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Supporting Information

Theoretical Study on the BINOL-Zinc Complex-Catalyzed Asymmetric Inverse-Electron-Demand Imino Diels-Alder Reaction: Mechanism and Stereochemistry

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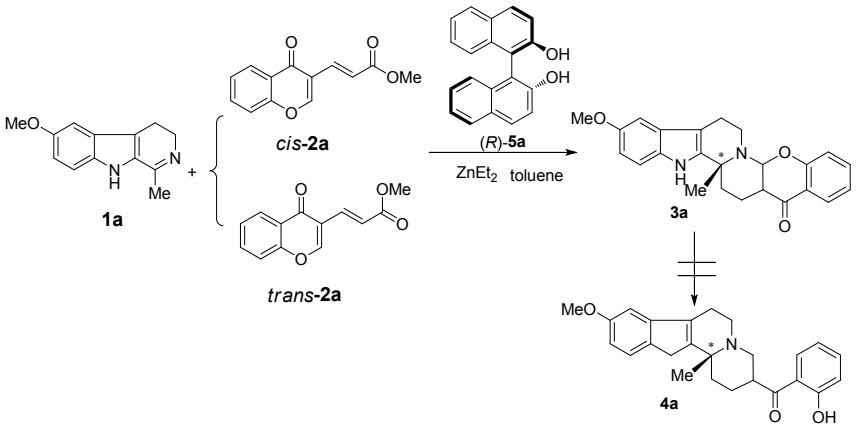
S1: Computational details.



Optimization and frequent calculation in gas phase: M05-2X/6-31G(d)

Solvation Method: M05-2X(SMD, toluene)/6–311+G(d,p)

For single-point energy calculation, the SCRF=Read keyword was used.

S2 Background reaction without catalyst.

2.1 The background reaction of imine 1a with diene *cis*-2a

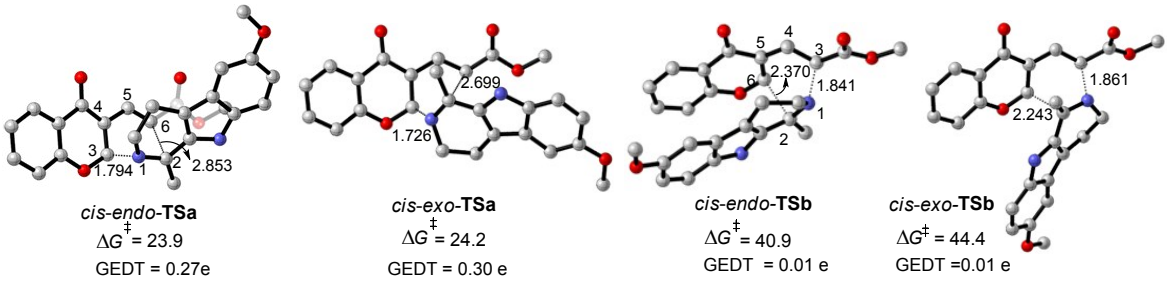


Figure S1. The M05-2X/6-31G(d)-optimized transition states structures for the IEDIDA reaction of **1a** and *cis*-**2a** (the forming bond distances are labeled in Å, the activation free energies are given in kcal mol^{-1}).

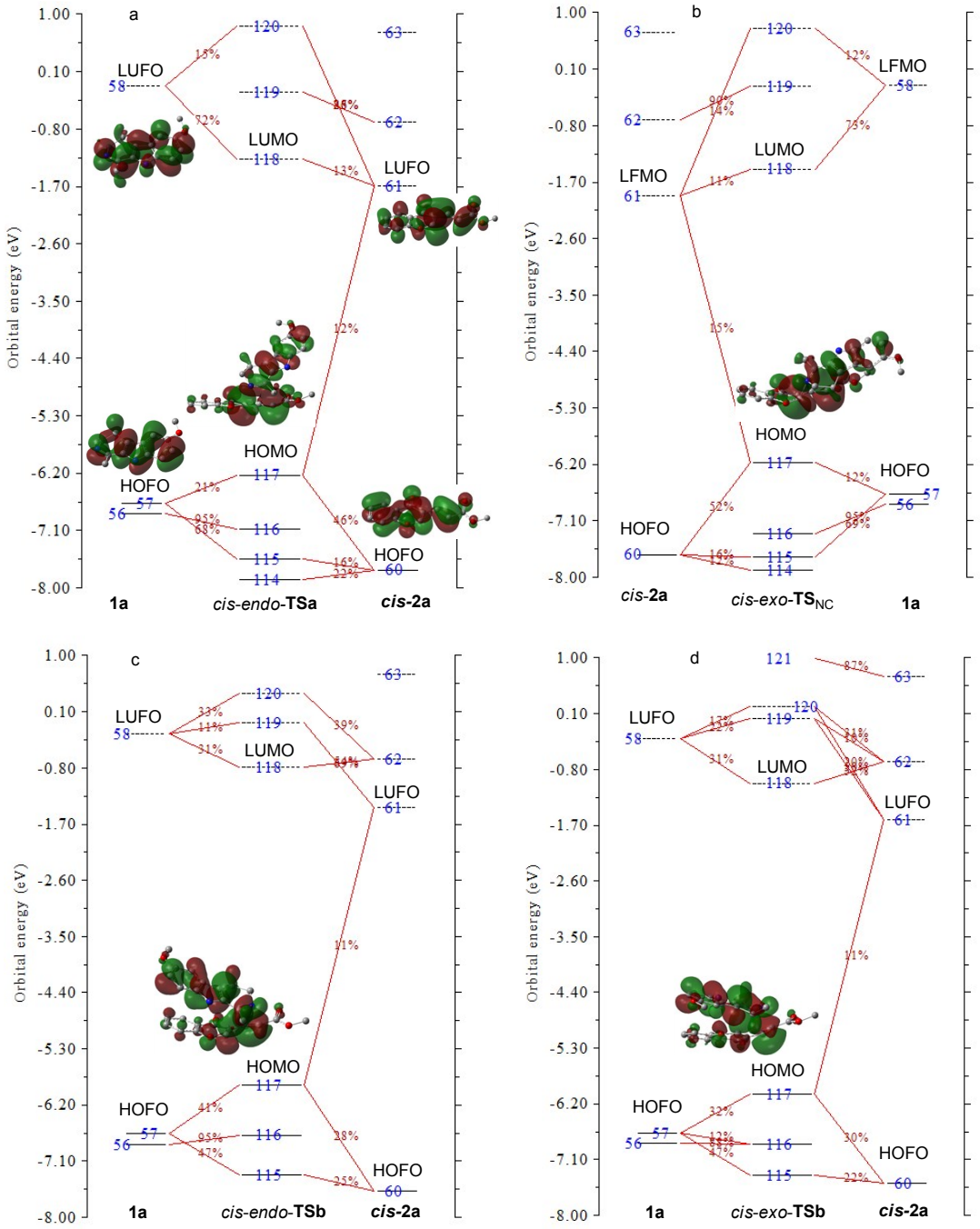


Figure S2. Orbital interaction diagrams for the four transition states from **1a** and *cis*-**2a** fragments (only α-spin orbitals presented).

Table S1 Activation barriers ($\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta G^{\neq}$), reaction energies (ΔG_{rxn}), distortion and interaction energies (all in kcal mol^{-1}), relative entropy (kcal mol^{-1} K^{-1}) and charge transfer (in e) for the transition states in uncatalyzed IEDIDA reaction of **1a** and *cis*-**2a**.

Structures	$\Delta E_{dist}^{\neq}$ [a]			$\Delta E_{int}^{\neq}$ [b]	$\Delta E^{\neq}$ [c]	$\Delta H^{\neq}$ [d]	$\Delta S^{\neq}$ [e]	$\Delta G^{\neq}$ [f]	ΔG_{rxn} [g]	GEDT[h]
	1a	*cis*-2a	total							
cis-endo-**TSa**	4.5	18.6	23.1	−14.2	8.8	8.3	−0.052	23.9	−2.1	0.27
cis -exo-**TSa**	3.9	27.3	31.2	−21.6	8.4	7.6	−0.050	24.4	−3.4	0.30
*cis-endo***TSb**	8.7	19.9	28.7	−3.5	19.7	24.5	−0.055	40.9	9.4	0.01
cis-exo-**TSb**	10.1	26.2	36.3	−7.0	24.5	28.6	−0.053	44.4	2.3	0.01

a: $\Delta E_{dist}^{\neq}$ is the energy to distort the 1a or *cis*-2a into the transition state;

b: $\Delta E_{int}^{\neq}$ is the interaction energy of the two fragments decomposed from the transition state ($\Delta E_{int}^{\neq} = \Delta E^{\neq} - \Delta E_{dist}^{\neq}$) ;

c: $\Delta E^{\neq}$ is the activation energy [$\Delta E^{\neq} = E$(TS)−E(1a)−E(*cis*-2a)], election energy $E = E_c + E_{sol}$, E_c is the zero-point correction in gas phase, E_{sol} is the electron energy in solvent after PCM correction;

d: $\Delta H^{\neq}$ is the activation enthalpy [$\Delta H^{\neq} = H$(TS)−H(1a)−H(*cis*-2a)], $H = H_c + E_{sol}$, H_c is thermal correction to enthalpy in gas phase;

e: $\Delta S^{\neq}$ is the change of entropy [$\Delta S^{\neq} = S$(TS)−S(1a)−S(*cis*-2a)], S is the entropy in gas phase;

f: $\Delta G^{\neq}$ is the activation Gibbs free energy [$\Delta G^{\neq} = G$(TS)−G(1a)−G(*cis*-2a)], $G = G_c + E_{sol}$, G_c is thermal correction to Gibbs Free Energy in gas phase;

g: ΔG_{rxn} is reaction free energy [$\Delta G_{rxn} = G$(cis-4a/5a) − G(1a) − G(*cis*-2a)];

h: GEDT is the global electron density transfer from nucleophilic 1a fragment to electrophilic *cis*-2 fragment.

2.2 The background reaction of imine 1a with diene *trans*-2a

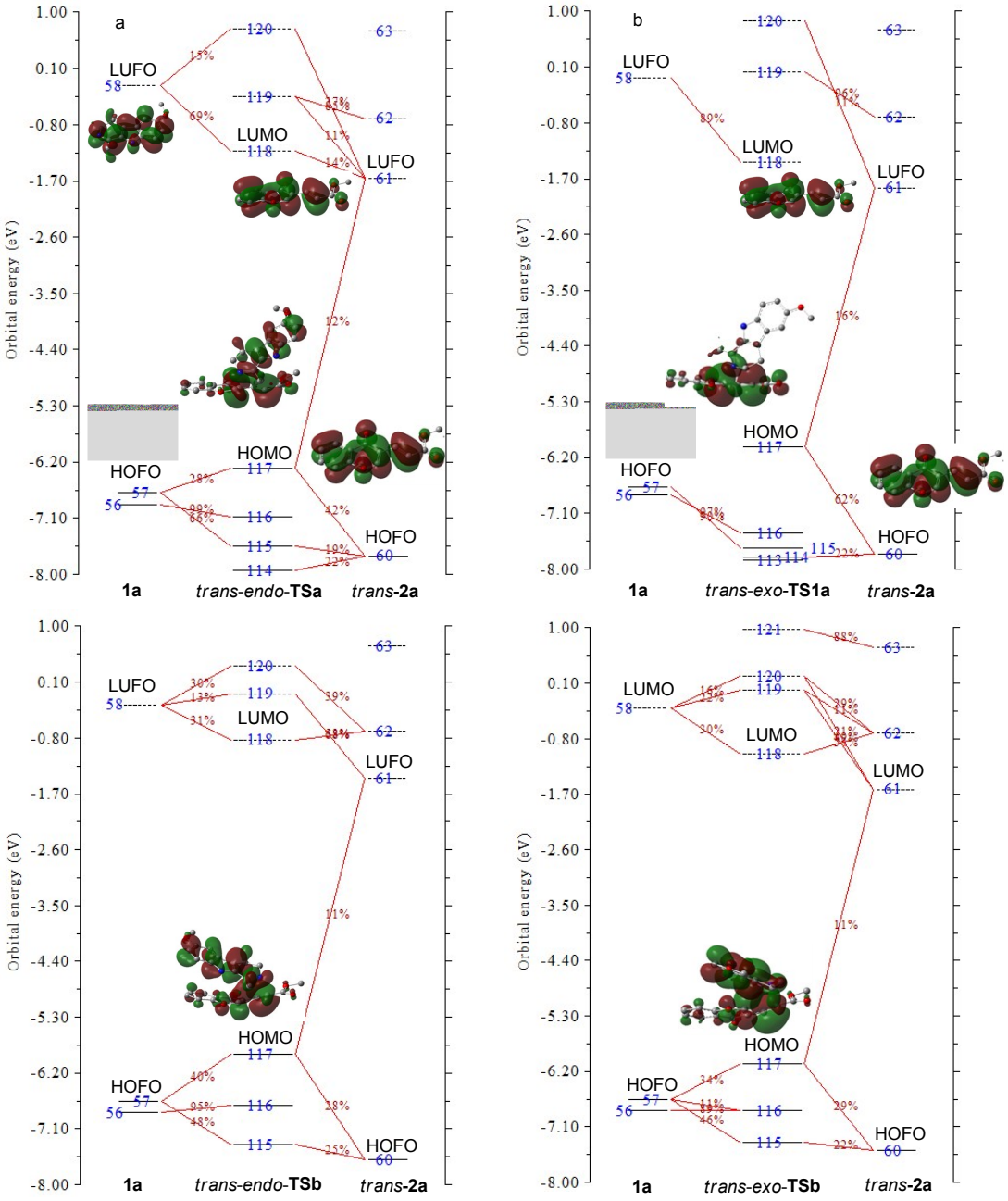


Figure S3. Orbital interaction diagrams for the four transition states from **1a** and *trans*-**2a** fragments (only α-spin orbitals presented).

Table S2 Activation barriers ($\Delta E^{\neq}$, $\Delta H,^{\neq}$ $\Delta G^{\neq}$), reaction energies (ΔG_{rxn}), distortion and interaction energies (all in kcal mol^{-1}), relative entropy (kcal mol^{-1} K^{-1}) and charge transfer (in e) for the transition states in uncatalyzed IEDIDA reaction of **1a** and *trans*-**2a**.

