 -3.270721
 H 1.447560 -4.238509 -2.788097
 H -0.125754 -3.641871 -2.266702
 H 2.518870 -3.451902 -0.791647
 H 0.903967 -3.787305 -0.152708
 H 0.476938 -1.348387 3.103255
 H 1.944831 -1.985622 3.818582
 H 1.225023 0.808084 -0.190742
 H 1.484543 -2.990189 1.597831
 H -2.813964 -0.494037 -1.061312
 H -3.515635 0.399160 -3.066901
 H -4.875848 -0.673912 -2.740331
 H -4.702571 2.305728 -2.134953
 H -5.838249 1.510371 -3.218315
 H -6.815409 2.095955 -0.970405
 H -6.937950 0.384347 -1.358961
 H -5.517515 1.850842 1.945092
 H -7.042448 1.789099 1.096732

H	2.559938	-1.128257	0.172151	H	-2.872153	0.936321	0.702690	H	-2.605053	-0.366697	1.010586
H	3.472808	-2.032749	-1.019546	H	-3.886628	2.070471	-0.168742	H	-3.488225	0.865305	1.892708
H	6.872547	-2.050939	0.942765	H	-7.318900	0.411611	0.749233	H	-7.043500	-0.744439	1.498287
H	7.176984	-3.383502	-0.150420	H	-7.891262	2.000154	0.289263	H	-7.362014	0.309615	2.858749
H	5.436213	-4.007255	1.438931	H	-6.605454	2.157904	2.354252	H	-5.849330	-1.478531	3.539997
H	4.829299	-4.004354	-0.200296	H	-5.848505	3.064366	1.065900	H	-5.087651	0.088058	3.684796
H	4.325538	-1.859519	1.904288	H	-4.956876	0.342813	2.105404	H	-4.596605	-1.944110	1.468639
H	3.194963	-3.053330	1.325076	H	-4.183943	1.882364	2.384200	H	-3.531212	-1.552896	2.794005
C	-3.670702	0.199410	-1.126484	C	3.952743	0.722308	-0.466379	C	3.777176	0.499743	-0.121916
H	-3.280872	0.128027	-2.130447	H	4.153749	1.109898	0.520345	H	3.496553	-0.029052	-1.019487
C	-4.520016	-0.921363	-0.706017	C	4.074872	-0.734652	-0.612024	C	3.691445	1.964774	-0.196421
C	-4.796686	-1.936385	-1.623709	C	4.512602	-1.483746	0.479539	C	3.107202	2.547541	-1.323322
C	-5.115596	-0.987151	0.556289	C	3.823920	-1.394065	-1.818337	C	4.201114	2.805313	0.795535
C	-5.629889	-2.992524	-1.288620	C	4.702038	-2.854042	0.370731	C	3.039220	3.923347	-1.460835
H	-4.363858	-1.888109	-2.612625	H	4.721204	-0.984373	1.415335	H	2.707061	1.910593	-2.100468
C	-5.945196	-3.053330	0.892183	C	4.001802	-2.761699	-1.922463	C	4.128009	4.183061	0.660884
H	-4.927684	-0.210504	1.283012	H	3.472063	-0.838258	-2.675441	H	4.663381	2.388088	1.677579
C	-6.203178	-3.053320	-0.026940	C	4.442803	-3.498873	-0.828462	C	3.548274	4.748256	-0.466145
H	-5.833300	-3.765829	-2.015262	H	5.050828	-3.416446	1.225047	H	2.589604	4.351961	-2.344830
H	-6.394441	-2.078846	1.874298	H	3.794047	-3.258193	-2.859391	H	4.528608	4.816709	1.439043
H	-6.851695	-3.875941	0.237428	H	4.582979	-4.566656	-0.914381	H	3.495566	5.822307	-0.569993
C	-3.942037	1.480938	-0.677963	C	4.292977	1.555978	-1.514572	C	4.745065	-0.120217	0.649866
H	-4.564604	1.726013	0.162322	H	4.296973	1.274167	-2.551368	H	5.285044	0.337506	1.457063
N	-3.457525	2.570039	-1.349262	N	4.687350	2.854480	-1.297274	N	5.124287	-1.413315	0.400998
O	-2.687213	2.416796	-2.308649	O	4.785764	3.999929	-0.147179	O	4.574911	-2.069118	-0.495731
O	-3.802743	3.700116	-0.974034	O	4.969155	3.550549	-2.282453	O	6.039722	-1.897853	1.084876
H	-2.864093	-1.237852	1.971813	H	2.711603	1.982236	2.243327	H	3.023703	-2.172957	1.653698
H	-1.467667	-3.886948	-0.335432	H	1.017563	4.240390	-0.242504	H	1.856367	0.493329	4.055019
H	-2.916796	-2.983914	0.048884	H	2.573975	3.612398	0.265204	H	3.199781	0.005839	3.041160
H	-2.041012	-2.012023	-1.971490	H	1.988345	2.370978	-1.693429	H	2.079359	1.852506	1.927426
H	-0.411271	-2.028609	-1.367382	H	0.335752	2.167416	-1.177083	H	0.515479	1.134211	2.173604

**Other conformations in enamine-DBU
carboxylate pathway**

(3-4)DBU3-anti (re-re)₆₀

E ₀	= -1610.5781509
E _{0+ZPE}	= -1609.901061
E ₂₉₈	= -1609.867669
H ₂₉₈	= -1609.866725
G ₂₉₈	= -1609.969740
NImag	= 1 (-321.3942)
N	-5.929504 0.637611 -0.252637
C	-6.272966 1.987364 -0.688884
C	-5.302970 2.478021 -1.737795
C	-3.889313 2.306251 -1.237704
N	-3.704254 0.952747 -0.760682
C	-4.678588 0.204121 -0.311105
C	-4.327511 -1.170089 0.159491
C	-4.509404 -1.372044 1.665133
C	-5.942619 -1.606270 2.108706
C	-6.903532 -0.479773 1.771175
C	-7.008563 -0.187230 0.283402
O	-1.192400 0.244864 -1.176378
C	-0.576335 -0.760631 -0.728964
O	-1.023954 -1.629592 0.026716
C	0.863896 -0.885184 -1.258309
N	1.702227 -1.747058 -0.437600
C	1.834629 -3.081695 -1.011437
C	0.953751 -3.053472 -2.250736
C	0.893273 -1.579198 -2.616874
C	2.162307 -1.398061 0.764113
C	2.155803 -0.070258 1.177967
C	2.47267 0.307313 2.594662
C	3.389396 -0.692145 3.281844
C	2.846929 -2.093945 3.092454
C	2.782316 -2.468573 1.620214
H	1.284605 0.111134 -1.320763

(3-4)DBU4-anti (re-re)₆₀

E ₀	= -1610.5786376
E _{0+ZPE}	= -1609.901211
E ₂₉₈	= -1609.867932
H ₂₉₈	= -1609.866988
G ₂₉₈	= -1609.969382
NImag	= 1 (-311.8496)
N	-5.726149 1.062790 0.327067
C	-5.996768 2.395335 -0.202026
C	-4.716712 3.180826 -0.362032
C	-3.721023 2.366401 -1.151036
N	-3.601471 1.048795 -0.564842
C	-4.556357 0.474805 0.120959
C	-4.295594 -0.896902 0.650939
C	-5.126561 -1.982024 -0.036207
C	-6.556202 -2.086361 0.465815
C	-7.382321 -0.820964 0.307365
C	-6.813622 0.389378 1.031138
O	-1.230934 0.050263 -1.170049
C	-0.601691 -0.830844 -0.523140
O	-1.020121 -1.483398 0.438905
C	0.814951 -1.094729 -1.066435
N	1.658909 -1.821581 -0.129234
C	1.751454 -3.237267 -0.468580
C	0.826594 -3.404154 -1.664299
C	0.784610 -2.016042 -2.282279
C	2.148912 -1.283504 0.988602
C	2.185575 0.094849 1.165413
C	2.538995 0.740525 2.490419
C	3.430516 -0.188839 3.333223
C	2.842264 -1.583607 3.396680
C	2.749348 -2.207099 2.013021
H	1.255216 -0.136790 -1.318304

(3-4)DBU5-anti (re-re)₆₀

E ₀	= -1610.5784448
E _{0+ZPE}	= -1609.901010
E ₂₉₈	= -1609.867709
H ₂₉₈	= -1609.866765
G ₂₉₈	= -1609.969370
NImag	= 1 (-319.9735)
N	-5.756195 0.130866 0.017797
C	-6.447800 -0.898359 0.786563
C	-5.826373 -2.254499 0.549101
C	-4.336720 -2.175021 0.779033
N	-3.790310 -1.071836 0.018684
C	-4.483393 -0.014660 -0.320430
C	-3.780680 1.049241 -1.097042
C	-3.555033 2.335771 -0.301147
C	-4.775751 3.234361 -0.208270
C	-5.991706 2.591645 0.436464
C	-6.498078 1.351739 -0.284551
O	-1.193116 -1.448704 -0.393115
C	-0.504076 -0.912069 -1.295738
O	-0.910331 -0.153083 -2.188749
C	0.999532 -1.242398 -1.345874
N	1.515161 -1.799726 -0.102946
C	1.652975 -3.250538 -0.175319
C	1.115391 -3.617788 -1.549816
C	1.295887 -2.343874 -2.359062
C	1.691532 -1.083926 1.008141
C	1.725772 0.305833 0.969910
C	1.710121 1.123805 2.228229
C	2.298549 0.390151 3.419238
C	1.676129 -0.986514 3.530673
C	1.956298 -1.822843 2.291837
H	1.523471 -0.329340 -1.603984