Structures	$\Delta E_{dist}^{\neq}$			$\Delta E_{int}^{\neq}$	$\Delta E^{\neq}$	$\Delta H^{\neq}$	$\Delta S^{\neq}$	$\Delta G^{\neq}$	ΔG_{rxn}	GEDT
	1a	2a	total							
trans-endo-**TSa**	4.5	18.5	23.0	−14.6	8.4	7.6	−0.056	24.4	−5.6	0.24
trans -exo-**TS1a**	4.4	18.6	22.9	−16.0	6.9	6.5	−0.050	21.4	-	0.39
trans -exo-**TS2a**	6.7	34.5	41.2	−29.6	11.6	10.9	−0.054	26.9	−7.4	0.38
trans-endo-**TSb**	8.6	20.2	28.8	−3.0	25.8	25.3	−0.057	42.0	14.2	0.01
trans-exo-**TSb**	10.0	25.9	36.0	−7.3	28.6	27.9	−0.053	43.9	4.3	0.01

S3 Catalytic reaction mechanism

3.1 The IEDIDA reaction of imine 1a with diene *cis*-2a catalyzed by $ZnCl_2$

Model I and II: the cycloaddition of the activated **1a** with diene *cis*-**2a**

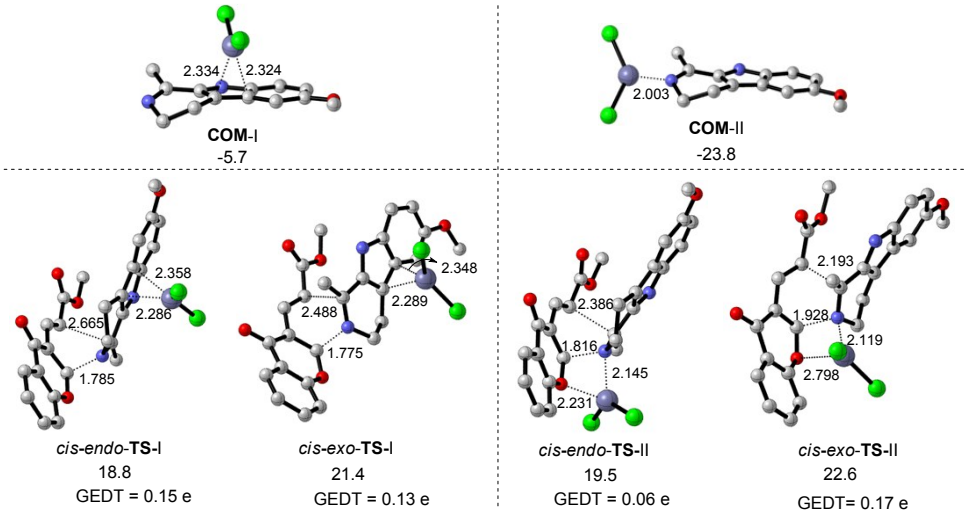


Figure S4. The M05-2X/6-31G(d)-optimized **1a**-$ZnCl_2$ complexes and transition states in the cycloaddition of **1a**-$ZnCl_2$ complexes with diene *cis*-**2a** (the bond distances are labeled in Å and the relative Gibbs free energies are given in kcal mol^{-1}).

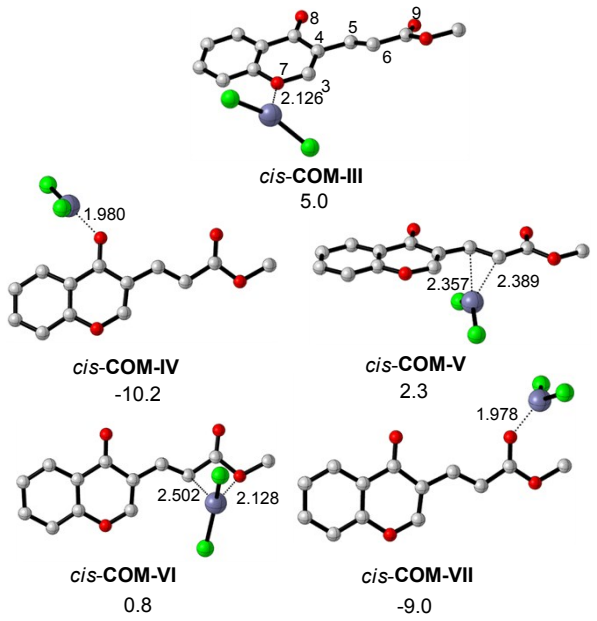


Figure S5. The M05-2X/6-31G(d)-optimized *cis*-**2a**-$ZnCl_2$ complexes (the bond distances are labeled in Å and the relative Gibbs free energies are given in kcal mol^{-1}).

Table S3 Electronic chemical potential μ, chemical hardness η, global electrophilicity ω, global nucleophilicity N, electrophilic Parr function P_k^+, local electrophilicity ω_k, electrophilic Parr function P_k^- and local nucleophilicity N_k indices for **1a**, *cis*-**2a** and molecular complexes.

Species	μ [eV]	η [eV]	ω [eV]	ω [eV]	P_k^+		ω_k [eV]		P_k^-		N_k [eV]	
					C3	C6	C3	C6	N1	C2	N1	C2
1a	−3.7	0.24	1.0	4.0		-		-	0.27	0.13	1.1	0.5
COM-I	−4.7	0.25	1.6	3.0		-		-	0.27	0.03	1.0	0.3
COM-II	−4.8	0.22	1.9	3.2		-		-	0.21	0.36	0.7	1.2
cis-**2a**	−4.7	7.0	1.6	2.8	0.57	0.10	0.9	0.2		-		-
cis-**COM-III**	−5.2	7.4	2.1	2.1	0.50	0.06	1.1	0.1		-		-
cis-**COM-IV**	−5.7	6.7	2.4	2.0	0.42	−0.01	1.0	0.0		-		-
cis-**COM-V**	−5.7	6.5	2.5	2.1	0.50	0.22	1.3	0.6		-		-
cis-**COM-VI**	−5.4	6.6	2.2	2.3	0.44	0.09	1.0	0.2		-		-
cis-**COM-VII**	−5.5	6.6	2.3	2.2	0.43	0.07	1.0	0.2		-		-

Model III: the cycloaddition of the complex *cis*-**COM**-III with **1a** undergoes a one-step concerted mechanism

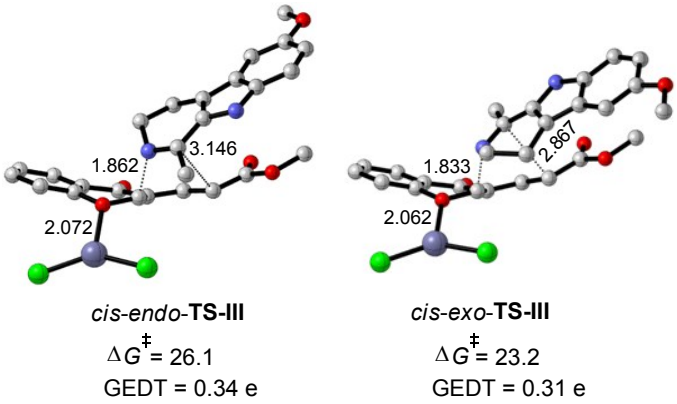


Figure S6. The M05-2X/6-31G(d)-optimized transtion states in the cycloaddition of the complex *cis*-**COM**-III with **1a** (the bond distances are labeled in Å and the relative Gibbs free energies are given in kcal mol^{-1}).

Model IV: the cycloaddition of the complex *cis*-**COM**-IV with **1a** undergoes a two-step stepwise mechanism

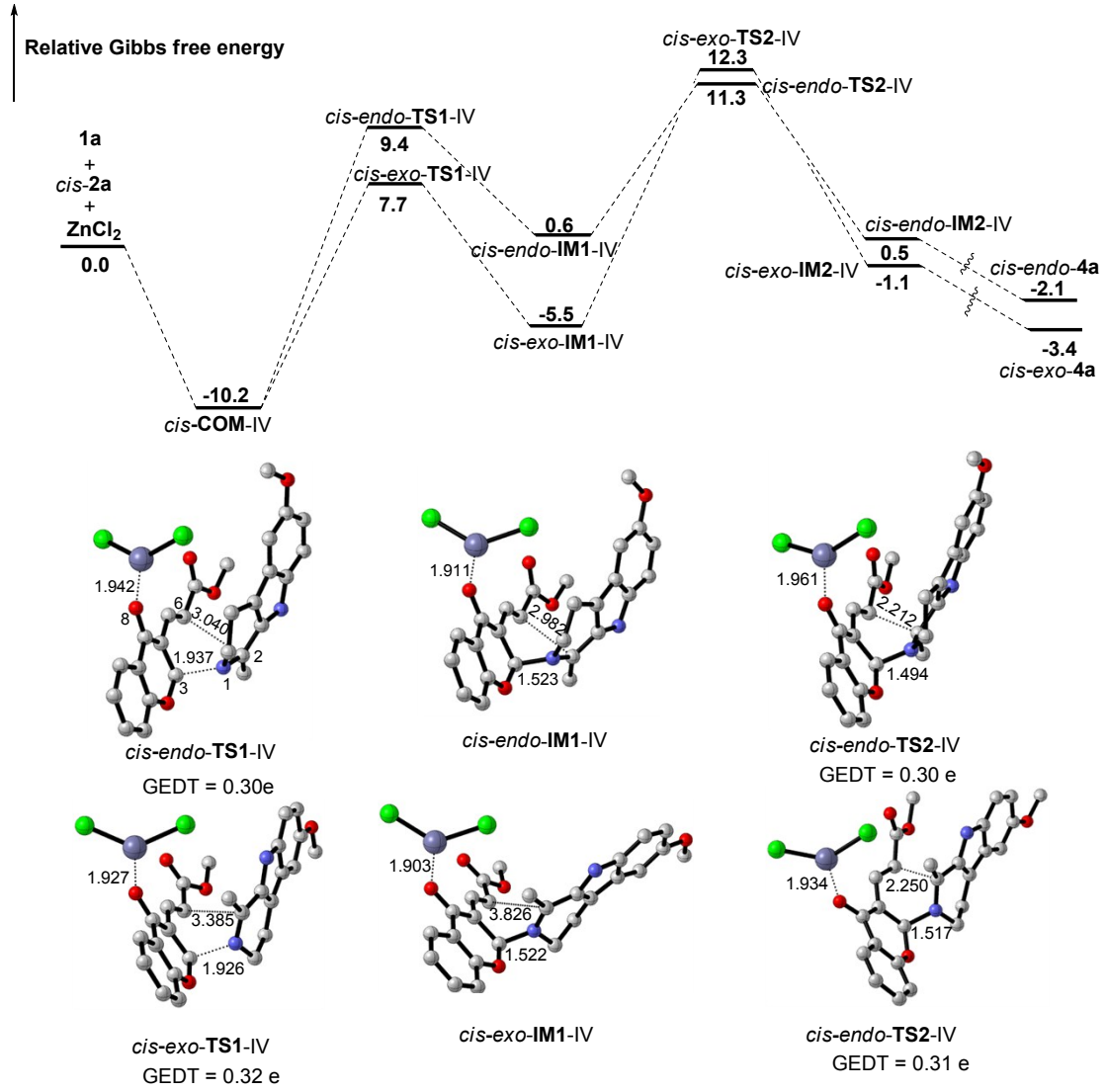


Figure S7. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *cis*-COM-IV and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Model V: the cycloaddition of the complex *cis*-**COM**-V with **1a** undergoes a two-step stepwise mechanism

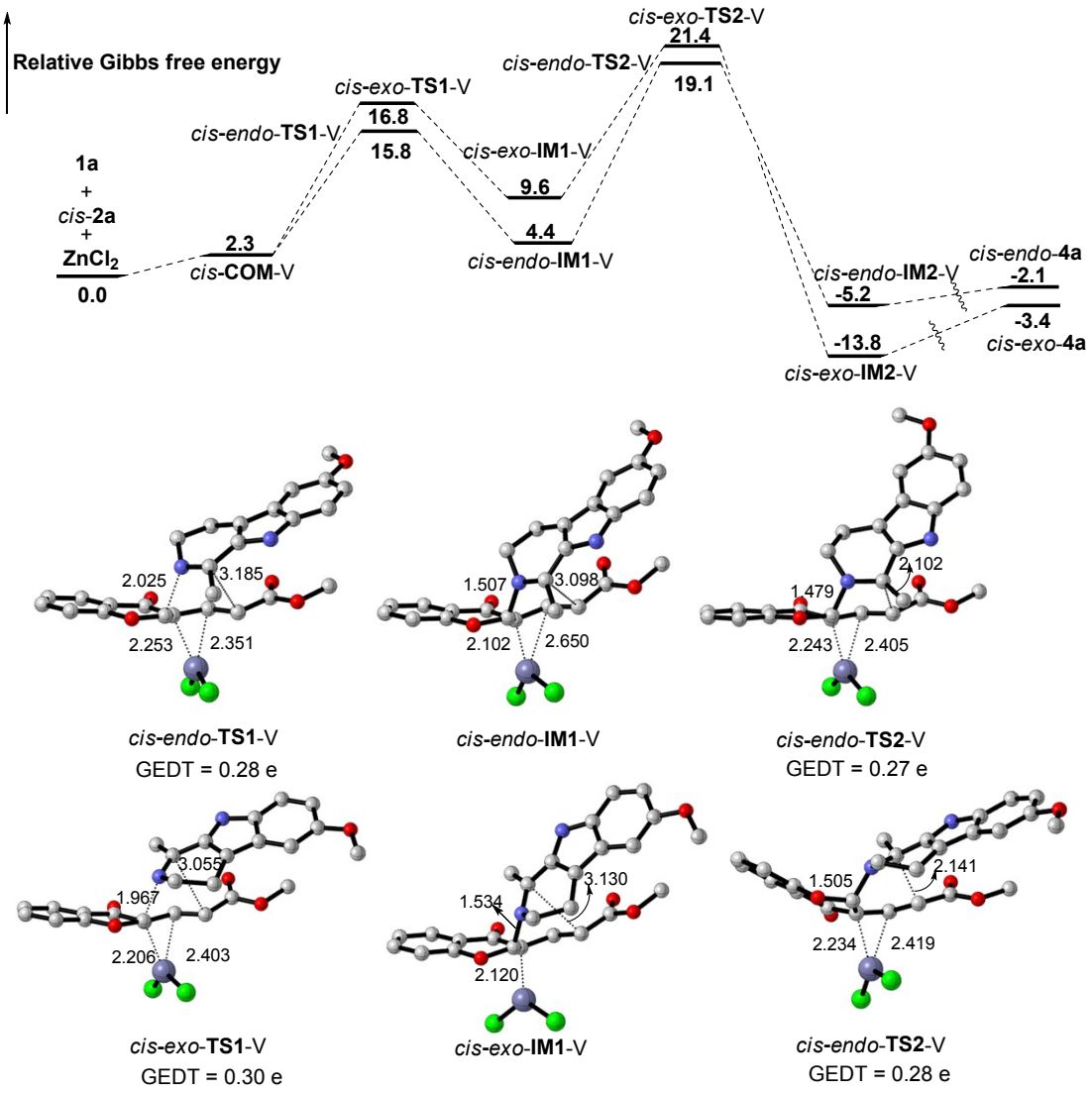


Figure S8. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *cis*-COM-V and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Model VI: the cycloaddition of the complex *cis*-**COM**-VI with **1a** undergoes a two-step stepwise mechanism

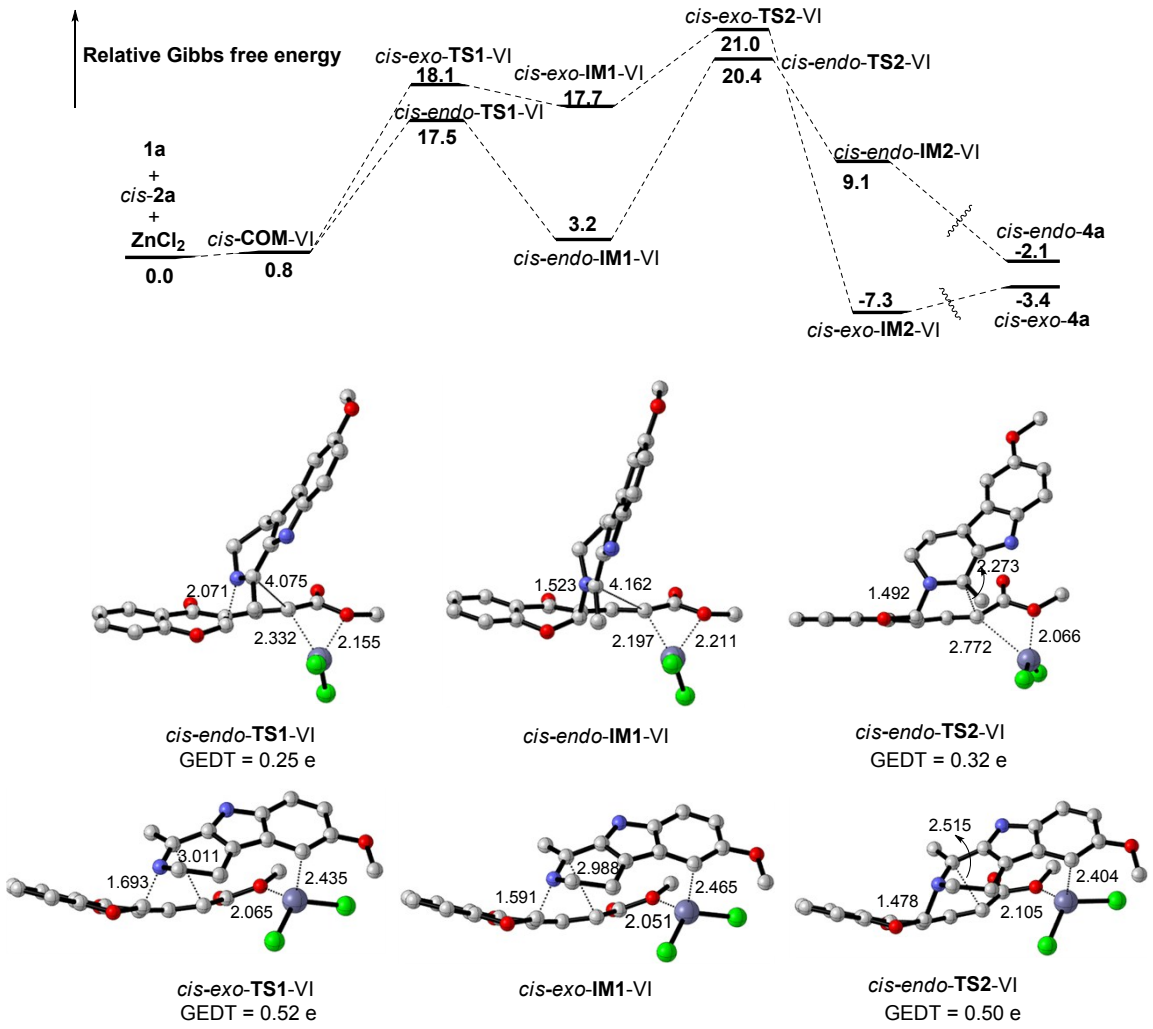


Figure S9. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *cis*-COM-VI and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Model VII: the cycloaddition of the complex *cis*-**COM**-VI with **1a**, the endo approach undergoes a one-step concerted mechanism, while the exo approach undergoes a two-step stepwise mechanism

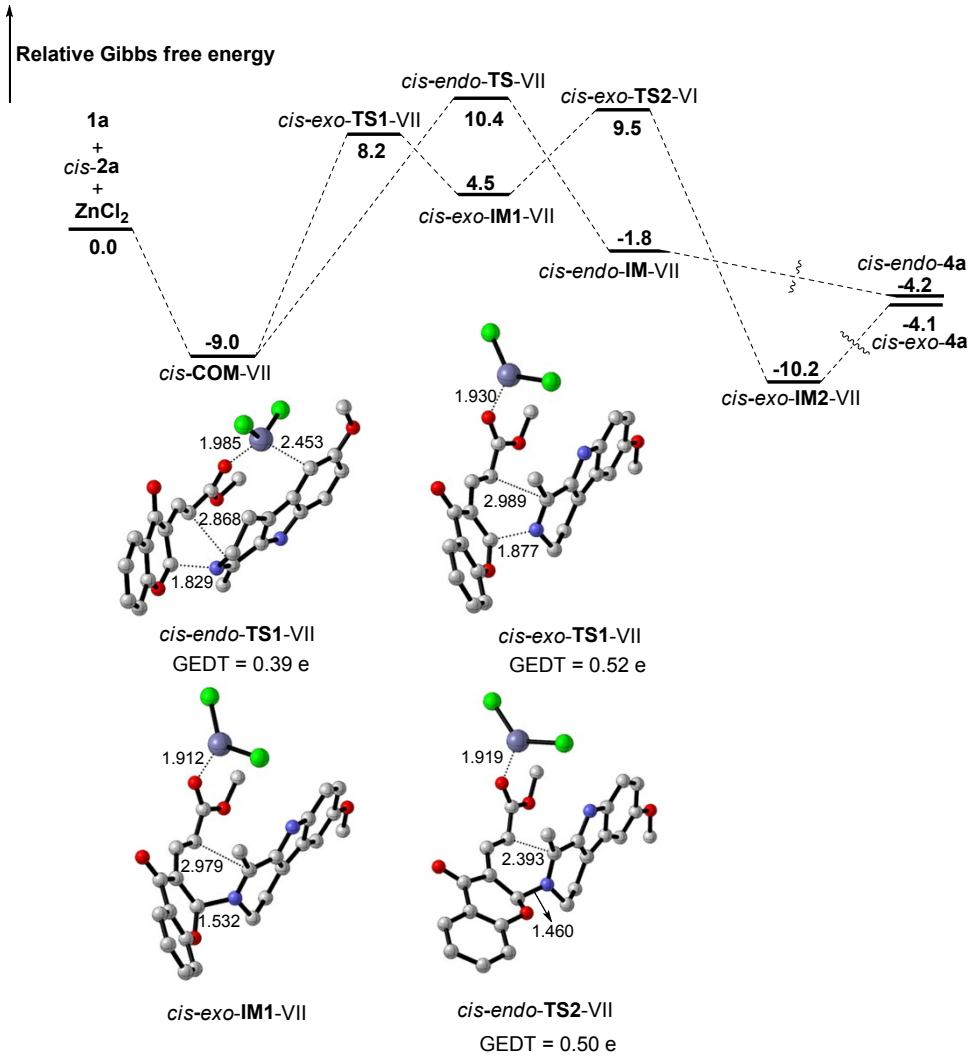


Figure S10. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *cis*-COM-VII and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Table S4 Activation barriers ($\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta G^{\neq}$), reaction energies (ΔG_{rxn}), distortion and interaction energies (all in kcal mol^{-1}), relative entropy (kcal mol^{-1} K^{-1}) and charge transfer (in e) for the transition states in $ZnCl_2$-catalyzed IEDIDA reaction of **1a** and *cis*-**2a**.

Structures	$\Delta E_{dist}^{\neq}$				$\Delta E_{int}^{\neq}$	$\Delta E^{\neq}$	$\Delta H^{\neq}$	$\Delta S^{\neq}$	$\Delta G^{\neq}$	GEDT
	1a	*cis*-**2a**	$ZnCl_2$	total						
cis-*endo*-**TS**-I	7.0	19.0	7.0	31.3	−32.6	−4.4	−4.8	−0.079	18.8	0.15
cis-*exo*-**TS**-I	6.4	25.9	3.6	35.9	−37.9	−1.9	−2.3	−0.079	21.4	0.13
cis-*endo*-**TS**-II	11.2	25.6	4.2	41.0	−49.8	−4.4	−4.9	−0.082	19.5	0.06
cis-*exo*-**TS**-II	14.7	27.9	7.2	49.8	−51.9	−2.1	−2.7	−0.085	22.6	0.17
cis-*endo*-**TS**-III	1.8	20.1	2.6	24.5	−21.0	3.5	3.4	−0.076	26.1	0.34
cis-*exo*-**TS**-III	2.5	23.9	2.7	29.1	−28.2	0.9	0.8	−0.075	23.2	0.31
cis-*endo*-**TS1**-IV	3.0	15.5	3.8	22.3	−36.0	−13.7	−14.2	−0.079	9.4	0.30
cis-*endo*-**TS2**-IV	16.4	51.1	3.0	70.5	−82.2	−11.7	−12.2	−0.079	11.3	0.30
cis-*exo*-**TS1**-IV	5.2	16.5	4.8	26.5	−40.5	−14.0	−14.1	−0.073	7.7	0.32
cis-*exo*-**TS2**- IV	14.9	49.5	3.3	67.6	−77.6	−10.0	−10.6	−0.077	12.3	0.31
cis-*endo*-**TS1**-V	1.6	12.9	3.3	17.8	−24.2	−6.4	−6.2	−0.074	15.8	0.28
cis-*endo*-**TS2**-V	17.9	55.0	3.4	76.4	−80.6	−4.2	−4.8	−0.080	19.1	0.27
cis-*exo*-**TS1**-V	1.7	16.3	3.6	21.6	−26.5	−4.9	−4.9	−0.073	16.8	0.30
cis-*exo*-**TS2**-V	16.6	53.2	3.9	73.7	−75.9	−1.8	−2.4	−0.080	21.4	0.28
cis-*endo*-**TS1**-VI	0.7	13.0	3.1	16.9	−19.9	−3.0	−2.7	−0.068	17.5	0.25
cis-*endo*-**TS2**-VI	13.5	54.8	2.0	70.2	−72.6	−2.4	−3.0	−0.078	20.4	0.32
cis-*exo*-**TS1**-VI	6.4	30.1	7.3	43.8	−50.2	−6.3	−6.9	−0.084	18.1	0.51
cis-*exo*-**TS2**-VI	12.8	67.8	3.3	83.8	−88.5	−4.7	−5.9	−0.090	21.0	0.50
cis-*endo*-**TS**-VII	2.8	20.9	4.8	28.6	−42.7	−14.1	−14.5	−0.084	10.4	0.39
cis-*exo*-**TS1**-VII	2.9	21.6	4.4	28.9	−43.6	−14.8	−15.2	−0.078	8.2	0.31
cis-*exo*-**TS2**-VII	10.9	87.2	4.7	102.9	−117.1	−14.3	−15.0	−0.082	9.5	0.41

2a.

3.2 The IEDIDA reaction of imine 1a with diene *trans*-2a catalyzed by $ZnCl_2$

Model III: the cycloaddition of the complex *trans*-**COM**-III with **1a**, the endo approach undergoes a one-step concerted mechanism, while the exo approach undergoes a two-step stepwise mechanism

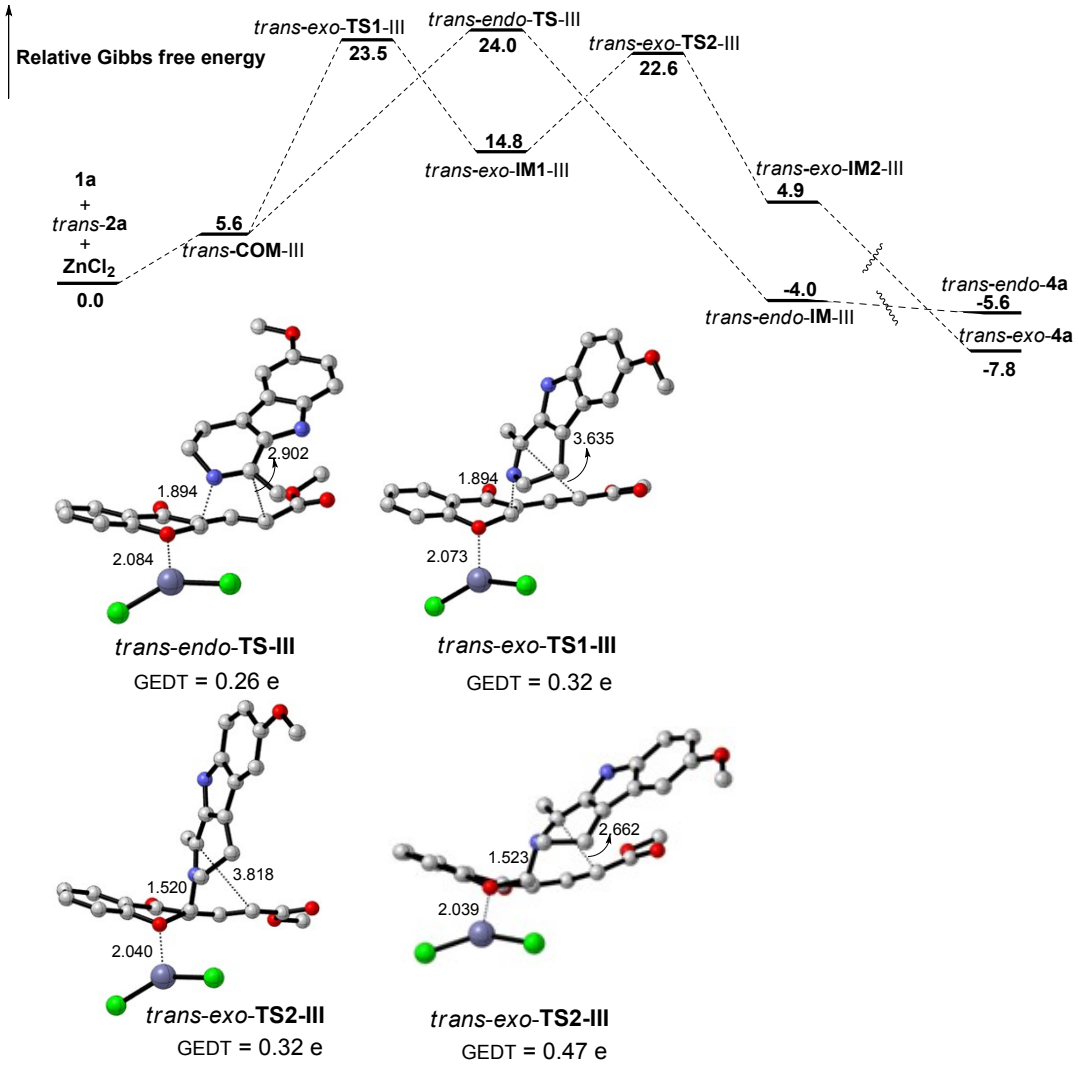


Figure S11. The M05-2X/6-31G(d)-optimized transtion states in the cycloaddition of the complex *cis*-**COM**-III with **1a** (the bond distances are labeled in Å and the relative Gibbs free energies are given in kcal mol^{-1}).