H	0.032103	-1.317371	-3.225851	H	-0.090729	-1.840117	-2.901320	H	0.645632	-2.282405	-3.227234
H	1.797333	-1.288724	-3.149869	H	1.676467	-1.847793	-2.883944	H	2.328696	-2.256785	-2.692756
H	1.360429	-3.671015	-3.047655	H	1.190868	-4.163342	-2.351912	H	1.643976	-4.467546	-1.974599
H	-0.040663	-3.421681	-2.006995	H	-0.166496	-3.697229	-1.328913	H	0.059946	-3.873992	-1.480794
H	2.883530	-3.260431	-1.259131	H	2.788093	-3.476070	-0.717871	H	2.707632	-3.513333	-0.065433
H	1.516017	-3.847870	-0.309488	H	1.450459	-3.866060	0.365217	H	1.097134	-3.742348	0.618771
H	1.846604	-2.151227	3.527226	H	1.845683	-1.531640	3.840368	H	0.597174	-0.880643	3.663525
H	3.460713	-2.826189	3.616532	H	3.439527	-2.232265	4.037089	H	2.050883	-1.516206	4.406188
H	1.496678	0.610459	0.661477	H	1.541154	0.695285	0.542216	H	1.302817	0.791573	0.104188
H	2.210576	-3.387223	1.508436	H	2.148964	-3.112657	2.066466	H	1.343393	-2.721059	2.317932
H	-2.734159	0.556214	-0.832751	H	-2.692274	0.543770	-0.717981	H	-2.775928	-1.129515	-0.242800
H	-6.281883	2.653582	0.174963	H	-2.735794	2.824009	-1.141224	H	-3.835600	-3.082750	0.454614
H	-7.280520	1.955078	-1.093117	H	-4.034344	2.274744	-2.191712	H	-4.115194	-2.033613	1.837618
H	-7.923643	0.360979	0.084414	H	-4.305236	3.416164	0.619015	H	-6.024379	-2.574070	-0.473496
H	-7.068863	-1.117406	-0.282576	H	-4.926911	4.118450	-0.870246	H	-6.275080	-2.982489	1.220039
H	-4.929507	-1.896073	-0.389172	H	-6.661846	2.896105	0.495962	H	-7.487836	-0.902294	0.472489
H	-3.282281	-1.344560	-0.090157	H	-6.519263	2.304908	-1.155466	H	-6.419618	-0.636990	1.845524
H	-7.899670	-0.751229	2.121892	H	-6.482466	0.114018	2.032869	H	-6.508237	1.514462	-1.362839
H	-6.625118	0.436096	2.295933	H	-7.591500	1.136050	1.152961	H	-7.523138	1.153763	0.011626
C	3.924189	0.647588	-0.037461	H	-3.233042	-1.100496	0.524594	H	-2.826614	0.640370	-1.427634
H	4.587852	0.162201	0.674860	H	-4.494527	-0.903754	1.723638	H	-4.361191	1.265458	-1.995046
C	3.692226	2.088957	0.148278	H	-7.512991	-0.574654	-0.748075	H	-5.786498	2.336924	1.478025
C	2.759941	2.801738	-0.609532	H	-8.378895	-1.002258	0.710811	H	-6.805571	3.317279	0.446819
C	4.446788	2.781642	1.095395	H	-7.056319	-2.905417	-0.051838	H	-4.513179	4.135715	0.346222
C	2.596116	4.163998	-0.428907	H	-6.535558	-2.357862	1.524421	H	-5.047587	3.560158	-1.215499
H	2.147556	2.287304	-1.336597	H	-5.112818	-1.824069	-1.115860	H	-3.189079	2.087189	0.696535
C	4.285413	4.148358	1.273658	H	-4.623740	-2.932482	0.138645	H	-2.751942	2.883281	-0.792655
H	5.176576	2.246523	1.686777	C	3.956272	0.535848	-0.180036	C	3.816603	0.540955	0.139907
C	3.359158	4.844743	0.512832	H	4.617015	0.172884	0.591962	H	4.221030	0.309384	1.113091
H	1.866918	4.696959	-1.022050	C	3.774037	1.994845	-0.235713	C	3.715816	1.971787	-0.188067
H	4.884572	4.666405	2.008611	C	2.848256	2.602035	-1.087695	C	3.086327	2.430826	-1.347161
H	3.228550	5.908077	0.652291	C	4.571813	2.809788	0.567880	C	4.293162	2.907257	0.670759
C	3.915531	0.111358	-1.311650	C	2.732352	3.980231	-1.137300	C	3.044505	3.782890	-1.639572
H	3.509617	0.598651	-2.178612	H	2.204734	1.992784	-1.706616	H	2.613428	1.726851	-2.017086
N	4.455892	-1.119788	-1.570818	C	4.458474	4.191838	0.515132	C	4.255077	4.262668	0.375568
O	4.947845	-1.792446	-0.654701	H	5.297107	2.356400	1.228822	H	4.788931	2.567027	1.569171
O	4.451877	-1.533585	-2.740385	C	3.538020	4.782170	-0.336836	C	3.630133	4.705399	-0.780002
H	3.780935	-2.675493	1.237045	H	2.008275	4.431679	-1.800293	H	2.549281	4.119810	-2.538886
H	3.472518	-0.451724	4.341851	H	5.090445	4.805019	1.141373	H	4.713881	4.970729	1.050617
H	4.396928	-0.631844	2.864046	H	3.444988	5.857780	-0.377306	H	3.595571	5.760343	-1.010557
H	2.919806	1.304183	2.614105	C	3.900044	-0.206579	-1.344122	C	4.067966	-0.374905	-0.864556
H	1.545510	0.391489	3.163811	H	3.491977	0.142991	-2.274402	H	3.951835	-0.179642	-1.914641
H	-3.163973	2.480853	-2.027307	N	4.389804	-1.484515	-1.398952	N	4.515231	-1.637660	-0.580939
H	-3.676306	3.007561	-0.430132	O	4.879860	-2.009917	-0.390485	O	4.680044	-1.993904	0.593904
H	-5.502935	3.523866	-1.956424	O	4.341846	-2.091304	-2.479738	O	4.762393	-2.404528	-1.524070
H	-5.440354	1.911616	-2.658431	H	3.737089	-2.508849	1.666487	H	2.993763	-2.155391	2.286893
H	-3.910439	-2.237808	1.944139	H	3.538224	0.230182	4.333764	H	2.129079	0.963824	4.330644
H	-4.081024	-0.522537	2.199231	H	4.432594	-0.237876	2.900816	H	3.380346	0.291676	3.304477
H	-5.956567	-1.778851	3.185273	H	3.010678	1.675122	2.330631	H	2.238712	2.062616	2.057877
H	-6.308259	-2.525786	1.644500	H	1.618529	0.916002	3.044699	H	0.677953	1.408601	2.458220

(3-4)DBU7-anti (re-re)₆₀

$E_0 = -1610.578597$

$E_{0+ZPE} = -1609.901082$

$E_{298} = -1609.867897$

$H_{298} = -1609.866952$

$G_{298} = -1609.968707$

$N_{\text{Imag}} = 1 (-318.7860)$

N	5.722129	-1.128986	0.270773
C	5.952026	-1.656195	1.611559
C	4.654910	-2.099977	2.245959
C	3.639913	-0.986581	2.155776
N	3.563083	-0.513176	0.790845
C	4.554898	-0.595017	-0.058664
C	4.337191	-0.043455	-1.429146
C	5.130955	1.235237	-1.701047
C	6.592983	1.001503	-2.041436
C	7.388566	0.265761	-0.976083
C	6.857462	-1.120833	-0.647056

O	1.249280	0.699120	0.345963
C	0.622780	0.639176	-0.741591
O	1.019391	0.126362	-1.798712
C	-0.765852	1.302157	-0.806819
N	-1.349714	1.553979	0.503610
C	-1.193788	2.947366	0.907424
C	-0.392174	3.584234	-0.217044
C	-0.687952	2.698618	-1.416551
C	-1.822590	0.590785	1.295748
C	-2.122520	-0.670131	0.792383
C	-2.447825	-1.818641	1.702106
C	-3.045077	-1.374923	3.024720
C	-2.185634	-0.286470	3.634338
C	-2.116155	0.934556	2.730751
H	-1.408116	0.658775	-1.397113
H	0.064260	2.758145	-2.198244
H	-1.655147	2.959081	-1.843303
H	-0.676986	4.621228	-0.376222
H	0.669731	3.555777	0.019449
H	-2.182796	3.399721	1.009933
H	-0.682718	3.029503	1.863200
H	-1.178503	-0.676446	3.798066
H	-2.568519	0.016492	4.608701
H	-1.686093	-0.946666	-0.154859
H	-1.345942	1.609329	3.098020
H	2.667115	-0.051704	0.493550
H	6.441520	-0.893040	2.218630
H	6.634413	-2.496792	1.521576
H	7.634570	-1.700979	-0.159875
H	6.592272	-1.654481	-1.560096
H	8.414150	0.147779	-1.327142
H	7.438925	0.853330	-0.057267
H	6.647965	0.430788	-2.971991
H	7.069144	1.961658	-2.241712
C	-4.076326	-0.135856	-0.215865
H	-4.562962	-0.116622	0.747139
C	-4.226548	-1.382481	-0.982832
C	-3.544641	-1.614920	-2.179559
C	-5.105348	-2.360926	-0.517355
C	-3.745757	-2.785333	-2.890436
H	-2.841439	-0.882667	-2.550871
C	-5.310080	-3.532414	-1.232074
H	-5.644898	-2.194247	0.404483
C	-4.630828	-3.749150	-2.421037
H	-3.206239	-2.949406	-3.812186
H	-6.000669	-4.274259	-0.857458
H	-4.785277	-4.662012	-2.977869
C	-3.980313	1.072967	-0.879144
H	-3.747782	1.183839	-1.922196
N	-4.196672	2.258820	-0.229186
O	-4.465212	2.269429	0.979990
O	-4.129891	3.312784	-0.880099
H	-3.055254	1.485657	2.766240
H	-3.126288	-2.226078	3.700889
H	-4.057482	-0.994447	2.871702
H	-3.120535	-2.508637	1.191030
H	-1.535242	-2.392374	1.895747
H	2.649869	-1.327458	2.445803
H	3.911776	-0.159589	2.812933
H	4.277779	-2.983590	1.732072
H	4.832062	-2.367944	3.284425
H	4.605429	-0.808808	-2.158845
H	3.269273	0.136903	-1.541719
H	4.653199	1.741018	-2.539088
H	5.041453	1.908841	-0.847134

syn-addition

(3-4)DBU-*syn* (re-re)₁₈₀

E₀ = -1610.5758495

E_{0+ZPE} = -1609.897980

(3-4)DBU2-*syn* (re-re)₁₈₀

E₀ = -1610.5758048

E_{0+ZPE} = -1609.898143

(3-4)DBUx-*syn* (re-re)₁₈₀

E₀ = -1610.5761759

E_{0+ZPE} = -1609.898270

$E_{298} = -1609.864859$
 $H_{298} = -1609.863914$
 $G_{298} = -1609.966232$
 $N_{\text{Imag}} = 1 (-370.9171)$