Model IV: the cycloaddition of the complex *trans*-**COM**-IV with **1a** undergoes a two-step stepwise mechanism

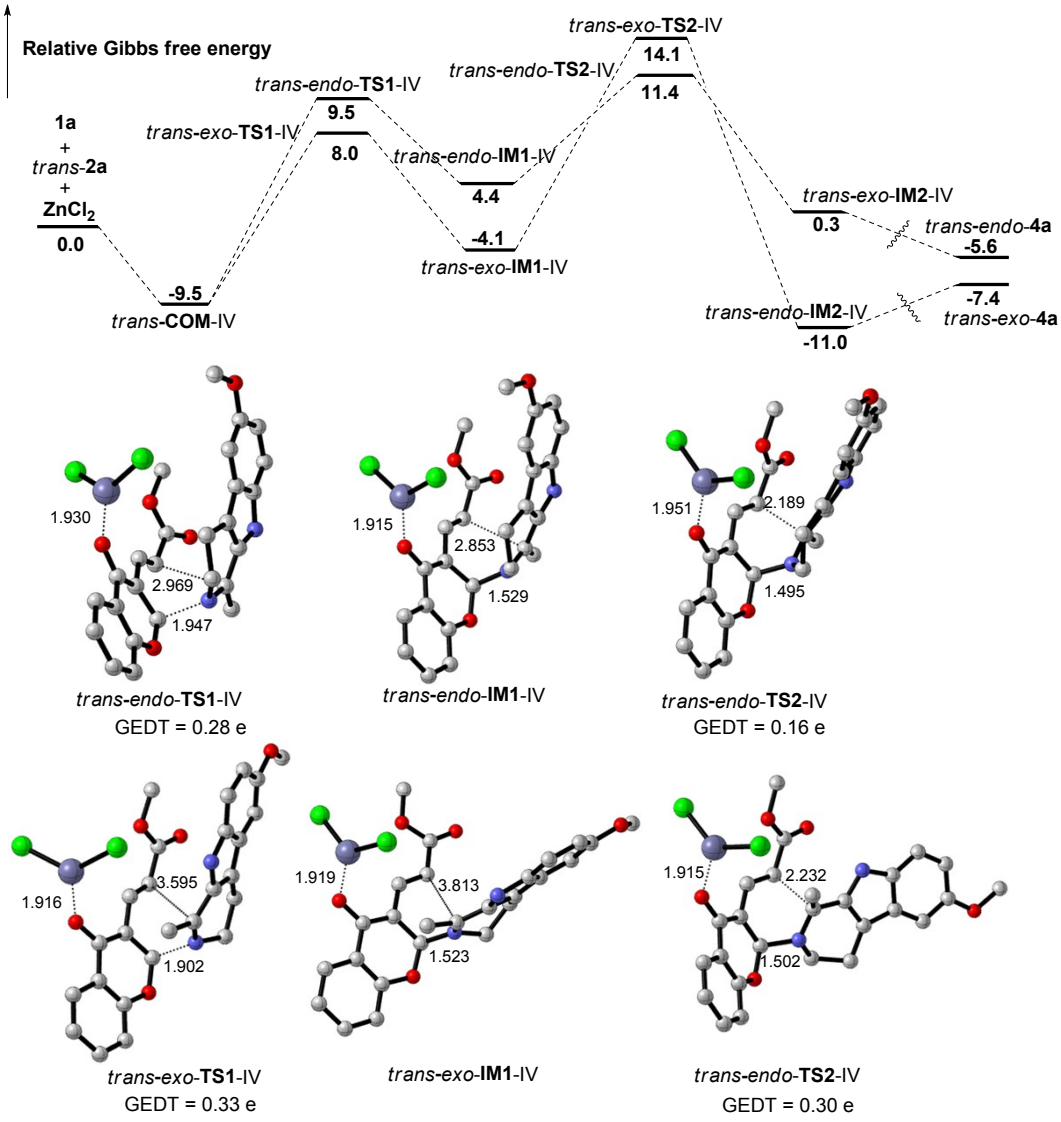


Figure S12. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *trans*-COM-IV and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Model V: the cycloaddition of the complex *trans*-**COM**-V with **1a** undergoes a two-step stepwise mechanism

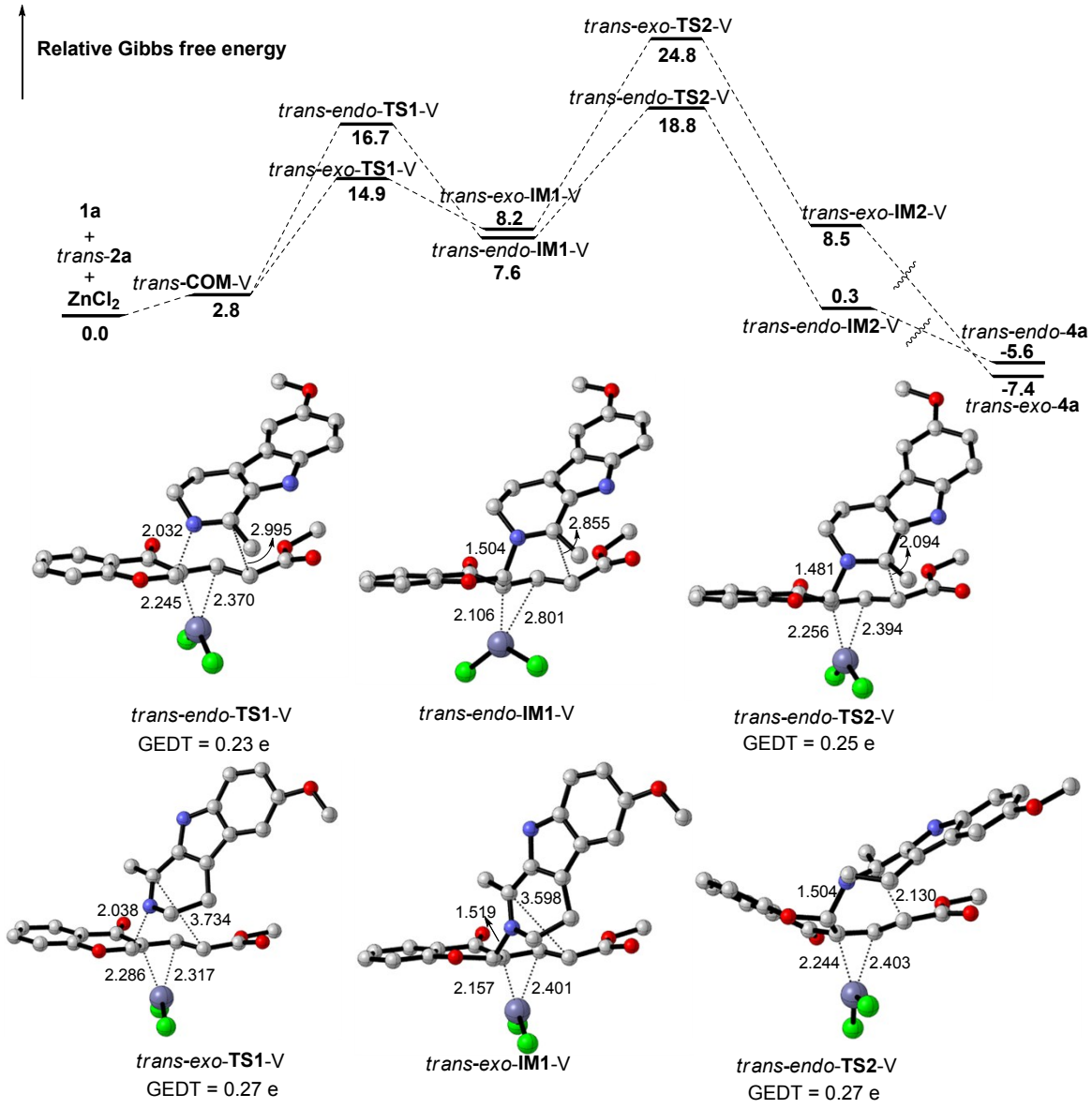


Figure S13. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *trans*-COM-V and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Model VI: the cycloaddition of the complex *trans*-**COM**-VI with **1a** undergoes a two-step stepwise mechanism

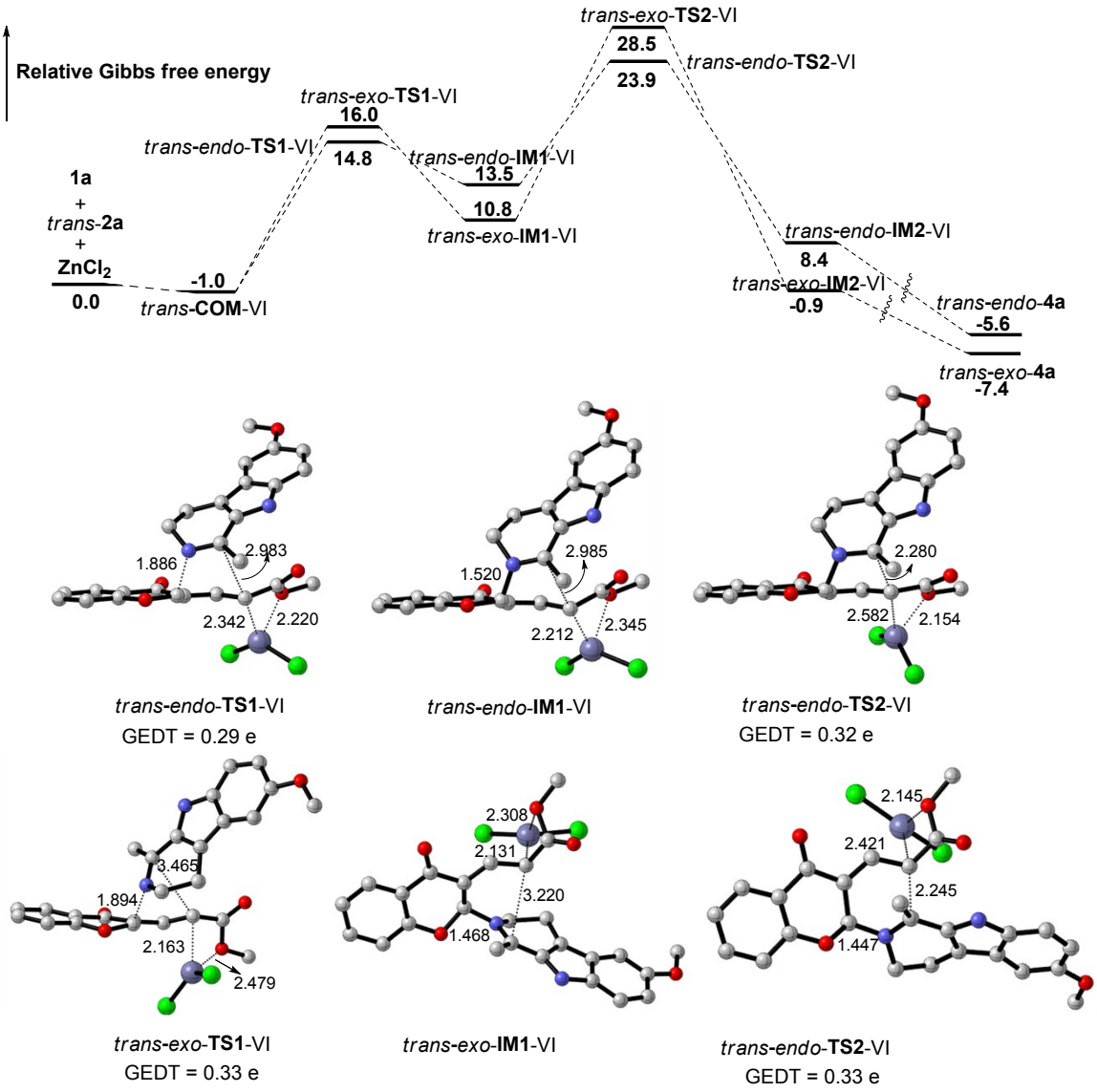


Figure S14. The free energy profile (in kcal mol^{-1}) of the cycloaddition reaction of the complex *trans*-COM-VI and **1a**, with the M05-2X/6-31G(d)-optimized transition states and intermediates shown below (the forming bond distances are labeled in Å).

Table S5 Activation barriers ($\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta G^{\neq}$), reaction energies (ΔG_{rxn}), distortion and interaction energies (all in kcal mol^{-1}), relative entropy (kcal mol^{-1} K^{-1}) and charge transfer (in e) for the transition states in $ZnCl_2$-catalyzed IEDIDA reaction of **1a** and *trans*-**2a**.