N	5.451061	1.125960	-0.583586
C	5.163415	1.871791	-1.805864
C	3.676218	1.933109	-2.067480
C	3.091657	0.543308	-2.003333
N	3.504437	-0.092543	-0.770856
C	4.606912	0.208017	-0.136240
C	4.905524	-0.551940	1.116369
C	6.097361	-1.502424	0.985177
C	7.452401	-0.825227	1.093918
C	7.713187	0.249196	0.052129
C	6.720658	1.400342	0.083373
O	1.813969	-1.502649	0.366802
C	0.621687	-1.540843	0.068551
O	0.241057	-0.606385	-0.645499
C	-0.410310	-2.509085	0.670833
N	-1.793267	-2.085536	0.493315
C	-2.479011	-2.888945	-0.515363
C	-1.374128	-3.708226	-1.153939
C	-0.371598	-3.868623	-0.025204
C	-2.406257	-1.126920	1.185732
C	-3.716911	-0.733367	0.894789
C	-4.546390	0.002551	1.911918
C	-3.734594	0.780490	2.935318
C	-2.567975	-0.405073	3.437018
C	-1.655111	-0.436365	2.284693
H	-0.170774	-2.620301	1.724807
H	0.632191	-4.117983	-0.355626
H	-0.704204	-4.642111	0.667034
H	-1.742645	-4.655849	-1.538589
H	-0.929702	-3.157291	-1.981555
H	-3.214193	-3.528358	-0.019739
H	-3.012077	-2.263007	-1.226352
H	-2.933259	-0.946273	3.934646
H	-1.990058	0.511470	4.174552
H	-4.279156	-1.403551	0.261357
H	-0.845884	-1.061841	2.647814
H	2.844352	-0.779800	-0.330647
H	5.685689	1.404390	-2.641879
H	5.566835	2.872813	-1.680478
H	7.143870	2.255984	-0.432457
H	6.533123	1.715071	1.110796
H	8.704466	0.669269	0.224721
H	7.726530	-0.181032	-0.950886
H	7.542013	-0.377079	2.086700
H	8.232889	-1.583640	1.027310
C	-3.573087	0.660374	-0.830125
H	-2.862789	-0.003374	-1.297397
C	-3.000679	1.889368	-0.263828
C	-3.786157	2.971608	0.142435
C	-1.611135	2.001898	-0.174130
C	-3.198434	4.126418	0.632265
H	-4.862531	2.922026	0.079898
C	-1.026223	3.161839	0.310347
H	-0.991726	1.166556	-0.477196
C	-1.816015	4.227617	0.718922
H	-3.822485	4.952084	0.943103
H	0.050834	3.231873	0.368919
H	-1.360255	5.131231	1.097670
C	-4.857674	0.670661	-1.355746
H	-5.610424	1.404392	-1.139243
N	-5.304969	-0.350213	-2.145491
O	-4.545393	-1.281969	-2.453876
O	-6.478846	-0.319180	-2.546780
H	-1.188496	0.458657	1.866975
H	-4.378759	1.078219	3.763098
H	-3.349004	1.696983	2.489530

$E_{298} = -1609.865014$
 $H_{298} = -1609.864070$
 $G_{298} = -1609.966252$
 $N_{\text{Imag}} = 1 (-375.7360)$

N	5.710876	0.886245	-0.922818
C	5.330658	2.208777	-1.410922
C	3.884527	2.228677	-1.850350
C	3.011400	1.673982	-0.751135
N	3.542534	0.402581	-0.311342
C	4.802226	0.068942	-0.412055
C	5.196473	-1.277355	0.105958
C	6.054193	-1.216580	1.371189
C	7.518238	-0.899006	1.120582
C	7.774710	0.426991	0.424836
C	7.129772	0.543581	-0.947458
O	1.859184	-1.407632	0.688495
C	0.683710	-1.255925	0.258887
O	0.285059	-0.361964	-0.495626
C	-0.293000	-2.341007	0.743077
N	-1.694759	-2.042190	0.479936
C	-2.237872	-2.881556	-0.583867
C	-1.019168	-3.556387	-1.182052
C	-0.071985	-3.659047	-0.000115
C	-2.438364	-1.166416	1.154036
C	-3.762428	-0.894785	0.791739
C	-4.715090	-0.257284	1.765750
C	-4.039851	0.580671	2.840067
C	-2.832600	-0.139347	3.404385
C	-1.820156	-0.435422	2.307896
H	-0.120548	-2.476602	1.807071
H	0.969427	-3.791580	-0.277921
H	-0.359968	-4.491538	0.641785
H	-1.263099	-4.520467	-1.621101
H	-0.589536	-2.928332	-1.960853
H	-2.923562	-3.612180	-0.146387
H	-2.798462	-2.294403	-1.306306
H	-3.142447	-1.074837	3.875446
H	-2.352593	0.459838	4.177892
H	-4.220067	-1.607865	0.121945
H	-0.987873	-1.000636	2.715914
H	2.868186	-0.303250	0.076512
H	1.992886	1.495611	-1.083344
H	2.973299	2.361748	0.094911
H	3.765637	1.629610	-2.752629
H	3.593278	3.248656	-2.088049
H	5.981877	2.496551	-2.246639
H	5.508469	2.945293	-0.625949
H	7.272889	-0.377220	-1.513735
H	7.614520	1.334831	-1.509634
H	4.276898	-1.816934	0.312666
H	5.722531	-1.823012	-0.677909
H	7.442691	1.260425	1.046692
H	8.850057	0.547359	0.290701
H	8.050145	-0.911131	2.072252
H	7.951521	-1.698933	0.514984
H	5.622119	-0.496172	2.067620
H	5.984894	-2.189399	1.856028
C	-3.666952	0.524558	-0.911112
H	-2.871706	-0.058371	-1.348461
C	-3.245817	1.794863	-0.304594
C	-4.150454	2.795802	0.059323
C	-1.880258	2.032772	-0.130691
C	-3.701682	3.994838	0.588514
H	-5.211830	2.647962	-0.068619
C	-1.434483	3.236692	0.392580
H	-1.169831	1.260520	-0.399503
C	-2.342118	4.221374	0.757905
H	-4.416124	4.756766	0.865424
H	-0.374029	3.405366	0.516115
H	-1.994305	5.159603	1.165882

$E_{298} = -1609.865114$
 $H_{298} = -1609.864170$
 $G_{298} = -1609.966761$
 $N_{\text{Imag}} = 1 (-367.9092)$

N	-5.076617	-0.172436	0.051283
C	-5.793661	0.464001	1.151887
C	-5.179522	1.802172	1.493788
C	-3.695163	1.637848	1.712984
N	-3.121850	0.916348	0.597985
C	-3.795876	0.090109	-0.159238
C	-3.055706	-0.580892	-1.271724
C	-2.866649	-2.084793	-1.064893
C	-4.090637	-2.921897	-1.392959
C	-5.330046	-2.583626	-0.582279
C	-5.805913	-1.149490	-0.751666
O	-0.571763	1.390822	-0.059280
C	-0.285611	2.609964	0.076131
O	-0.968102	3.469286	0.647793
C	1.019191	3.107059	-0.568745
N	1.968993	2.048357	-0.884512
C	2.005547	1.758965	-2.314885
C	0.861459	2.570120	-2.893354
C	0.743093	3.740559	-1.932540
C	2.744186	1.417173	-0.004219
C	3.530810	0.320730	-0.372832
C	4.694498	-0.117833	0.473167
C	4.582393	0.272329	1.938651
C	4.104370	1.702553	2.078083
C	2.744302	1.884449	1.428055
H	1.457887	3.836420	0.105005
H	-0.223864	4.235020	-1.957833
H	1.509274	4.485238	-2.147630
H	1.059762	2.876788	-3.917329
H	-0.053461	1.980615	-2.872666
H	2.969519	2.082326	-2.716011
H	1.907531	0.693317	-2.507684
H	4.823406	2.383500	1.617140
H	4.030643	1.984310	3.128238
H	3.671854	0.178472	-1.433810
H	2.444743	2.926169	1.479218
H	-2.120986	1.108562	0.357018
H	-5.785023	-0.200418	2.017305
H	-6.826701	0.589948	0.840568
H	-6.842789	-1.069506	-0.442291
H	-5.768330	-0.857630	-1.801688
H	-6.143362	-3.238079	-0.897059
H	-5.162427	-2.779517	0.478483
H	-4.324540	-2.800898	-2.453614
H	-3.846220	-3.974617	-1.249982
C	2.148258	-1.421978	-0.398504
H	1.399993	-0.814504	-0.883067
C	1.898003	-1.704148	1.021185
C	2.610593	-2.667636	1.740061
C	0.868026	-1.015936	1.666624
C	2.307166	-2.924886	3.067008
H	3.407717	-3.224428	1.271121
C	0.561986	-1.280829	2.992427
H	0.313499	-0.265275	1.116868
C	1.282536	-2.233337	3.699937
H	2.870537	-3.671753	3.607888
H	-0.240177	-0.740083	3.474596
H	1.046101	-2.439139	4.734022
C	2.799772	-2.357930	-1.189035
H	3.425695	-3.149482	-0.823605
N	2.764569	-2.277881	-2.552255
O	2.092861	-1.396182	-3.111086
O	3.409717	-3.108051	-3.211369
H	1.990958	1.316689	1.971890
H	5.548530	0.141416	2.426875
H	3.878705	-0.384432	2.449397

H	-5.244053	0.668216	1.396635	C	-4.916766	0.416586	-1.505803	H	4.824903	-1.199158	0.377894
H	-5.174925	-0.723952	2.436846	H	-5.751824	1.064171	-1.317357	H	5.607986	0.320717	0.059033
H	2.005564	0.550128	-2.007203	N	-5.216542	-0.629680	-2.331445	H	-5.356395	2.505879	0.681031
H	3.429142	-0.056475	-2.849813	O	-4.349091	-1.470218	-2.616912	H	-5.652662	2.200352	2.387813
H	3.196755	2.568108	-1.323100	O	-6.366834	-0.713693	-2.789009	H	-3.179928	2.592349	1.772427
H	3.499526	2.374980	-3.044738	H	-1.400967	0.500277	1.930935	H	-3.500773	1.090310	2.636247
H	5.078722	0.153026	1.929700	H	-4.755616	0.807277	3.630646	H	-2.541115	-2.273634	-0.040979
H	4.011274	-1.116525	1.363798	H	-3.717133	1.534177	2.422856	H	-2.045614	-2.397589	-1.708400
H	6.010589	-2.241416	1.780638	H	-5.442789	0.346630	1.216977	H	-3.580483	-0.396198	-2.209690
H	6.021903	-2.053148	0.046290	H	-5.299496	-1.047492	2.247811	H	-2.086209	-0.096676	-1.343617

3DBU

$E_0 = -1096.5680552$
 $E_{0+ZPE} = -1096.034119$
 $E_{298} = -1096.010082$
 $H_{298} = -1096.009138$
 $G_{298} = -1096.091391$
 $N_{\text{Imag}} = 0$