Structures	$\Delta E_{dist}^{\neq}$				$\Delta E_{int}^{\neq}$	$\Delta E^{\neq}$	$\Delta H^{\neq}$	$\Delta S^{\neq}$	$\Delta G^{\neq}$	GEDT
	1a	*trans* **-2a**	$ZnCl_2$	total						
trans-endo-**TS-**I	5.9	19.9	3.5	28.6	−33.3	−4.8	−5.1	−0.079	18.6	0.14
trans-exo-**TS-**I	6.2	26.3	3.6	36.1	−36.8	−0.7	−1.1	−0.078	22.2	0.16
trans-endo-**TS-**II	12.0	25.8	4.1	42.0	−47.6	−5.6	−6.6	−0.088	19.7	0.05
trans-exo-**TS-**II	14.8	28.8	7.3	50.8	−50.1	0.7	0.1	−0.085	25.4	0.15
trans-endo-**TS-**III	3.5	17.8	2.5	23.8	−22.6	1.2	1.0	−0.077	24.0	0.26
trans-exo-**TS1-**III	2.1	15.1	2.1	19.3	−17.3	2.0	1.8	−0.073	23.5	0.32
trans-exo-**TS2-**III	7.4	45.0	2.4	54.8	−54.8	0.0	−0.4	−0.077	22.6	0.47
trans-endo-**TS1-**IV	3.9	15.9	5.0	24.8	−38.8	−14.0	−14.3	−0.080	9.5	0.28
trans-endo-**TS2-**IV	18.8	71.9	5.7	96.4	−109.2	−12.8	−13.7	−0.084	11.4	0.16
trans-exo-**TS1-**IV	5.0	19.1	5.5	29.6	−44.4	−14.6	−14.6	−0.076	8.0	0.33
trans-exo-**TS2-** IV	17.7	54.6	5.5	77.8	−86.3	−8.5	−9.0	−0.077	14.1	0.30
trans-endo-**TS1-**V	2.3	12.7	3.0	17.9	−23.3	−5.4	−5.3	−0.074	16.7	0.23
trans-endo-**TS2-**V	19.3	53.9	3.1	76.3	−81.5	−5.2	−5.9	−0.083	18.8	0.25
trans-exo-**TS1-**V	1.1	11.6	3.2	15.9	−21.3	−5.6	−5.3	−0.068	14.9	0.27
trans-exo-**TS2-**V	18.3	52.7	3.7	74.7	−73.1	1.6	1.1	−0.079	24.8	0.27
trans-endo-**TS1-**VI	3.6	18.7	3.0	25.3	−33.1	−7.8	−8.0	−0.076	14.8	0.29
trans-endo-**TS2-**VI	14.9	44.8	2.7	66.4	−65.9	0.6	−0.1	−0.080	23.9	0.32
trans-exo-**TS1-**VI	1.9	18.4	4.4	24.7	−29.6	−4.9	−4.7	−0.069	16.0	0.33
trans-exo-**TS2-**VI	18.5	90.9	3.3	112.7	−106.1	6.6	6.3	−0.074	28.5	0.33
trans-endo-**TS1-**VII	3.7	19.4	5.1	28.2	−42.1	−14.1	−14.6	−0.074	10.4	0.37
trans-endo-**TS2-**VII	10.1	50.5	7.6	68.2	−83.1	−14.9	−15.9	−0.087	10.1	0.43
trans-exo-**TS1-**VII	2.6	21.3	4.3	28.2	−45.7	−17.5	−18.2	−0.083	6.5	0.48
trans -exo-**TS2-**VII	9.5	80.3	6.2	96.0	−110.0	−15.0	−16.1	−0.088	10.2	0.55

S4 Stereochemistry in the presence of BINOL-Zn complex.

4.1 Kumar's transition state models for the IEDIDA reaction of 1a with *cis*-2a or trans-2a catalyzed by chiral BINOL-Zn complex

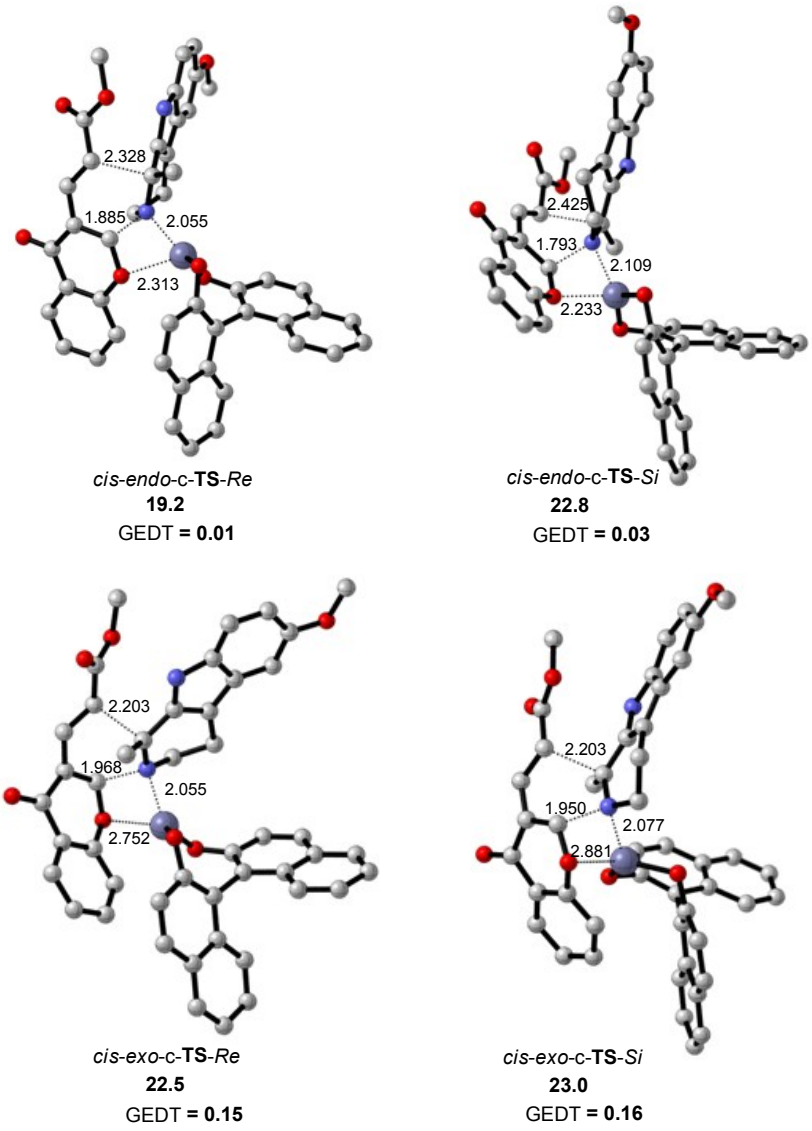


Figure S15. The M05-2X/6-31G(d)-optimized Kumar's transition state models for the IEDIDA reaction of **1a** with *cis*-**2a** catalyzed by chiral BINOL-Zn complex (the forming bond distances are labeled in Å, the relative free energies are give in kcal mol^{-1} and the values of charge transfer are given in e).

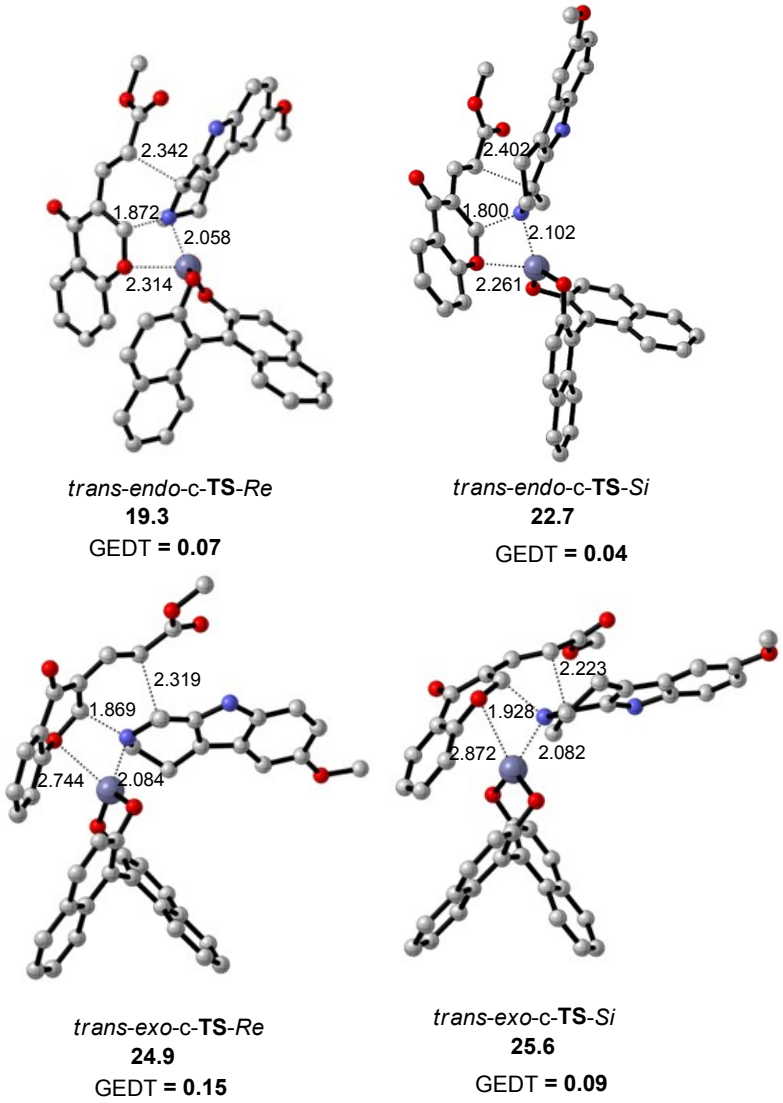


Figure S16. The M05-2X/6-31G(d)-optimized Kumar's transition state models for the IEDIDA reaction of **1a** with diene *trans*-**2a** catalyzed by chiral BINOL-Zn complex (the forming bond distances are labeled in Å, the relative free energies are give in kcal mol^{-1} and the values of charge transfer are given in e).

4.2 The models of activation of ester carbonyl group of diene 2a for IEDIDA reaction of imine 1a with diene 2a catalyzed by chiral BINOL-Zn complex

*4.2.1 trans-**2a** diene as the substrate*

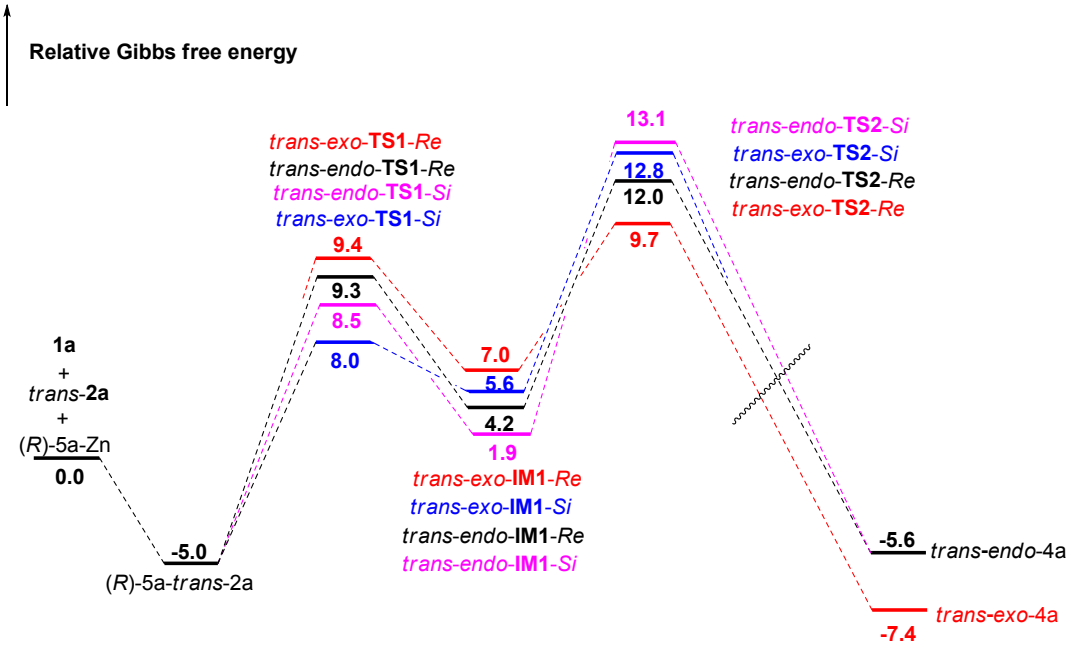


Figure S17. Energy profile of the IEDIDA reaction of **1a** with diene *trans*-**2a** catalyzed by chiral BINOL-Zn complex (the relative free energies are gieve in kcal mol^{-1}).

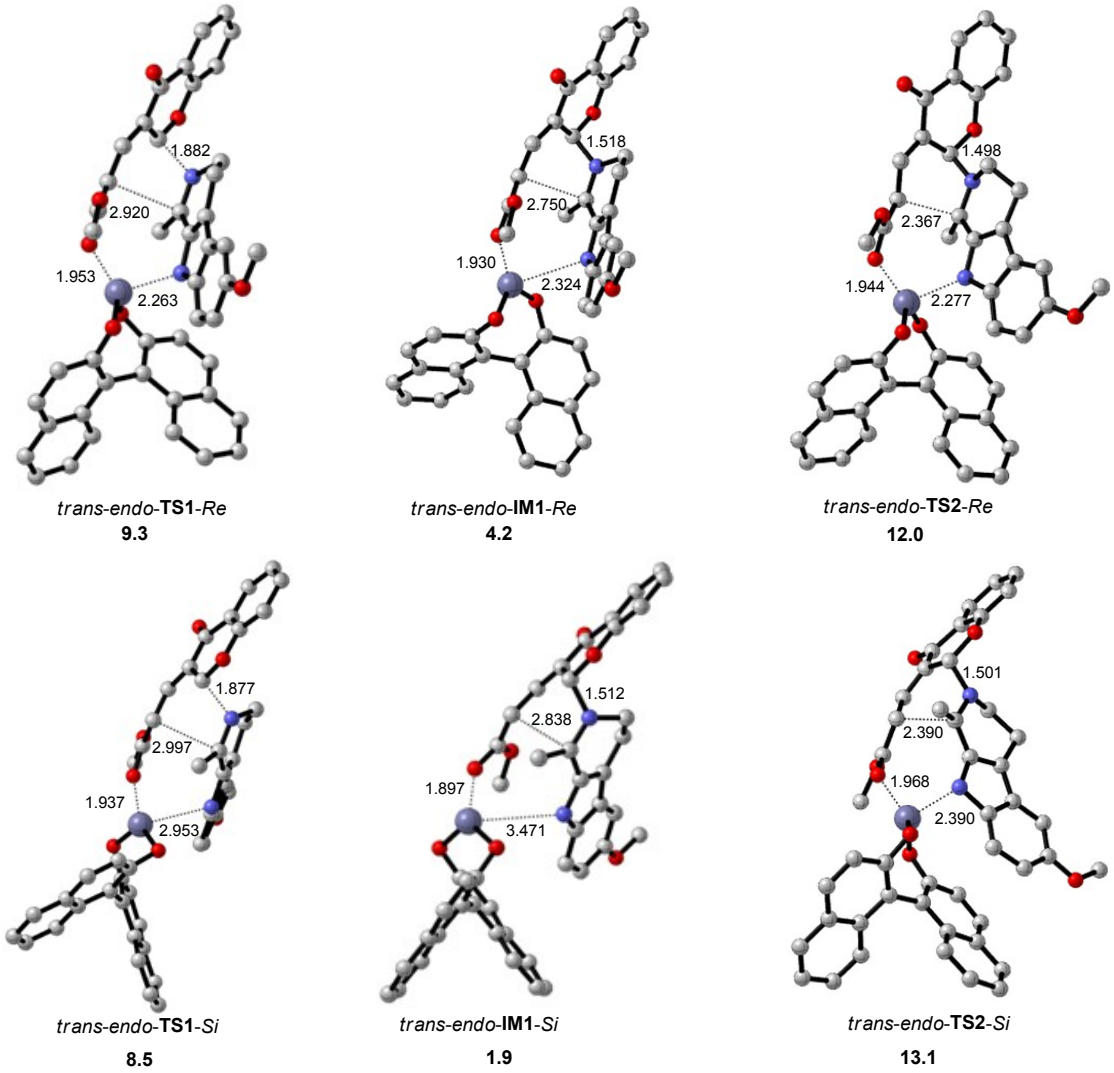


Figure S18. The M05-2X/6-31G(d)-optimized transition states and intermediates for the IEDIDA reaction of **1a** with *trans*-**2a** catalyzed by chiral BINOL-Zn complex along the *endo* pathways (the forming bond distances are labeled in Å).