C	-5.037874	-0.741660	0.463817
C	-4.012129	-0.268937	-0.276231
C	-3.337497	-1.127040	-1.313266
C	-4.111153	-2.396216	-1.631664
C	-4.609507	-3.066115	-0.366069
C	-5.571803	-2.140401	0.357214
N	-3.541504	1.016505	-0.162698
C	-2.277556	1.474671	-0.693354
C	-2.381457	2.985310	-0.491241
C	-3.105465	3.103664	0.843327
C	-4.043911	1.899376	0.866123
C	-1.028221	0.920093	0.009716
O	-1.137930	0.368417	1.110436
O	0.052149	1.112242	-0.622922
N	2.128937	0.182107	0.710218
C	2.035568	1.040896	2.152668
C	2.848829	-1.018739	2.674655
C	4.243381	-0.964084	2.094484
N	4.202609	-0.822278	0.642080
C	3.152729	-0.276853	0.042881
C	5.388018	-1.233471	-0.103434
C	6.145229	-0.090832	-0.762227
C	5.545329	0.375802	-2.077761
C	4.117639	0.885166	-1.984039
C	3.117996	-0.139905	-1.445817
H	-2.185191	1.237503	-1.750773
H	-1.409551	3.471404	-0.501697
H	-2.984876	3.412082	-1.292360
H	-3.639870	4.045144	0.950399
H	-2.391528	3.033467	1.661631
H	-5.079373	2.177610	0.649262
H	-4.039801	1.408414	1.842890
H	-5.777305	-2.528354	1.357399
H	-6.537056	-2.149972	-0.162812
H	-2.333892	-1.377934	-0.962141
H	-5.516153	-0.094849	1.185750
H	-3.202737	-0.549750	-2.227832
H	-3.477494	-3.069864	-2.209102
H	-4.967929	-2.150978	-2.264070
H	-3.759150	-3.289184	0.283087
H	-5.094752	-4.015247	-0.596473
H	1.294546	0.555422	0.174623
H	4.808944	-0.133788	2.520137
H	4.781486	-1.881413	2.318586
H	6.033040	-1.727156	0.616388
H	5.110989	-1.984422	-0.844367

3DBU1

$E_0 = -1096.5682627$
 $E_{0+ZPE} = -1096.034206$
 $E_{298} = -1096.010225$
 $H_{298} = -1096.009281$
 $G_{298} = -1096.090772$
 $N_{\text{Imag}} = 0$

N	3.991761	1.175408	-0.003564
C	3.999407	2.393687	-0.805984
C	2.633490	3.039161	-0.814352
C	1.595187	2.018168	-1.210789
N	1.745692	0.833362	-0.393918
C	2.877475	0.474335	0.154422
C	2.882634	-0.782455	0.961340
C	3.663261	-1.923835	0.307820
C	5.170101	-1.828035	0.475279
C	5.796164	-0.562210	-0.085089
C	5.268773	0.720834	0.537838
O	-0.525762	-0.492857	-0.311025
C	-0.905794	-1.279354	0.595675
O	-0.239917	-1.645907	1.577722
C	-2.315778	-1.878528	0.464729
N	-3.246366	-1.121548	-0.343832
C	-3.265353	-1.569669	-1.717936
C	-2.367806	-2.803178	-1.739663
C	-2.268991	-3.213852	-0.276736
C	-3.753670	0.105731	0.004059
C	-4.389241	0.913574	-0.872270
C	-4.959749	2.254457	-0.511573
C	-4.416827	2.772200	0.808571
C	-4.470511	1.671628	1.849898
C	-3.595147	0.494969	1.450150
H	-2.695417	-2.017744	1.473941
H	-1.373234	-3.785692	-0.047033
H	-3.134500	-3.810886	0.010975
H	-2.766180	-3.593154	-2.372725
H	-1.383427	-2.535505	-2.117020
H	-4.290707	-1.797866	-2.024305
H	-2.893603	-0.793400	-2.391903
H	-5.504440	1.334712	1.957310
H	-4.156577	2.039440	2.826957
H	-4.511960	0.595484	-1.898034
H	-3.833189	-0.360573	2.081599
H	0.888493	0.232695	-0.261290
H	4.322802	2.155659	-1.820587
H	4.732986	3.068672	-0.373667
H	5.970385	1.527874	0.354113
H	5.189182	0.614763	1.620365
H	3.301786	-0.564954	1.944738
H	1.845160	-1.077870	1.116561
H	6.870904	-0.595179	0.096431
H	5.663506	-0.512126	-1.167555
H	-4.741192	2.969472	-1.307982

3DBU2

$E_0 = -1096.5679216$
 $E_{0+ZPE} = -1096.034121$
 $E_{298} = -1096.009994$
 $H_{298} = -1096.009050$
 $G_{298} = -1096.091968$
 $N_{\text{Imag}} = 0$

N	-4.348036	-0.709561	-0.654754
C	-4.209508	-1.987600	-1.346485
C	-2.820531	-2.144300	-1.921905
C	-1.793658	-1.870564	-0.849989
N	-2.087038	-0.603470	-0.217747
C	-3.287079	-0.093724	-0.150738
C	-3.437901	1.215498	0.556216
C	-4.189788	1.106462	1.884268
C	-5.700237	1.035036	1.742336
C	-6.209601	-0.140156	0.925323
C	-5.696384	-0.171295	-0.505342
O	-0.045104	0.808435	0.680716
C	0.988407	0.605660	-0.022792
O	1.101369	-0.233523	-0.923420
C	2.165411	1.541312	0.297201
N	3.443436	1.135619	-0.242929
C	3.685456	1.711515	-1.546800
C	2.535045	2.691735	-1.761430
C	1.962899	2.902764	-0.366259
C	4.157507	0.044013	0.186735
C	3.742202	-0.531099	1.514889
C	4.769302	-1.488459	2.096636
C	5.285384	-2.444719	1.039246
C	5.990583	-1.664203	-0.056048
C	5.193058	-0.475062	-0.507104
H	2.210236	1.647267	1.378624
H	0.920873	3.211692	-0.367299
H	2.540127	3.653114	0.173998
H	2.863420	3.618325	-2.227294
H	1.782737	2.243233	-2.407169
H	4.660517	2.207446	-1.563619
H	3.702465	0.940146	-2.321233
H	6.184073	-2.317563	-0.909823
H	6.979071	-1.354995	0.303948
H	2.783054	-1.039679	1.392474
H	5.481531	-0.027065	-1.447470
H	3.566644	0.280086	2.221166
H	4.325365	-2.029668	2.932408
H	5.609550	-0.918728	2.500829
H	4.444785	-2.996600	0.611665
H	5.961079	-3.179446	1.478599
H	-1.271033	-0.038565	0.151346
H	-0.875740	-1.795527	-1.248184
H	-1.802810	-2.660777	-0.097534
H	-2.683650	-1.446321	-2.747499
H	-2.703129	-3.151445	-2.313976

H 7.162799 -0.436394 -0.946838
H 6.219912 0.738784 -0.056623
H 5.575109 -0.454653 -2.787718
H 6.174172 1.161396 -2.497421
H 0.980491 0.051448 2.396066
H 2.399731 1.082984 2.565663
H 2.908014 -0.984741 3.759700
H 2.370012 -1.957042 2.396513
H 4.074357 1.788496 -1.373246
H 3.783042 1.173545 -2.979683
H 3.299285 -1.114298 -1.900299
H 2.107816 0.158386 -1.710640

H -6.053741 2.207776 -0.454803
H -3.380671 3.094110 0.678050
H -4.983751 3.643816 1.137476
H -2.544883 0.727624 1.642043
H 3.319021 -2.851676 0.763103
H 3.399736 -1.987961 -0.749351
H 5.407350 -1.889408 1.540519
H 5.636690 -2.694687 0.005954
H 0.587642 2.397034 -1.064184
H 1.697781 1.750518 -2.263226
H 2.406227 3.428929 0.177393
H 2.629880 3.873889 -1.510567

H -4.951774 -2.013194 -2.139820
H -4.436109 -2.798133 -0.652042
H -5.742052 0.824662 -0.947968
H -6.336278 -0.809617 -1.105787
H -2.435982 1.596873 0.730163
H -3.944910 1.922173 -0.101353
H -5.962186 -1.085011 1.412879
H -7.297827 -0.087627 0.880630
H -6.147692 0.999272 2.735984
H -6.052752 1.959989 1.278896
H -3.818715 0.245312 2.442346
H -3.934939 1.986074 2.473999

3DBU3

E₀ = -1096.5681456
E_{0+ZPE} = -1096.033940
E₂₉₈ = -1096.009994
H₂₉₈ = -1096.009050
G₂₉₈ = -1096.090453
NImag = 0

N 4.343898 0.066607 -0.247980
C 5.290067 -0.810408 0.432851
C 4.741372 -2.213982 0.540156
C 3.354110 -2.171117 1.134171
N 2.544814 -1.217576 0.406949
C 3.042729 -0.185597 -0.223644
C 2.083540 0.730247 -0.910720
C 1.956770 2.096895 -0.236041
C 3.086535 3.060586 -0.556161
C 4.475149 2.567397 -0.185059
C 4.880167 1.272059 -0.871776
O -0.015821 -1.702917 0.759371
C -0.967061 -1.339241 0.010176
O -0.862191 -0.756198 -1.076013
C -2.362131 -1.710436 0.538242
N -3.460323 -0.968983 -0.040639
C -4.020384 -1.643048 -1.191102
C -3.319842 -2.998612 -1.231867
C -2.716097 -3.147199 0.158294
C -3.678900 0.371786 0.164634
C -2.956988 0.981527 1.336685
C -3.490205 2.352958 1.718638
C -3.716279 3.214053 0.491365
C -4.765804 2.571107 -0.398236
C -4.512381 1.105901 -0.603083
H -2.337293 -1.597077 1.619556
H -1.853035 -3.807663 0.187041
H -3.459131 -3.529012 0.858469
H -4.001793 -3.808293 -1.482497
H -2.530896 -2.984645 -1.980773
H -5.104218 -1.740224 -1.078730
H -3.841052 -1.074567 -2.107450
H -4.788561 3.074865 -1.367290
H -5.757117 2.736902 0.039820
H -1.891810 1.045419 1.101659
H -5.036953 0.633946 -1.421919
H -3.036951 0.313917 2.194316
H -2.796158 2.830182 2.410936
H -4.437499 2.238631 2.251230
H -2.777731 3.308658 -0.060634
H -4.023561 4.220908 0.776669
H 1.497663 -1.352452 0.437444
H 5.512285 -0.403038 1.420412
H 6.211867 -0.808307 -0.142222
H 5.959441 1.164727 -0.838867
H 4.597986 1.293827 -1.924799
H 2.401597 0.858548 -1.946310
H 1.114374 0.233288 -0.935307
H 5.202364 3.329064 -0.468136
H 4.563034 2.437875 0.895382

3DBU4

E₀ = -1096.5680525
E_{0+ZPE} = -1096.034012
E₂₉₈ = -1096.009948
H₂₉₈ = -1096.009004
G₂₉₈ = -1096.091462
NImag = 0

N -4.377337 -0.755740 -0.357104
C -5.055279 -1.706024 0.517916
C -4.065518 -2.656632 1.149126
C -2.949538 -1.870043 1.793071
N -2.414822 -0.920909 0.841239
C -3.110439 -0.424311 -0.148544
C -2.432528 0.566223 -1.037647
C -2.971636 1.989820 -0.885977
C -4.273520 2.247542 -1.624206
C -5.429631 1.354527 -1.207497
C -5.173520 -0.130849 -1.409227
O 0.047123 -0.284004 1.519405
C 0.928219 0.241620 0.780867
O 0.804551 0.530044 -0.415650
C 2.247672 0.556672 1.505427
N 3.373072 0.849411 0.647179
C 3.496068 2.264872 0.381057
C 2.458861 2.924588 1.286055
C 2.123849 1.848985 2.310864
C 4.013325 -0.074313 -0.141576
C 3.743076 -1.518775 0.186538
C 4.729944 -2.472411 -0.467474
C 4.966433 -2.104425 -1.919327
C 5.582196 -0.718691 -2.001645
C 4.864949 0.271321 -1.130820
H 2.461483 -0.283132 2.162653
H 1.139498 1.965876 2.756573
H 2.862807 1.841915 3.112124
H 2.831116 3.839660 1.741493
H 1.571615 3.177804 0.709269
H 4.513024 2.601469 0.603981
H 3.306816 2.487440 -0.672395
H 5.570000 -0.369224 -3.036473
H 6.642155 -0.781052 -1.727678
H 2.723709 -1.765540 -0.119813
H 5.055115 1.316948 -1.327786
H 3.775064 -1.654519 1.267302
H 4.359876 -3.493901 -0.376460
H 5.681923 -2.433127 0.067584
H 4.013081 -2.113459 -2.453234
H 5.612323 -2.837654 -2.403731
H -1.416528 -0.610519 0.988019
H -2.136921 -2.518920 2.107702
H -3.308877 -1.338300 2.675084
H -3.655828 -3.318867 0.387051
H -4.572498 -3.271334 1.888520
H -5.773056 -2.254809 -0.085652
H -5.610881 -1.159517 1.281607
H -4.703708 -0.309348 -2.376955
H -6.118950 -0.663159 -1.417679

3DBU5

E₀ = -1096.5681425
E_{0+ZPE} = -1096.033983
E₂₉₈ = -1096.010005
H₂₉₈ = -1096.009061
G₂₉₈ = -1096.090736
NImag = 0

N -4.108682 -0.307864 0.549066
C -4.378096 -0.727770 1.920043
C -3.384852 -1.773941 2.368695
C -1.981057 -1.286845 2.102968
N -1.874155 -0.842214 0.730416
C -2.887747 -0.389809 0.038969
C -2.623659 0.055437 -1.361759
C -2.739961 1.568216 -1.555248
C -4.166581 2.076204 -1.678246
C -5.059982 1.765608 -0.488945
C -5.215524 0.280781 -0.198407
O 0.639002 -0.951735 -0.043092
C 1.067445 -0.994031 -1.225688
O 0.378975 -0.887550 -2.259214
C 2.589072 -1.092667 -1.424863
N 3.398090 -0.727689 -0.282932
C 3.721678 -1.872692 0.538586
C 3.199614 -3.075786 -0.242262
C 3.007855 -2.543463 -1.655847
C 3.500799 0.546292 0.218561
C 3.028323 1.650132 -0.690007
C 3.479992 3.029864 -0.239085
C 3.293782 3.208027 1.255245
C 4.150365 2.200364 2.001758
C 4.020840 0.816502 1.435210
H 2.834451 -0.483874 -2.292067
H 2.272338 -3.098211 -2.232582
H 3.951543 -2.560886 -2.201052
H 3.880272 -3.923238 -0.199261
H 2.243163 -3.395260 0.166522
H 4.801874 -1.923681 0.704227
H 3.248572 -1.797768 1.521413
H 3.872370 2.188968 3.058175
H 5.195052 2.532538 1.979471
H 1.938082 1.612985 -0.750240
H 4.375176 0.004771 2.054894
H 3.391946 1.466053 -1.700547
H 2.931040 3.789403 -0.796236
H 4.536748 3.163799 -0.482684
H 2.241998 3.054138 1.509260
H 3.550708 4.223974 1.557604
H -0.914379 -0.869965 0.293741
H -1.251259 -2.077430 2.253466
H -1.722338 -0.465608 2.772471
H -3.560544 -2.703630 1.828394
H -3.522305 -1.973747 3.428320
H -5.387353 -1.128891 1.947961
H -4.347983 0.143482 2.576110
H -5.366745 -0.275346 -1.124250
H -6.099341 0.120839 0.410732

H 4.704602 -2.670506 -0.448433
H 5.400583 -2.815512 1.160847
H 2.865569 -3.139502 1.070486
H 3.392997 -1.887859 2.186846
H 2.898671 4.008842 -0.051773
H 3.069643 3.273896 -1.627984
H 1.017900 2.535505 -0.571174
H 1.862359 1.962983 0.842876

H -1.368208 0.543363 -0.805060
H -2.540006 0.239189 -2.072834
H -5.694771 1.530025 -0.163106
H -6.305973 1.617932 -1.800470
H -4.560777 3.290419 -1.486365
H -4.099817 2.114710 -2.695006
H -3.080465 2.228144 0.173518
H -2.210024 2.665646 -1.272926

H -1.622190 -0.279953 -1.630623
H -3.320375 -0.454405 -2.028478
H -4.694193 2.266272 0.409601
H -6.054775 2.166036 -0.686193
H -4.147873 3.154581 -1.838776
H -4.616764 1.639519 -2.573377
H -2.221799 2.082038 -0.744064
H -2.199540 1.818600 -2.467388

3DBU6

E₀ = -1096.568233
E_{0+ZPE} = -1096.034190
E₂₉₈ = -1096.010170
H₂₉₈ = -1096.009226
G₂₉₈ = -1096.091084
NImag = 0
N -4.021193 -0.004117 -0.411209
C -4.729030 -1.245507 -0.707699
C -3.797723 -2.262782 -1.326256
C -2.570791 -2.411901 -0.460982
N -2.016645 -1.164488 -0.169386
C -2.717361 -0.014897 -0.168141
C -1.994395 1.255878 0.144953
C -2.389659 1.873488 1.487315
C -3.696795 2.646184 1.458806
C -4.910810 1.828642 1.051872
C -4.812006 1.220204 -0.338198
O 0.566917 -0.964794 0.325808
C 1.233673 -1.772375 -0.376950
O 0.770287 -2.589976 -1.186911
C 2.761067 -1.775643 -0.199430
N 3.322203 -0.614907 0.456087
C 3.447213 -0.806144 1.883558
C 3.071574 -2.266699 2.116928
C 3.190589 -2.902639 0.738644
C 3.364933 0.643681 -0.089885
C 3.115513 0.726638 -1.572174
C 3.510082 2.067986 -2.169493
C 3.035001 3.216951 -1.301340
C 3.696575 3.134911 0.063093
C 3.640550 1.748992 0.636121
H 3.193405 -1.917371 -1.187357
H 2.582381 -3.795270 0.618336
H 4.227237 -3.166121 0.528796
H 3.708853 -2.743920 2.858218
H 2.044149 -2.332646 2.468910
H 4.469924 -0.586170 2.204241
H 2.785317 -0.129456 2.430878
H 3.214331 3.833046 0.751119
H 4.734090 3.479449 -0.020985
H 2.058346 0.526485 -1.762330
H 3.839877 1.655068 1.694354
H 3.666871 -0.066666 -2.076221
H 3.106865 2.146209 -3.179359
H 4.597790 2.118822 -2.260089
H 1.949780 3.156916 -1.186081
H 3.254036 4.174819 -1.774477
H -0.975352 -1.058106 0.013843
H -1.789159 -2.991339 -0.954021
H -2.819848 -2.925209 0.473368
H -3.505660 -1.933983 -2.323281
H -4.315394 -3.213288 -1.427844
H -5.537038 -1.007463 -1.393925
H -5.174772 -1.634332 0.209263
H -4.419016 1.951405 -1.045751
H -5.803747 0.950576 -0.686112
H -0.933611 1.022994 0.146739
H -2.169367 1.970659 -0.659978
H -5.100452 1.033624 1.775460
H -5.787629 2.476781 1.062399

3DBU7

E₀ = -1096.568193
E_{0+ZPE} = -1096.033982
E₂₉₈ = -1096.009960
H₂₉₈ = -1096.009016
G₂₉₈ = -1096.090932
NImag = 0
N 4.018421 1.149056 0.099211
C 4.016126 2.514897 -0.413426
C 2.695586 3.194289 -0.135658
C 1.563628 2.316909 -0.612833
N 1.725108 0.984751 -0.072820
C 2.886214 0.474724 0.244830
C 2.902697 -0.924542 0.767328
C 3.498127 -1.930768 -0.217992
C 5.017063 -1.937802 -0.255103
C 5.656492 -0.606443 -0.613258
C 5.317639 0.529175 0.340296
O -0.533083 -0.367408 -0.078364
C -0.893889 -1.112146 0.870595
O -0.226229 -1.390312 1.879742
C -2.279043 -1.772487 0.767327
N -3.172738 -1.210409 -0.221106
C -3.040244 -1.871819 -1.499905
C -2.137724 -3.074113 -1.229305
C -2.153219 -3.216594 0.287229
C -3.738975 0.037806 -0.133605
C -3.725541 0.669927 1.232771
C -4.662896 1.861327 1.347885
C -4.543476 2.771071 0.140878
C -4.949907 2.015623 -1.111987
C -4.311190 0.659442 -1.186969
H -2.719947 -1.738341 1.761004
H -1.270656 -3.709471 0.686307
H -3.031208 -3.776989 0.608331
H -2.481147 -3.971262 -1.739725
H -1.126986 -2.863537 -1.573169
H -4.024914 -2.168510 -1.872314
H -2.601090 -1.202536 -2.244748
H -4.680295 2.595082 -1.997957
H -6.042774 1.931969 -1.140500
H -2.702776 0.927058 1.470524
H -4.325657 0.169836 -2.150527
H -4.000711 -0.076348 1.977600
H -4.448360 2.402279 2.269956
H -5.693527 1.506240 1.423476
H -3.508401 3.108442 0.045311
H -5.160539 3.661717 0.265684
H 0.858189 0.386954 0.015414
H 4.226847 2.497412 -1.483928
H 4.825454 3.050223 0.076022
H 6.048128 1.324163 0.229539
H 5.375764 0.190672 1.375411
H 3.466366 -0.943147 1.700828
H 1.876221 -1.188288 1.016252
H 6.740002 -0.728457 -0.603063
H 5.385703 -0.308961 -1.628320
H 2.593266 3.377326 0.933525
H 2.669719 4.155695 -0.642425
H 0.600520 2.695780 -0.282387
H 1.544035 2.268758 -1.702436