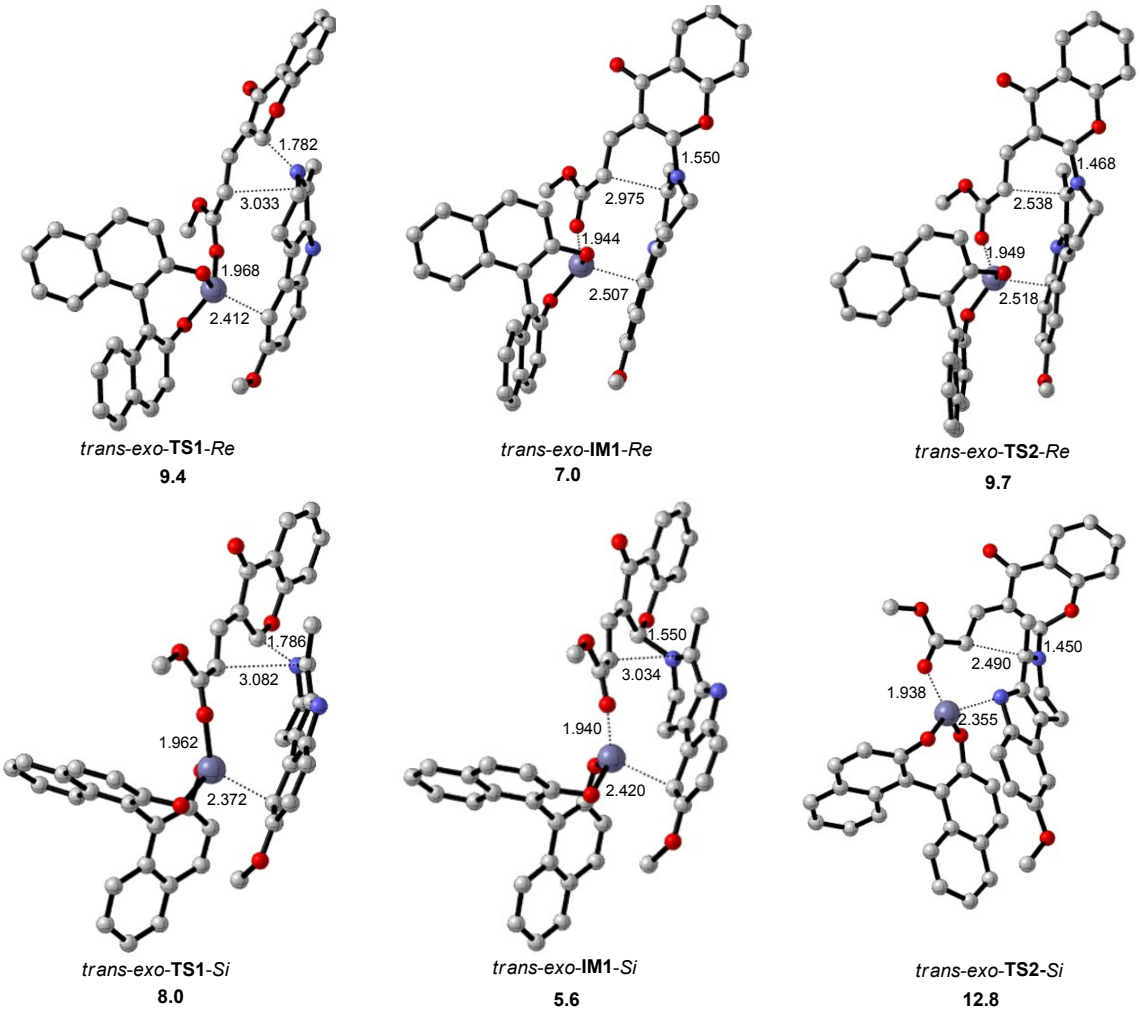


Figure S19. The M05-2X/6-31G(d)-optimized transition states and intermediates for the IEDIDA reaction of **1a** with *trans*-**2a** catalyzed by chiral BINOL-Zn complex along the *exo* pathways (the forming bond distances are labeled in Å).

*4.2.2 cis-**2a** diene as the substrate*

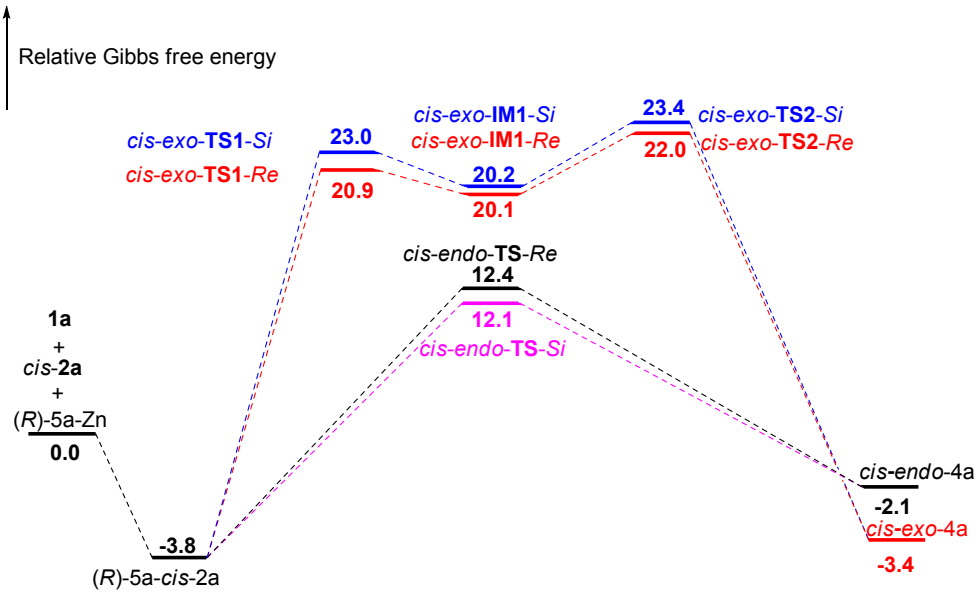


Figure S20. Energy profile of the IEDIDA reaction of **1a** with *cis*-**2a** catalyzed by chiral BINOL-Zn complex (the relative free energies gieve in kcal mol^{-1}).

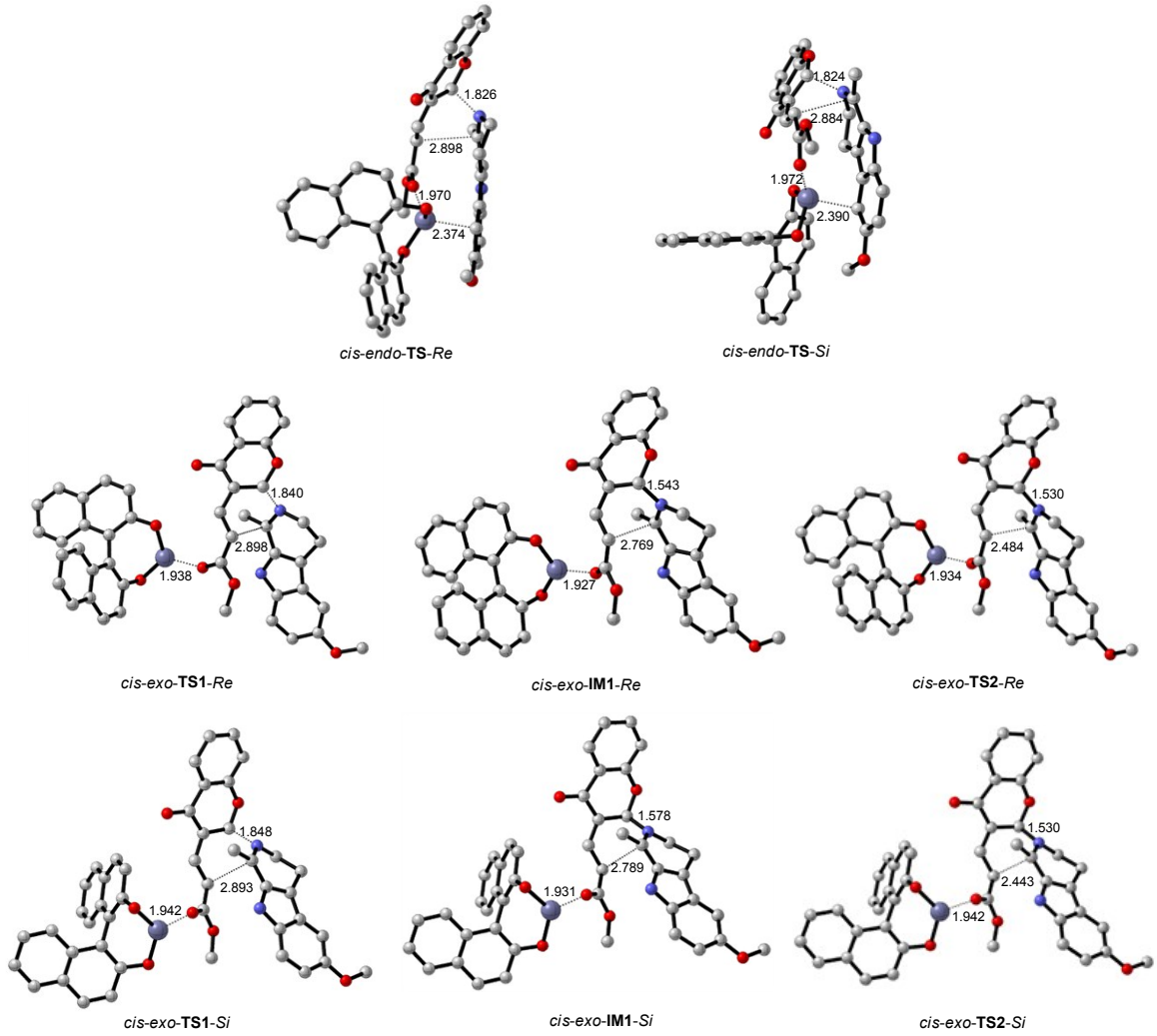


Figure S21. The M05-2X/6-31G(d)-optimized transition states and intermediates for the IEDIDA reaction of **1a** with diene *cis*-**2a** catalyzed by chiral BINOL-Zn complex (the forming bond distances are labeled in Å).

S5 Cartesian coordinate, frequency and energy information of optimized-structures.

5.1 Background reaction

1a

Imaginary frequency: none

Standard orientation:

Electronic energy E = -688.20304 a.u.

Enthalpy H = -688.20304 a.u.

Entropy S =114.473 cal/mol/K

Gibbs free energy G = -688.20304 a.u.

Total free energy in solution E_{sol} = -688.64976 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.667403	0.950368	-0.059612
2	6	0	-2.771980	2.053714	-0.424778
3	6	0	-3.146510	-0.209108	0.066916
4	6	0	-4.022406	-1.397260	0.354911
5	1	0	-3.715112	-1.893068	1.278974
6	1	0	-3.957590	-2.128823	-0.456489
7	1	0	-5.053326	-1.063113	0.445299
8	6	0	-1.700842	-0.402714	-0.038590
9	6	0	-0.819382	0.644882	0.031775
10	7	0	-1.011533	-1.592941	-0.099758
11	6	0	0.336471	-1.314521	-0.090262
12	6	0	0.495606	0.087744	0.010315
13	1	0	-1.418806	-2.503690	-0.212848
14	6	0	-1.370813	2.025489	0.202777
15	1	0	-3.279468	2.985210	-0.175377
16	1	0	-2.664166	2.023667	-1.516096
17	1	0	-0.746821	2.778632	-0.283579
18	1	0	-1.420829	2.285438	1.266348
19	6	0	1.787571	0.648325	0.059382
20	6	0	2.871891	-0.206425	-0.002097
21	6	0	2.695652	-1.606207	-0.113176
22	6	0	1.440996	-2.171991	-0.159361
23	8	0	4.176888	0.193750	0.035058
24	6	0	4.418142	1.581315	0.142289
25	1	0	5.498381	1.700865	0.157332
26	1	0	4.002496	2.120982	-0.713493
27	1	0	1.906280	1.719301	0.140683
28	1	0	3.586785	-2.217584	-0.159096
29	1	0	1.320495	-3.244896	-0.242218
30	1	0	3.992742	1.985629	1.065095

cis-2a

Imaginary frequency: none

Standard orientation:

Electronic energy E = -801.991311 a.u.

Enthalpy H = -801.976062 a.u.

Entropy S = 122.314 cal/mol/K

Gibbs free energy G = -802.034178 a.u.