3DBU-conf

E₀ = -1096.5686704
E_{0+ZPE} = -1096.034544
E₂₉₈ = -1096.010591
H₂₉₈ = -1096.009646
G₂₉₈ = -1096.091407
NImag = 0
N -4.384357 -0.359631 0.545272
C -4.448852 -0.880109 1.906963
C -3.075381 -0.935842 2.534419
C -2.117651 -1.626292 1.592231
N -2.182955 -0.987352 0.296869
C -3.260881 -0.406943 -0.155606
C -3.184673 0.240189 -1.502425
C -3.440330 1.748412 -1.489588
C -4.905930 2.145505 -1.425287
C -5.648496 1.665336 -0.189997
C -5.626305 0.156190 -0.017754
O 0.010627 -0.896917 -1.157502
C 1.060383 -0.964414 -0.451786
O 1.104440 -1.023239 0.782124
C 2.363342 -1.013455 -1.265107
N 3.570142 -0.734094 -0.520223
C 4.169593 -1.938746 0.009133
C 3.357543 -3.079768 -0.598007
C 2.624159 -2.433291 -1.765715
C 3.904725 0.498538 -0.015575
C 3.137449 1.667192 -0.574197
C 3.768641 3.009753 -0.241639
C 4.202337 3.066327 1.210164
C 5.263793 2.011424 1.467542
C 4.880111 0.675598 0.901398
H 2.249206 -0.328618 -1.022207
H 1.707611 -2.948964 -2.040325
H 3.267195 -2.390208 -2.644650
H 3.983921 -3.914839 -0.904374
H 2.640226 -3.451880 0.130546
H 5.225841 -1.987648 -0.271920
H 4.125848 -1.953754 1.101430
H 5.436965 1.914837 2.541707
H 6.217769 2.352936 1.048376
H 2.113991 1.629570 -0.193376
H 5.427732 -0.181005 1.268344
H 3.061644 1.564055 -1.656463
H 3.062239 3.807631 -0.471823
H 4.641885 3.168808 -0.878999
H 3.338058 2.878963 1.852136
H 4.580547 4.057668 1.462491
H -1.293945 -0.941234 -0.278671
H -4.908380 -1.869591 1.886434
H -5.101767 -0.222872 2.476654
H -5.826950 -0.338823 -0.967948
H -6.411461 -0.152938 0.665804
H -2.191004 0.038768 -1.891589
H -3.895214 -0.252457 -2.168126
H -5.242897 2.131061 0.710038
H -6.690728 1.977269 -0.262956
H -4.978912 3.231606 -1.485946
H -5.412802 1.752891 -2.310562
H -2.885468 2.205083 -0.668755
H -3.013281 2.152729 -2.406518

H -3.872505 3.081221 2.442976
H -3.593029 3.484195 0.764890
H -2.425733 1.093596 2.249769
H -1.588338 2.550408 1.780182

H 5.352573 -2.695279 -0.964076
H 5.387983 -2.247817 0.725260
H 3.150700 -2.920121 0.076897
H 3.091671 -1.748437 -1.214372

H -1.085849 -1.557279 1.924497
H -2.371703 -2.682781 1.491583
H -3.131590 -1.467778 3.480782
H -2.720527 0.073965 2.738976

3DBUS

E₀ = -1096.5677059
E_{0+ZPE} = -1096.033596
E₂₉₈ = -1096.009572
H₂₉₈ = -1096.008628
G₂₉₈ = -1096.090416
NImag = 0
N 3.521201 -0.801561 -0.355498
C 4.153368 -1.937179 0.276947
C 3.391504 -3.150266 -0.247750
C 2.687357 -2.631172 -1.493689
C 2.360516 -1.183695 -1.127510
C 1.017543 -1.108195 -0.382304
O 0.003393 -1.129052 -1.142867
C 3.802512 0.478231 0.052713
C 3.006721 1.570832 -0.610753
C 5.073312 2.152561 1.438266
O 1.001666 -1.063790 0.851350
H 2.267017 -0.577709 -0.225472
H 1.800283 -3.200260 -1.759635
H 3.365728 -2.640678 -2.346819
H 4.047685 -3.993118 -0.453766
H 2.656618 -3.471744 0.487384
H 5.215443 -1.971523 0.015165
H 4.092897 -1.865407 1.365990
C 4.750639 0.762888 0.971768
C 3.581348 2.958028 -0.371885
C 3.980484 3.143708 1.078999
H 5.226897 2.146713 2.519724
H 6.022834 2.496518 1.011011
H 1.976980 1.523761 -0.248537
H 5.320509 -0.041538 1.415118
H 2.958910 1.382676 -1.683064
H 2.851790 3.708299 -0.677859
H 4.462189 3.100163 -1.002778
H 3.109656 2.974605 1.717067
H 4.317383 4.165168 1.259741
H -1.362314 -1.107868 -0.374514
N -2.317192 -1.126770 0.088665
C -2.547668 -2.108756 1.124422
H -1.960656 -2.990464 0.883096
H -2.184058 -1.722543 2.076691
C -4.021640 -2.427372 1.199603
H -4.325217 -2.980604 0.311279
H -4.231693 -3.048570 2.066642
C -4.813728 -1.144160 1.296926
H -5.875384 -1.345811 1.185031
H -4.665198 -0.669124 2.267961
C -3.215569 -0.258846 -0.291136
N -4.428962 -0.212210 0.242068
C -5.395837 0.815991 -0.128346
H -5.590969 0.764528 -1.200147
H -6.320217 0.544989 0.371342
C -4.995356 2.227435 0.271148
C -2.817529 0.719057 -1.350614
H -1.861656 0.384985 -1.743246
H -3.540605 0.674824 -2.165805
C -2.690071 2.155316 -0.839903
C -4.012629 2.885201 -0.682569
H -4.593796 2.208365 1.286072
H -5.903963 2.829176 0.305600
H -3.816037 3.903498 -0.346364
H -4.485242 2.970734 -1.664374
H -2.139346 2.157226 0.101814
H -2.073931 2.698992 -1.554851

3DBU9

E₀ = -1096.5676643
E_{0+ZPE} = -1096.033580
E₂₉₈ = -1096.009553
H₂₉₈ = -1096.008609
G₂₉₈ = -1096.090305
NImag = 0
N -4.388220 -1.083295 -0.073630
C -4.363905 -2.172488 -1.044194
C -3.033543 -2.888579 -1.016179
C -1.913688 -1.884955 -1.149048
N -2.099398 -0.820384 -0.187468
C -3.265493 -0.480086 0.293410
C -3.302559 0.658271 1.262429
C -3.973911 1.911393 0.696904
C -5.491946 1.874636 0.724284
C -6.115844 0.732829 -0.059675
C -5.693113 -0.648511 0.414205
O -0.033081 0.538237 0.732041
C 0.981862 0.550665 -0.026315
O 1.109817 -0.078236 -1.081425
C 2.111217 1.480640 0.443940
N 3.410765 1.207473 -0.128195
C 3.647847 1.980022 -1.327313
C 2.457920 2.930524 -1.422890
C 1.855455 2.912543 -0.024607
C 4.153601 0.084162 0.142750
C 3.740329 -0.698710 1.360318
C 4.786176 -1.709473 1.803743
C 5.349560 -2.472332 0.620384
C 6.044083 -1.509744 -0.326738
C 5.213206 -0.291645 -0.604849
H 2.141143 1.434212 1.529991
H 0.799997 3.172685 -0.005355
H 2.387329 3.603028 0.629938
H 2.750670 3.928385 -1.742440
H 1.737023 2.547624 -2.141871
H 4.599319 2.514341 -1.247917
H 3.713360 1.333109 -2.205996
H 6.272680 -2.016479 -1.266948
H 7.015901 -1.228777 0.096382
H 2.795226 -1.204923 1.149387
H 5.499454 0.303532 -1.460599
H 3.537253 -0.010133 2.180211
H 4.345463 -2.388298 2.534205
H 5.601986 -1.188389 2.310686
H 4.534433 -2.977024 0.095811
H 6.043103 -3.245053 0.954420
H -1.245345 -0.288902 0.145939
H -4.569076 -1.773443 -2.038717
H -5.167901 -2.857269 -0.789005
H -6.402692 -1.387347 0.056571
H -5.710044 -0.698836 1.503374
H -7.200112 0.794033 0.037871
H -5.891659 0.827546 -1.123695
H -5.821240 1.804305 1.764104
H -5.876201 2.821153 0.343320
H -0.944153 -2.335576 -0.961226
H -1.887711 -1.463596 -2.154147
H -2.992769 -3.609938 -1.828495
H -2.930831 -3.435798 -0.079523
H -3.615185 2.085398 -0.318880
H -3.633485 2.758256 1.291156
H -3.812051 0.338694 2.172113
H -2.273317 0.881935 1.526124

3DBU10

E₀ = -1096.5679001
E_{0+ZPE} = -1096.033825
E₂₉₈ = -1096.009845
H₂₉₈ = -1096.008901
G₂₉₈ = -1096.090302
NImag = 0
N -4.271481 -0.925009 -0.429361
C -4.722545 -2.190237 0.139421
C -3.548745 -3.091813 0.443456
C -2.530570 -2.339227 1.266063
N -2.226975 -1.078009 0.626259
C -3.064335 -0.450088 -0.156510
C -2.623229 0.858597 -0.727338
C -3.353927 2.059282 -0.124524
C -4.742054 2.291857 -0.575899
C -5.704065 1.125846 -0.541589
C -5.239250 -0.159944 -1.208554
O 0.057336 -0.030155 1.402325
C 0.894609 0.435576 0.575898
O 0.755272 0.487538 -0.652073
C 2.161315 1.021990 1.219678
N 3.318982 1.094350 0.356330
C 3.410309 2.365965 -0.325269
C 2.305000 3.220346 0.288762
C 1.944830 2.492582 1.577173
C 4.021734 0.002986 -0.093094
C 3.775761 -1.286901 0.643379
C 4.816805 -2.353235 0.342006
C 5.112555 -2.427200 -1.143384
C 5.690454 -1.105349 -1.617238
C 4.904966 0.069589 -1.112478
H 2.372000 0.439549 2.113124
H 0.932102 2.693419 1.918388
H 2.632357 2.768142 2.377101
H 2.623808 4.246357 0.461916
H 1.445580 3.244932 -0.377195
H 4.402546 2.801711 -0.175129
H 3.270409 2.246332 -1.402611
H 5.716382 -1.082976 -2.709182
H 6.737604 -1.037261 -1.299758
H 2.778877 -1.655368 0.388922
H 5.076479 1.014690 -1.608013
H 3.761549 -1.092568 1.715362
H 4.468700 -3.314345 0.720789
H 5.740329 -2.119607 0.876805
H 4.187544 -2.637914 -1.685141
H 5.803080 -3.243561 -1.359150
H -1.294768 -0.627044 0.845867
H -1.603242 -2.898404 1.357170
H -2.906704 -2.155686 2.273251
H -3.093253 -3.428462 -0.487511
H -3.895487 -3.970433 0.981211
H -5.381551 -2.660245 -0.585930
H -5.305451 -1.992555 1.040384
H -4.829894 0.049319 -2.197260
H -6.087666 -0.820328 -1.354624
H -1.550844 0.933848 -0.563698
H -2.773845 0.839205 -1.860794
H -5.901696 0.926192 0.513471
H -6.658796 1.400717 -0.991157
H -5.175992 3.176203 -0.229541
H -4.645968 2.521976 -1.761261
H -3.402018 1.950784 0.960488
H -2.744431 2.941275 -0.316359

3DBU11E₀ = -1096.5683306E_{0+ZPE} = -1096.034086E₂₉₈ = -1096.010136H₂₉₈ = -1096.009192G₂₉₈ = -1096.090577

NImag = 0

N	-3.969851	0.067836	-0.530325
C	-4.631948	-1.098043	-1.107223
C	-3.631821	-2.018101	-1.768838
C	-2.507428	-2.320125	-0.807766
N	-1.989751	-1.082020	-0.268171
C	-2.698346	0.009407	-0.157930
C	-2.027579	1.205510	0.438295
C	-2.561921	1.574820	1.822977
C	-3.873829	2.339975	1.804167
C	-5.028139	1.611276	1.137339
C	-4.782984	1.261458	-0.321731
O	0.560618	-0.968147	0.397835
C	1.261304	-1.785484	-0.259277
O	0.836498	-2.629555	-1.063368
C	2.779981	-1.765440	-0.023013
N	3.311749	-0.545152	0.543326
C	3.388556	-0.603644	1.985861
C	3.007967	-2.038251	2.340411
C	3.174386	-2.798239	1.031673
C	3.365549	0.658034	-0.115170
C	3.174773	0.598262	-1.607781
C	3.583277	1.880675	-2.314156
C	3.065157	3.100352	-1.577639
C	3.674079	3.155493	-0.187606
C	3.606500	1.829435	0.512893
H	3.251783	-1.995682	-0.975301
H	2.570687	-3.700498	0.974296
H	4.217449	-3.077600	0.882834
H	3.621709	-2.442079	3.142749
H	1.969653	-2.076470	2.662520
H	4.399414	-0.349616	2.318886
H	2.706977	0.116863	2.445960
H	3.160506	3.910610	0.411822
H	4.711533	3.501718	-0.264709
H	2.127660	0.370405	-1.820841
H	3.766389	1.837752	1.581906
H	3.751445	-0.233291	-2.011780
H	3.220072	1.858114	-3.341875
H	4.673315	1.934810	-2.366858
H	1.976844	3.038369	-1.498471
H	3.294470	4.012190	-2.130498
H	-0.966555	-1.052440	0.001206
H	-1.674571	-2.827623	-1.286308
H	-2.860046	-2.950651	0.009939
H	-3.232894	-1.544866	-2.665700
H	-4.130295	-2.935694	-2.071058
H	-5.353135	-0.736908	-1.835410
H	-5.182821	-1.621969	-0.324408
H	-4.334927	2.106320	-0.846047
H	-5.730950	1.059315	-0.809708
H	-0.968653	0.973632	0.503884
H	-2.132688	2.051007	-0.242167
H	-5.275802	0.699550	1.684298
H	-5.912045	2.248564	1.176125
H	-4.152836	2.588486	2.828422
H	-3.717276	3.290731	1.288385
H	-2.656595	0.670658	2.426686
H	-1.804980	2.189030	2.308784

Different conformation of Enamine intermediate

1_i (Cyhex_{Conf})

$E_0 = -634.5121219$
 $E_{0+ZPE} = -634.232212$
 $E_{298} = -634.219850$
 $H_{298} = -634.218906$
 $G_{298} = -634.271259$
 $N\text{Imag} = 0$

N	0.429174	0.556919	0.168744
C	0.850716	1.944364	0.339694
C	2.340376	1.912056	0.066273
C	2.438676	0.885663	-1.049497
C	1.406925	-0.170159	-0.640985
C	2.064270	-1.276208	0.174932
O	1.759830	-1.264690	1.460519
C	-0.941911	0.279354	0.042229
C	-1.295427	-1.129760	-0.351401
C	-3.357286	0.916966	0.242995
O	2.815424	-2.087093	-0.299844
H	0.966018	-0.642131	-1.514941
H	3.430182	0.462110	-1.181910
H	2.130320	1.328643	-1.994670
H	2.725562	2.887318	-0.219367
H	2.887764	1.579793	0.948610
H	0.340572	2.586772	-0.384865
H	0.602602	2.300074	1.337789
C	-1.885197	1.193108	0.310012
C	-2.734633	-1.478652	-0.010149
C	-3.674595	-0.382990	-0.475580
H	-3.770649	0.886469	1.256444
H	-3.858733	1.750867	-0.251586
H	-0.623357	-1.833225	0.141166
H	-1.597707	2.187035	0.622183
H	-1.135582	-1.259352	-1.424364
H	1.119188	-0.532801	1.559394
H	-2.992209	-2.434045	-0.466145
H	-3.556375	-0.244538	-1.552792
H	-4.713142	-0.664930	-0.303010
H	-2.832175	-1.604678	1.070323

1_i

$E_0 = -634.5116771$
 $E_{0+ZPE} = -634.231616$
 $E_{298} = -634.219261$
 $H_{298} = -634.218317$
 $G_{298} = -634.270692$
 $N\text{Imag} = 0$

N	0.440206	0.577722	0.148412
C	0.859575	1.965803	0.310052
C	2.365056	1.904825	0.167629
C	2.533658	0.875858	-0.937510
C	1.436462	-0.154048	-0.636837
C	2.003889	-1.317824	0.163034
O	1.685904	-1.308393	1.445160
C	-0.929776	0.299677	-0.014842
C	-1.288375	-1.152474	-0.177574
C	-3.343562	0.973899	0.046506
O	2.710340	-2.165496	-0.316464
H	1.033512	-0.565141	-1.559301
H	3.520621	0.423814	-0.980823
H	2.330149	1.331284	-1.904849
H	2.794273	2.870624	-0.085759
H	2.826925	1.563103	1.093987
H	0.432414	2.594987	-0.477135
H	0.524241	2.351745	1.270621
C	-1.870011	1.250104	0.072649
C	-2.737158	-1.351225	-0.592758
C	-3.662135	-0.496845	0.251989
H	-3.836170	1.575806	0.812445
H	-3.763352	1.311978	-0.906153
H	-1.101260	-1.670263	0.767119
H	-1.579331	2.283734	0.193303
H	-0.637868	-1.625605	-0.912234
H	-2.993377	-2.406838	-0.508527
H	-2.855381	-1.079500	-1.643963
H	-3.528793	-0.756831	1.304817
H	-4.705088	-0.694971	0.005563
H	1.081349	-0.547362	1.548408

1_i (down)

$E_0 = -634.5076091$
 $E_{0+ZPE} = -634.227694$
 $E_{298} = -634.215177$
 $H_{298} = -634.214233$
 $G_{298} = -634.266710$
 $N\text{Imag} = 0$

N	0.517020	0.652260	0.139246
C	0.956517	2.043420	0.255810
C	2.278145	2.096756	-0.492210
C	2.807899	0.681340	-0.376816
C	1.535887	-0.165348	-0.496148
C	1.757966	-1.474378	0.233230
O	1.415170	-1.454929	1.513722
C	-0.851007	0.371270	0.005719
C	-1.208561	-0.993033	-0.521707
C	-3.270635	0.954802	0.341057
O	2.265261	-2.440005	-0.270963
H	1.330059	-0.388983	-1.542998
H	3.270534	0.530173	0.598941
H	3.533052	0.415320	-1.139736
C	-1.799160	1.242553	0.385621
C	-2.673561	-1.102987	-0.912909
C	-3.567728	-0.523564	0.165112
H	-3.735805	1.324115	1.256966
H	-3.736735	1.520552	-0.472205
H	-0.979829	-1.746627	0.236130
H	-1.514505	2.208428	0.777747
H	-0.592032	-1.233445	-1.386606
H	-2.914243	-2.148501	-1.102864
H	-2.841520	-0.564091	-1.847938
H	-3.385587	-1.049936	1.105170
H	-4.618489	-0.671559	-0.083762
H	0.979535	-0.601455	1.670954
H	1.066997	2.325644	1.304068
H	0.220046	2.709328	-0.190614
H	2.960338	2.837096	-0.082001
H	2.101021	2.342606	-1.538603

1_{iii}

$E_0 = -634.5066239$
 $E_{0+ZPE} = -634.227352$
 $E_{298} = -634.214552$
 $H_{298} = -634.213608$
 $G_{298} = -634.267540$
 $N\text{Imag} = 0$

N	0.419858	0.660896	-0.077249
C	0.878163	2.001900	0.211003
C	2.389600	1.883203	0.180099
C	2.618873	0.814897	-0.875981
C	1.447681	-0.158942	-0.667137
C	1.896418	-1.326273	0.188226
O	1.813714	-1.106570	1.494824
C	-0.926862	0.356177	-0.110573
C	-1.275028	-1.088897	-0.345833
C	-3.344255	0.966197	0.209778
O	2.337827	-2.350735	-0.268955
H	1.149088	-0.593271	-1.619415
H	3.588438	0.327468	-0.807119
H	2.530738	1.243142	-1.872856
H	2.875363	2.824401	-0.065005
H	2.760835	1.551063	1.148194
H	0.521052	2.711837	-0.544433
H	0.499924	2.334295	1.178151
C	-1.880318	1.280093	0.115049
C	-2.756215	-1.302691	-0.613742
C	-3.604114	-0.521577	0.371016
H	-3.780294	1.512340	1.049002
H	-3.868806	1.331104	-0.680002

1_{iv}

$E_0 = -634.5070037$
 $E_{0+ZPE} = -634.227800$
 $E_{298} = -634.215013$
 $H_{298} = -634.214069$
 $G_{298} = -634.267788$
 $N\text{Imag} = 0$

N	0.389938	0.683279	-0.035153
C	0.807578	2.044683	0.217032
C	2.321378	1.965222	0.207994
C	2.590995	0.883740	-0.824573
C	1.444839	-0.116778	-0.598764
C	1.909632	-1.221967	0.328170
O	2.540787	-2.180792	-0.350177
C	-0.948786	0.346087	-0.092249
C	-1.260164	-1.113584	-0.286102
C	-3.386605	0.911083	0.148331
O	1.782476	-1.253352	1.522610
H	1.165904	-0.580819	-1.543850
H	3.573396	0.426448	-0.735087
H	2.500972	1.288697	-1.830874
H	2.786192	2.913953	-0.048415
H	2.688529	1.660638	1.186866
H	0.443643	2.721728	-0.565210
H	0.407122	2.396149	1.168166
C	-1.927852	1.254478	0.079779
C	-2.727557	-1.367724	-0.590928
C	-3.619330	-0.576787	0.346232
H	-3.855039	1.471186	0.960474
H	-3.896233	1.239225	-0.764151