Total free energy in solution E_{sol} = -802.43299 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.995585	0.994231	-0.038344
2	6	0	2.379399	0.483413	0.022304
3	6	0	-0.031875	-0.055794	-0.145738
4	6	0	0.349845	-1.348046	-0.244254
5	6	0	2.631484	-0.884223	-0.056404
6	8	0	1.615933	-1.791707	-0.202864
7	8	0	0.728646	2.183945	-0.002227
8	6	0	-1.434956	0.352349	-0.194884
9	6	0	-2.483519	-0.415851	0.119287
10	1	0	-0.343309	-2.165141	-0.387011
11	1	0	-1.615680	1.378366	-0.496273
12	6	0	-3.850703	0.128708	-0.018744
13	8	0	-4.135306	1.237923	-0.406223

14	1	0	-2.394630	-1.427830	0.493361
15	8	0	-4.770293	-0.783524	0.348767
16	6	0	-6.124692	-0.332079	0.241300
17	1	0	-6.352331	-0.069943	-0.790515
18	1	0	-6.280540	0.541881	0.871418
19	1	0	-6.738635	-1.163642	0.573542
20	6	0	3.461216	1.361191	0.159801
21	6	0	4.752725	0.872189	0.217327
22	6	0	4.981022	-0.508448	0.136501
23	6	0	3.926767	-1.394806	-0.001413
24	1	0	3.242189	2.419159	0.218311
25	1	0	5.587943	1.551269	0.324235
26	1	0	5.992603	-0.890588	0.181289
27	1	0	4.076765	-2.463628	-0.068411

trans-2a

Imaginary frequency: none

Standard orientation:

Electronic energy E = -801.990603 a.u.

Enthalpy H = -801.975281 a.u.

Entropy S = 123.616 cal/mol/K

Gibbs free energy G = -801.975281 a.u.

Total free energy in solution E_{sol} = -802.43256 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854954	0.905833	-0.012293
2	6	0	-2.280658	0.526025	-0.022520
3	6	0	0.074672	-0.232961	0.079871
4	6	0	-0.420984	-1.482835	0.210436
5	6	0	-2.654636	-0.811403	0.084623
6	8	0	-1.723536	-1.807196	0.212646
7	8	0	-0.479421	2.065469	-0.073614
8	6	0	1.509612	0.052469	0.081345
9	6	0	2.475213	-0.818534	-0.233006
10	1	0	0.196940	-2.359672	0.344845
11	1	0	1.770818	1.070384	0.343327
12	6	0	3.914543	-0.490717	-0.175953
13	8	0	4.789565	-1.281841	-0.445537
14	1	0	2.275285	-1.829451	-0.565405
15	8	0	4.158381	0.774302	0.207477
16	6	0	5.546894	1.116768	0.268465
17	1	0	6.006176	1.001183	-0.711516
18	1	0	6.061497	0.474028	0.980522
19	1	0	5.577976	2.153259	0.589796
20	6	0	-3.281122	1.498570	-0.139342
21	6	0	-4.613086	1.130748	-0.150257
22	6	0	-4.964448	-0.221995	-0.041523
23	6	0	-3.992707	-1.200263	0.076556
24	1	0	-2.967404	2.530938	-0.220702
25	1	0	-5.385416	1.882605	-0.241997
26	1	0	-6.007939	-0.509559	-0.049404
27	1	0	-4.237894	-2.249807	0.164335

cis-endo-TSa

Imaginary frequency: -306.0935 cm^{-1}

Standard orientation:

Electronic energy E = -1490.182372 a.u.

Enthalpy H = -1490.153499 a.u.

Entropy S = 184.501 cal/mol/K

Gibbs free energy G = -1490.241162 a.u.

Total free energy in solution E_{sol}= -1491.07119 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.094663	-0.589982	-1.367633

2	7	0	1.276968	-0.591389	-1.391092
3	6	0	0.168870	-1.270715	-1.518764
4	6	0	0.172736	-2.705437	-1.967685
5	6	0	-1.212182	0.676765	-0.842287
6	6	0	1.178840	0.880614	-1.326779
7	6	0	0.022092	1.446828	-0.493260
8	1	0	-0.521372	-3.308059	-1.381188
9	1	0	1.166731	-3.145113	-1.927977
10	1	0	-0.145391	-2.725410	-3.014914
11	6	0	-2.603126	0.925558	-0.670668
12	6	0	-3.280613	-0.231269	-1.123942
13	7	0	-2.344889	-1.139224	-1.557099
14	1	0	-2.532718	-2.099088	-1.785647
15	1	0	1.047865	1.200731	-2.364474
16	1	0	2.135893	1.261794	-0.980330
17	1	0	-0.084208	2.505602	-0.741978
18	1	0	0.229199	1.385806	0.578870
19	6	0	-3.333204	2.024064	-0.171727
20	6	0	-4.679198	-0.317798	-1.094966
21	6	0	-4.709912	1.926394	-0.139125
22	6	0	-5.373878	0.761512	-0.599859
23	1	0	-2.812174	2.902907	0.179562
24	8	0	-5.544592	2.900069	0.319875
25	1	0	-6.454165	0.753059	-0.545553
26	1	0	-5.199357	-1.200391	-1.445283
27	6	0	-4.940249	4.067618	0.841321
28	1	0	-5.754347	4.705286	1.175113
29	1	0	-4.360851	4.587094	0.072976
30	1	0	-4.290161	3.827945	1.686846
31	6	0	2.912570	0.444147	1.447791
32	6	0	4.126821	0.825295	0.678998
33	6	0	2.227209	-0.728009	0.953086
34	6	0	2.560921	-1.260924	-0.330529
35	6	0	4.484950	0.117069	-0.465739
36	8	0	3.746929	-0.945645	-0.929108
37	8	0	2.555259	1.093109	2.429355
38	6	0	1.018395	-1.135129	1.577197
39	6	0	0.233260	-2.173253	1.186644
40	1	0	2.348022	-2.303765	-0.516615
41	1	0	0.656808	-0.489906	2.372353
42	6	0	-1.135508	-2.287807	1.677028
43	8	0	-1.666818	-1.619133	2.534820
44	1	0	0.562975	-2.932012	0.493883
45	8	0	-1.817990	-3.244467	0.979689
46	6	0	-3.195440	-3.352204	1.346153
47	1	0	-3.291364	-3.585111	2.405043
48	1	0	-3.714337	-2.414869	1.144408
49	1	0	-3.601259	-4.159183	0.740757
50	6	0	4.928706	1.892535	1.088721
51	6	0	6.065422	2.234868	0.373659
52	6	0	6.408368	1.507114	-0.769322
53	6	0	5.621312	0.447074	-1.197048
54	1	0	4.625930	2.426305	1.980041
55	1	0	6.686030	3.059773	0.697544
56	1	0	7.295538	1.769156	-1.331579
57	1	0	5.864842	-0.129299	-2.079165

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cis-exo-TSa

Imaginary frequency: -268.2487 cm^{-1}

Standard orientation: Electronic energy E =-1490.179994 a.u.

Enthalpy H = -1490.151034 a.u.

Center Atomic Atomic Coordinates (Angstroms) Entropy S =114.473 cal/mol/K

Gibbs free energy G = -1490.239484 a.u.
Total free energy in solution E_{sol}= -1491.06901 a.u.

Number	Number	Type	X	Y	Z
1	6	0	-3.886455	1.250638	-0.374294
2	6	0	-4.762915	0.100592	-0.021789
3	6	0	-2.610472	0.880074	-0.940878
4	6	0	-2.265154	-0.511249	-1.077499
5	8	0	-3.254249	-1.463512	-1.075095
6	8	0	-4.233420	2.405535	-0.137702
7	6	0	-1.569469	1.828470	-0.967620
8	6	0	-0.257561	1.554979	-1.246009
9	1	0	-1.604709	-0.732964	-1.912441
10	1	0	-1.818940	2.813626	-0.584236
11	6	0	0.798924	2.455187	-0.816139
12	8	0	0.674839	3.403677	-0.059966
13	1	0	0.062565	0.655630	-1.753443
14	8	0	2.006446	2.054563	-1.281235
15	6	0	3.113207	2.835838	-0.832923
16	1	0	3.078108	3.830533	-1.276568
17	1	0	3.097484	2.932920	0.251150
18	1	0	4.002824	2.299850	-1.152560
19	6	0	-4.402044	-1.199596	-0.368043
20	6	0	-5.963781	0.306409	0.660462
21	6	0	-6.782504	-0.763487	0.985343
22	6	0	-6.404306	-2.058929	0.621285
23	6	0	-5.215025	-2.284759	-0.057673
24	1	0	-4.902872	-3.277418	-0.352777
25	1	0	-7.041432	-2.898419	0.869216
26	1	0	-7.712130	-0.598497	1.513717
27	1	0	-6.221577	1.326927	0.912318
28	6	0	0.984871	-0.324944	0.916528
29	7	0	-1.127958	-1.038192	0.108483
30	6	0	-0.446202	-0.168176	0.822769
31	6	0	-1.123821	0.829976	1.711295
32	6	0	1.718028	-1.147317	0.090048
33	6	0	-0.419718	-2.239711	-0.368291
34	6	0	0.998563	-2.004813	-0.901712
35	1	0	-0.678527	1.821280	1.609825
36	1	0	-0.986133	0.475155	2.739046
37	1	0	-2.189930	0.885226	1.521449
38	6	0	3.090509	-0.869217	0.339422
39	6	0	3.122923	0.124691	1.346728
40	7	0	1.830773	0.436768	1.691127
41	1	0	1.552164	1.213064	2.266570
42	1	0	-1.059523	-2.716893	-1.109485
43	1	0	-0.356621	-2.909504	0.492854
44	1	0	0.990692	-1.521737	-1.885275
45	1	0	1.482266	-2.975829	-1.029234
46	6	0	4.293642	-1.364835	-0.206468
47	6	0	5.482129	-0.848122	0.269629
48	6	0	5.497504	0.143550	1.283559
49	6	0	4.335622	0.633330	1.832572
50	8	0	6.717994	-1.220794	-0.164594
51	6	0	6.771974	-2.202012	-1.181130
52	1	0	7.825925	-2.360166	-1.392565
53	1	0	6.264008	-1.857653	-2.086134
54	1	0	6.321048	-3.140007	-0.845670
55	1	0	4.265684	-2.121180	-0.977687
56	1	0	6.464137	0.500516	1.612315
57	1	0	4.362090	1.390334	2.606060

cis-endo-TSb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.441277	-0.827786	0.809622
2	6	0	-1.541906	-0.141065	1.518190
3	6	0	-2.010615	0.517332	2.793802
4	6	0	-1.963801	-1.962376	-0.013240
5	1	0	-1.406846	1.389140	3.055267
6	1	0	-1.958385	-0.202441	3.615502
7	1	0	-3.053266	0.824393	2.700946
8	6	0	-0.133952	-0.488783	1.359628
9	6	0	-0.569850	-1.873390	-0.655033
10	6	0	0.364357	-1.264066	0.342069
11	7	0	0.899810	-0.032532	2.147066
12	6	0	2.087375	-0.496324	1.624143
13	6	0	1.784617	-1.275223	0.482875
14	1	0	0.811839	0.607147	2.915460
15	1	0	-1.958181	-2.803751	0.686433
16	1	0	-2.720425	-2.163164	-0.768009
17	1	0	-0.257324	-2.889712	-0.913625
18	1	0	-0.591643	-1.304790	-1.587045
19	6	0	3.405084	-0.298187	2.047073
20	6	0	2.825578	-1.866142	-0.259534
21	6	0	4.126588	-1.656784	0.160118
22	6	0	4.412134	-0.880175	1.307070
23	8	0	5.230894	-2.159186	-0.469163
24	6	0	5.006976	-2.936434	-1.626630
25	1	0	2.593485	-2.453988	-1.136003
26	1	0	3.634568	0.297905	2.921819
27	1	0	5.451151	-0.758810	1.582028
28	1	0	4.412215	-3.825072	-1.397177
29	1	0	5.988272	-3.238928	-1.983248
30	1	0	4.499647	-2.354020	-2.401011
31	6	0	-0.333967	1.411223	-1.813546
32	6	0	0.927598	1.885259	-1.217572
33	6	0	-1.493861	1.428564	-0.894173
34	6	0	-1.324868	1.930359	0.386910
35	6	0	0.953402	2.395952	0.080632
36	8	0	-0.176029	2.507520	0.836984
37	8	0	-0.405994	0.987690	-2.956400
38	6	0	-2.633462	0.682436	-1.222816
39	6	0	-3.504579	0.287539	-0.198291
40	1	0	-2.154347	2.226671	1.008057
41	1	0	-2.675246	0.193201	-2.186821
42	6	0	-4.679755	-0.558301	-0.569288
43	8	0	-4.730006	-1.302897	-1.520336
44	8	0	-5.682272	-0.403522	0.304354
45	6	0	-6.837671	-1.207683	0.032252
46	1	0	-6.570435	-2.262501	0.053032
47	1	0	-7.549081	-0.972251	0.817463
48	1	0	-7.243106	-0.960577	-0.947070
49	1	0	-3.746546	0.968681	0.608251
50	6	0	2.129059	1.787310	-1.930295
51	6	0	3.319489	2.195285	-1.359937
52	6	0	3.320984	2.715425	-0.059234
53	6	0	2.145583	2.823819	0.663284
54	1	0	2.082402	1.377373	-2.930562
55	1	0	4.247613	2.108092	-1.908295

Imaginary frequency: -506.9835 cm^{-1}

Electronic energy E =-1490.161497 a.u.

Enthalpy H = -1490.132800 a.u.

Entropy S =114.473 cal/mol/K

Gibbs free energy G = -1490.219222 a.u.

Total free energy in solution E_{sol}= -1491.04499 a.u.

56	1	0	4.252541	3.030361	0.393241
57	1	0	2.125423	3.219003	1.670305

cis-exo-TSb

Imaginary frequency: -532.3827 cm^{-1}

Standard orientation:

Electronic energy E = -1490.173142 a.u.

Enthalpy H = -1490.144410 a.u.

Entropy S =184.511 cal/mol/K

Gibbs free energy G = -1490.232077 a.u.