1_{ii}

$E_0 = -634.5016601$
 $E_{0+ZPE} = -634.222666$
 $E_{298} = -634.209810$
 $H_{298} = -634.208866$
 $G_{298} = -634.262846$
 $N\text{Imag} = 0$

N	0.392938	0.674816	-0.074338
C	0.826532	2.026448	0.202818
C	2.340425	1.934496	0.186266
C	2.599185	0.842049	-0.837635
C	1.449533	-0.148374	-0.588330
C	1.900582	-1.225339	0.390562
O	2.606329	-2.221129	-0.155340
C	-0.947324	0.343565	-0.110323
C	-1.272768	-1.108568	-0.334036
C	-3.377010	0.921262	0.178344
O	1.703461	-1.215535	1.571720
H	1.171973	-0.639140	-1.523808
H	3.582849	0.386176	-0.748022
H	2.502147	1.236543	-1.847511
H	2.811276	2.877181	-0.080503
H	2.711119	1.635374	1.165298
H	0.462225	2.720499	-0.563457
H	0.436226	2.363510	1.163534
C	-1.916881	1.255310	0.095578
C	-2.746835	-1.344669	-0.621008
C	-3.617855	-0.568757	0.347486
H	-3.828235	1.466663	1.009933
H	-3.898371	1.273156	-0.718594

H -0.969117 -1.669061 0.528918
H -1.596551 2.312353 0.264921
H -0.702048 -1.481372 -1.185174
H -2.979833 -2.368303 -0.566190
H -2.992998 -0.975304 -1.628643
H -3.349095 -0.829861 1.387935
H -4.662680 -0.739499 0.227627
H 2.160981 -1.883686 1.946457

H -0.969026 -1.653816 0.617815
H -1.670893 2.296936 0.204759
H -0.652979 -1.523209 -1.093026
H -2.930204 -2.436076 -0.516768
H -2.942285 -1.076118 -1.621600
H -3.386171 -0.849807 1.378319
H -4.668697 -0.821901 0.180399
H 2.865335 -2.833729 0.279268

H -0.970459 -1.673765 0.550539
H -1.650240 2.292697 0.240632
H -0.682898 -1.502413 -1.161377
H -2.956227 -2.412938 -0.567846
H -2.975570 -1.027892 -1.641233
H -3.370448 -0.866157 1.369361
H -4.671401 -0.802843 0.192836
H 2.671644 -2.121580 -1.108775

\mathbf{I}_{iv} (Cyhex_{Conf})

$E_0 = -634.5074761$
 $E_{0+ZPE} = -634.228349$
 $E_{298} = -634.215512$
 $H_{298} = -634.214568$
 $G_{298} = -634.268602$
NImag = 0

N 0.369386 0.657322 -0.080297
C 0.820717 1.990419 0.252369
C 2.325535 1.941725 0.038541
C 2.496114 0.851494 -1.007408
C 1.413225 -0.163624 -0.621077
C 1.966143 -1.157792 0.383574
O 2.697511 -2.095472 -0.219192
C -0.962181 0.310457 -0.030151
C -1.308244 -1.074866 -0.507962
C -3.377172 0.832733 0.434995
O 1.807995 -1.127423 1.574441
H 1.092028 -0.730437 -1.492931
H 3.493135 0.419569 -1.033924
H 2.265471 1.233280 -2.000412
H 2.726793 2.898879 -0.284532
H 2.829407 1.662759 0.962687
H 0.341611 2.726434 -0.402384
H 0.561078 2.249878 1.279870
C -1.913815 1.161929 0.400408
C -2.714043 -1.497340 -0.115024
C -3.712394 -0.391812 -0.398230
H -0.594634 -1.795065 -0.107635
H -1.630093 2.142413 0.756157
H -1.200409 -1.113234 -1.595218
H -2.735625 -1.736064 0.950604
H -2.977857 -2.410068 -0.649060
H 3.054992 -2.682252 0.455890
H -3.952648 1.691012 0.081870
H -3.704487 0.666923 1.467460
H -4.728503 -0.726776 -0.188706
H -3.673315 -0.135280 -1.459845

\mathbf{I}_{iv} (down)

$E_0 = -634.505846$
 $E_{0+ZPE} = -634.226735$
 $E_{298} = -634.213871$
 $H_{298} = -634.212926$
 $G_{298} = -634.267008$
NImag = 0

N -0.502111 -0.756039 -0.265757
C -1.057302 -1.972772 0.275926
C -2.424990 -2.024949 -0.376189
C -2.854162 -0.564700 -0.395520
C -1.528765 0.220436 -0.530987
C -1.558980 1.365324 0.454817
O -2.147976 2.440097 -0.068499
C 0.835934 -0.429354 -0.132691
C 1.281103 0.795136 -0.887935
C 3.171222 -0.887257 0.665590
O -1.153950 1.333771 1.586233
H -1.430193 0.645845 -1.529247
H -3.344057 -0.312349 0.544050
H -3.541072 -0.324256 -1.201318
C 1.704315 -1.181623 0.565026
C 2.789163 0.848089 -1.075025
C 3.507911 0.525632 0.221163
H 3.500684 -1.041237 1.694921
H 3.743851 -1.602950 0.065375
H 0.951906 1.693592 -0.359407
H 1.347151 -2.057133 1.089499
H 0.790290 0.813534 -1.861529
H 3.073697 1.833120 -1.444712
H 3.085496 0.125627 -1.838993
H 3.195504 1.235160 0.991025
H 4.585735 0.638382 0.102378
H -2.198681 3.119891 0.612365
H -1.133277 -1.944372 1.369358
H -0.430802 -2.821385 0.006338
H -3.127590 -2.654618 0.164128
H -2.331140 -2.409303 -1.390858

\mathbf{I}_{iii} (down)

$E_0 = -634.5057508$
 $E_{0+ZPE} = -634.226642$
 $E_{298} = -634.213813$
 $H_{298} = -634.212869$
 $G_{298} = -634.266630$
NImag = 0

N -0.537761 -0.727635 -0.280364
C -1.124074 -1.929267 0.262878
C -2.492871 -1.948837 -0.387779
C -2.881803 -0.478256 -0.407917
C -1.540208 0.267470 -0.582514
C -1.555782 1.480875 0.318109
O -1.205625 1.214408 1.571456
C 0.807496 -0.436503 -0.143943
C 1.288487 0.775268 -0.897737
C 3.124361 -0.947211 0.676058
O -1.901040 -2.578057 -0.041763
H -1.435529 0.650534 -1.596552
H -3.339158 -0.206378 0.542355
H -3.581273 -0.221665 -1.197740
C 1.651426 -1.206578 0.565025
C 2.798364 0.788582 -1.075406
C 3.498912 0.454813 0.227912
H 3.442313 -1.104700 1.708519
H 3.683771 -1.679282 0.083354
H 0.982147 1.684027 -0.373212
H 1.269659 -2.072925 1.087307
H 0.802640 0.807313 -1.873235
H 3.110151 1.764053 -1.448269
H 3.080974 0.054473 -1.833339
H 3.198219 1.175965 0.991802
H 4.580044 0.540669 0.117406
H -1.284119 2.026382 2.083861
H -1.198482 -1.897049 1.356584
H -0.518554 -2.793760 -0.004564
H -3.210695 -2.559131 0.154672
H -2.410304 -2.336944 -1.402062

\mathbf{I}_{i-syn}

$E_0 = -634.5071916$
 $E_{0+ZPE} = -634.228103$
 $E_{298} = -634.215271$
 $H_{298} = -634.214327$
 $G_{298} = -634.268093$
NImag = 0

N 0.409833 0.672368 -0.083688
C 0.826414 2.049045 0.120708
C 2.338135 1.945438 0.177773
C 2.637089 0.827077 -0.806558
C 1.465844 -0.146303 -0.599867
C 1.867347 -1.248508 0.360648
O 2.451237 -2.259100 -0.284655
C -0.905276 0.258271 -0.133110
C -1.916273 1.263240 0.348107
C -2.691415 -1.471229 -0.507361
O 1.743081 -1.232517 1.555557
H 1.192010 -0.620153 -1.544647
H 3.607408 0.359953 -0.656573
H 2.600805 1.199599 -1.828693

\mathbf{I}_{i-syn} (Cyhex_{Conf})

$E_0 = -634.5071025$
 $E_{0+ZPE} = -634.228011$
 $E_{298} = -634.215161$
 $H_{298} = -634.214217$
 $G_{298} = -634.268141$
NImag = 0

N 0.407945 0.656782 -0.035759
C 0.786960 2.060187 -0.005172
C 2.300622 2.002546 0.019344
C 2.604753 0.812038 -0.874770
C 1.454088 -0.164050 -0.573999
C 1.908989 -1.226295 0.405432
O 2.491084 -2.245379 -0.228398
C -0.905776 0.226810 -0.061829
C -1.920350 1.233172 0.410873
C -2.691731 -1.491277 -0.475437
O 1.821961 -1.176660 1.602515
H 1.143010 -0.674788 -1.488099
H 3.585470 0.375618 -0.701379
H 2.550441 1.100218 -1.922885

H	2.827442	2.879775	-0.086024	H	2.757128	2.922569	-0.337234
H	2.655561	1.665540	1.181018	H	2.649382	1.818311	1.034341
H	0.515221	2.693104	-0.709173	H	0.434590	2.593557	-0.895147
H	0.408612	2.457439	1.038098	H	0.380397	2.561688	0.869116
C	-1.276613	-0.971468	-0.538602	C	-1.271118	-1.011068	-0.445912
C	-3.346040	0.865503	0.022116	C	-3.279215	0.615458	0.698133
C	-3.591447	-0.595358	0.346349	C	-3.687161	-0.347453	-0.399846
H	-3.098649	-1.527753	-1.522755	H	-2.858843	-2.070751	-1.385708
H	-2.704953	-2.496127	-0.130680	H	-2.874752	-2.186157	0.351528
H	-0.531664	-1.674497	-0.885081	H	-2.018065	2.022244	-0.339384
H	-4.637760	-0.856691	0.185967	H	-0.521037	-1.731817	-0.740966
H	-3.375941	-0.770219	1.403140	H	-1.546536	1.718513	1.312006
H	2.742883	-2.905465	0.367225	H	-4.017426	1.408063	0.819426
H	-1.702301	2.236418	-0.092883	H	-3.236745	0.075651	1.646688
H	-1.798670	1.388551	1.427647	H	-3.710749	0.182591	-1.355282
H	-3.537090	1.033180	-1.040438	H	-4.692329	-0.730889	-0.223186
H	-4.032872	1.509459	0.571236	H	2.815722	-2.866183	0.432645