Total free energy in solution E_{sol}= -1491.03785 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.476838	-1.701457	0.646730
2	6	0	0.816635	-0.572153	0.962581
3	6	0	1.510807	0.332538	1.944107
4	6	0	0.666733	-2.851852	0.202175
5	1	0	1.116093	1.350468	1.924248
6	1	0	2.579406	0.359563	1.728233
7	1	0	1.392543	-0.082979	2.948489
8	6	0	-0.640943	-0.588779	0.888839
9	6	0	-0.617636	-2.560040	-0.591996
10	6	0	-1.359338	-1.482692	0.134240
11	7	0	-1.483718	0.345104	1.438564
12	6	0	-2.770575	0.064922	1.032354
13	6	0	-2.728640	-1.083289	0.205676
14	1	0	-1.204781	1.128954	2.000934
15	1	0	1.322642	-3.529479	-0.340659
16	1	0	0.374782	-3.355539	1.128660
17	1	0	-0.389773	-2.269377	-1.624694
18	1	0	-1.199610	-3.483362	-0.654892
19	6	0	-3.919463	-1.590149	-0.350118
20	6	0	-5.104714	-0.936816	-0.063108
21	6	0	-5.129382	0.206839	0.767930
22	6	0	-3.974021	0.713948	1.323710
23	8	0	-6.328552	-1.314494	-0.537104
24	6	0	-6.370568	-2.457729	-1.365144
25	1	0	-4.004192	1.588446	1.961756
26	1	0	-6.089543	0.668989	0.952754
27	1	0	-3.888909	-2.464657	-0.984143
28	1	0	-6.003281	-3.341826	-0.836092
29	1	0	-7.414801	-2.601146	-1.630660
30	1	0	-5.779806	-2.309394	-2.273704
31	6	0	2.653159	2.354379	-0.562024
32	6	0	1.505548	3.274183	-0.433617
33	6	0	2.287729	0.940636	-0.821192
34	6	0	0.937124	0.605208	-0.942403
35	6	0	0.201964	2.813667	-0.630370
36	8	0	-0.065114	1.530821	-0.987954
37	8	0	3.807900	2.723288	-0.436191
38	6	0	3.241258	-0.052533	-0.625968
39	6	0	2.850474	-1.404327	-0.574542
40	1	0	0.614730	-0.304524	-1.420757
41	1	0	4.217319	0.236823	-0.259936
42	6	0	3.901825	-2.345482	-0.073025
43	8	0	4.825021	-2.033759	0.635933
44	8	0	3.684964	-3.603437	-0.495179
45	6	0	4.630692	-4.563552	-0.003435
46	1	0	4.608977	-4.584388	1.084429
47	1	0	4.320848	-5.517989	-0.417378
48	1	0	5.633037	-4.302236	-0.336448
49	1	0	2.255883	-1.801947	-1.391872
50	6	0	1.703925	4.616936	-0.086729
51	6	0	0.626764	5.470288	0.059865
52	6	0	-0.674419	4.985900	-0.137439

53	6	0	-0.895874	3.663396	-0.480178
54	1	0	2.723559	4.948298	0.060455
55	1	0	0.783437	6.506745	0.326952
56	1	0	-1.519821	5.652190	-0.021177
57	1	0	-1.888700	3.262798	-0.638720

cis-endo-3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.900357	0.940092	0.640508
2	7	0	1.145304	-1.280993	1.621801
3	6	0	1.883212	-0.132302	1.056546
4	6	0	2.877262	0.405777	2.093637
5	6	0	-0.415133	0.984823	1.021052
6	6	0	0.073934	-0.874080	2.541352
7	6	0	-1.045410	-0.055300	1.889951
8	1	0	3.389080	1.286826	1.699077
9	1	0	3.611664	-0.361261	2.342337
10	1	0	2.358627	0.712160	3.000285
11	6	0	-0.977920	2.167637	0.437120
12	6	0	0.057883	2.792920	-0.285505
13	7	0	1.204061	2.042979	-0.126415
14	1	0	2.033244	2.120974	-0.696072
15	1	0	0.546794	-0.266644	3.314050
16	1	0	-0.315116	-1.764049	3.027552
17	1	0	-1.655780	0.405675	2.673111
18	1	0	-1.714671	-0.699741	1.310570
19	6	0	-2.262739	2.739172	0.468550
20	6	0	-0.160283	3.976160	-0.997935
21	6	0	-2.470848	3.912328	-0.236366
22	6	0	-1.426347	4.522327	-0.965819
23	1	0	-3.054664	2.258930	1.026053
24	8	0	-3.666328	4.574953	-0.296283
25	1	0	-1.655513	5.435592	-1.498010
26	1	0	0.634545	4.452435	-1.558077
27	6	0	-4.746283	4.006453	0.411579
28	1	0	-5.596083	4.665109	0.249586
29	1	0	-4.529958	3.946352	1.482349
30	1	0	-4.982615	3.006462	0.036258
31	6	0	-0.445439	-2.179824	-1.685642
32	6	0	-1.564109	-2.870503	-1.023902
33	6	0	0.684201	-1.838265	-0.790646
34	6	0	0.769874	-2.333710	0.634389
35	6	0	-1.475859	-3.225670	0.325148
36	8	0	-0.386984	-3.006977	1.107602
37	8	0	-0.448036	-1.886917	-2.867781
38	6	0	1.693882	-1.073254	-1.207833
39	6	0	2.695398	-0.708060	-0.160515
40	1	0	1.560850	-3.089848	0.673359
41	1	0	1.724634	-0.665167	-2.210247
42	6	0	3.789340	0.208361	-0.653162
43	8	0	3.633747	1.177013	-1.366123
44	1	0	3.191621	-1.600498	0.235465
45	8	0	4.986682	-0.176435	-0.209788
46	6	0	6.080856	0.667625	-0.605483
47	1	0	6.156611	0.692685	-1.690315
48	1	0	5.924418	1.677243	-0.230742
49	1	0	6.964749	0.221109	-0.162687

Imaginary frequency: none
Electronic energy E = -1490.21574 a.u.
Enthalpy H = -1490.18778 a.u.
Entropy S = 182.531 cal/mol/K
Gibbs free energy G = -1490.27451 a.u.
Total free energy in solution E_{sol}=-1491.10112 a.u.

50	6	0	-2.732077	-3.160840	-1.738801
51	6	0	-3.797466	-3.792433	-1.125475
52	6	0	-3.696267	-4.142081	0.225953
53	6	0	-2.548749	-3.865595	0.950600
54	1	0	-2.761537	-2.867673	-2.780231
55	1	0	-4.699111	-4.013278	-1.680281
56	1	0	-4.523986	-4.637190	0.718021
57	1	0	-2.453628	-4.133753	1.994077

cis-endo-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.354027	-1.639321	0.291221
2	6	0	0.316408	-1.476484	1.320543
3	6	0	-0.649361	-2.451911	-0.889065
4	6	0	0.976966	-0.848653	2.412533
5	8	0	-1.774687	-3.170157	-0.738031
6	8	0	0.043837	-2.471280	-1.891008
7	8	0	1.929440	-0.079267	2.288092
8	8	0	0.464269	-1.207221	3.612216
9	6	0	-2.168408	-3.964932	-1.873148
10	6	0	1.079759	-0.603827	4.762092
11	1	0	-3.084564	-4.468619	-1.564267
12	1	0	-1.390040	-4.692762	-2.117036
13	1	0	0.534408	-1.002290	5.618303
14	1	0	2.138063	-0.874688	4.818666
15	1	0	0.987056	0.485138	4.720699
16	6	0	0.339052	1.126387	-0.902884
17	7	0	1.453448	1.006844	-1.186492
18	6	0	2.864264	0.807049	-1.398976
19	6	0	3.202456	-0.687533	-1.234310
20	6	0	4.709836	-0.900581	-1.446557
21	6	0	5.175344	1.460245	-0.640633
22	6	0	5.546177	-0.024421	-0.500703
23	1	0	2.917008	-0.993294	-0.221428
24	1	0	2.609666	-1.284640	-1.934765
25	1	0	4.973602	-0.672182	-2.490709
26	1	0	4.942651	-1.961262	-1.292986
27	1	0	5.734492	2.065766	0.083067
28	1	0	5.372542	-0.343988	0.536512
29	1	0	6.615829	-0.164772	-0.701994
30	6	0	3.669727	1.695096	-0.429751
31	1	0	3.412621	2.748467	-0.592535
32	1	0	3.380102	1.432397	0.594751
33	1	0	5.467562	1.819330	-1.639335
34	6	0	-1.508602	2.640619	-0.481099
35	6	0	-1.032643	1.223838	-0.538503
36	6	0	-1.669912	0.049540	-0.288743
37	6	0	-3.038872	-0.076665	0.183462
38	8	0	-2.790126	2.739530	-0.110693
39	8	0	-0.791813	3.589364	-0.755515
40	8	0	-3.341860	-0.143059	1.363928
41	8	0	-3.916417	-0.243745	-0.839364
42	6	0	-3.320766	4.075868	-0.014217
43	6	0	-5.278027	-0.496011	-0.449632
44	1	0	-3.278860	4.570067	-0.988272
45	1	0	-4.352344	3.949063	0.313441
46	1	0	-2.750819	4.656222	0.715632

Imaginary frequency: none
Electronic energy E = -1490.21586 a.u.
Enthalpy H = -1490.18651 a.u.
Entropy S = 188.540 cal/mol/K
Gibbs free energy G = -1490.27609 a.u.
Total free energy in solution E_{sol} = -1491.11304 a.u.

47	1	0	-5.826085	-0.619730	-1.384670
48	1	0	-5.340890	-1.402838	0.158256
49	1	0	-5.676983	0.347824	0.120420
50	1	0	3.055282	1.117891	-2.434734
51	1	0	-2.351801	-3.322137	-2.738351

cis-endo-3a’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.071617	-2.083586	1.696422
2	6	0	0.949543	-2.915285	1.032084
3	6	0	-1.117359	-1.549412	0.795621
4	6	0	-1.137683	-1.845432	-0.676505
5	6	0	0.906382	-3.128718	-0.348668
6	8	0	-0.030509	-2.595202	-1.179849
7	8	0	-0.066291	-1.858848	2.892588
8	6	0	-2.074165	-0.728374	1.231164
9	6	0	-3.058228	-0.275211	0.193334
10	1	0	-2.033054	-2.421517	-0.938457
11	1	0	-2.135862	-0.407538	2.263145
12	6	0	-4.049735	0.730773	0.756041
13	8	0	-3.897542	1.357494	1.774985
14	8	0	-5.138164	0.819711	-0.016139
15	6	0	-6.113645	1.771206	0.435265
16	1	0	-5.674136	2.766721	0.470720
17	1	0	-6.919210	1.728572	-0.290501
18	1	0	-6.467523	1.500451	1.427899
19	1	0	-3.666356	-1.140797	-0.100881
20	6	0	1.980256	-3.488408	1.784055
21	6	0	2.954347	-4.261543	1.178413
22	6	0	2.899084	-4.467545	-0.203618
23	6	0	1.885748	-3.909069	-0.967281
24	1	0	1.982098	-3.296341	2.849073
25	1	0	3.750054	-4.700869	1.764470
26	1	0	3.653867	-5.072780	-0.689837
27	1	0	1.824006	-4.068430	-2.035875
28	7	0	-2.420521	0.230466	-1.048648
29	6	0	-1.196797	-0.500236	-1.459764
30	6	0	-1.280627	-0.787874	-2.962668
31	6	0	-2.274598	1.689201	-1.121656
32	1	0	-0.387752	-1.303273	-3.316154
33	1	0	-1.380019	0.149268	-3.510514
34	1	0	-2.156928	-1.405097	-3.166782
35	6	0	0.037866	0.299189	-1.116501
36	6	0	-1.199963	2.261719	-0.193664
37	6	0	0.061888	1.524746	-0.506742
38	7	0	1.326567	-0.111631	-1.379121
39	6	0	2.201740	0.846010	-0.914468
40	6	0	1.439113	1.896466	-0.363490
41	1	0	1.581566	-1.005773	-1.757357
42	1	0	-2.007686	1.929116	-2.153334
43	1	0	-3.251980	2.137368	-0.943277
44	1	0	-1.084598	3.332984	-0.384432
45	1	0	-1.500296	2.150828	0.853297
46	6	0	3.599273	0.886270	-0.932220
47	6	0	2.082720	3.025845	0.174965
48	6	0	3.466073	3.061121	0.151599
49	6	0	4.216314	1.997025	-0.396790

Imaginary frequency: none
Electronic energy E = -1490.213372 a.u.
Enthalpy H = -1490.18530 a.u.
Entropy S = 179.937 cal/mol/K
Gibbs free energy G = -1490.27079 a.u.
Total free energy in solution E_{sol}= -1491.09875 a.u.

50	8	0	4.220729	4.091215	0.640794
51	6	0	3.523282	5.180966	1.205212
52	1	0	1.497523	3.829015	0.599895
53	1	0	4.182970	0.075214	-1.349327
54	1	0	5.294226	2.085440	-0.380476
55	1	0	2.872629	5.658903	0.466942
56	1	0	4.280459	5.888513	1.533715
57	1	0	2.922611	4.864159	2.062563

cis-exo-3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.372733	0.572373	0.493479
2	7	0	-0.887516	0.148877	1.300837
3	6	0	0.066984	1.213634	0.907864
4	6	0	0.248203	2.135756	2.125459
5	6	0	1.704594	-0.749226	0.645291
6	6	0	-0.242897	-0.907457	2.102746
7	6	0	0.795640	-1.722313	1.325946
8	1	0	1.025554	2.877914	1.936158
9	1	0	0.553860	1.561681	2.997372
10	1	0	-0.695075	2.636885	2.343866
11	6	0	3.020145	-0.914473	0.096942
12	6	0	3.429329	0.353051	-0.366496
13	7	0	2.410630	1.245278	-0.109770
14	1	0	2.388028	2.220094	-0.359906
15	1	0	-1.028131	-1.539433	2.506020
16	1	0	0.249564	-0.421169	2.943711
17	1	0	0.304340	-2.393057	0.612817
18	1	0	1.351556	-2.357230	2.021994
19	6	0	3.876439	-2.023039	-0.032542
20	6	0	5.111455	-1.827498	-0.626266
21	6	0	5.506213	-0.552623	-1.089444
22	6	0	4.678519	0.543466	-0.965666
23	8	0	6.040396	-2.811648	-0.818824
24	6	0	5.704397	-4.105823	-0.365991
25	1	0	6.556746	-4.739177	-0.598491
26	1	0	4.816410	-4.486425	-0.879023
27	1	0	5.527477	-4.113289	0.713462
28	1	0	3.561174	-2.993458	0.323946
29	1	0	6.483652	-0.467132	-1.544696
30	1	0	4.992561	1.516133	-1.323116
31	6	0	-3.898542	0.431752	-0.849378
32	6	0	-4.381373	-0.938830	-0.608613
33	6	0	-2.507750	0.690640	-0.397335
34	6	0	-1.672247	-0.403722	0.203208
35	8	0	-2.456279	-1.453743	0.771873
36	8	0	-4.572540	1.286377	-1.396131
37	6	0	-1.949490	1.882872	-0.576355
38	6	0	-0.489631	2.066804	-0.310837
39	1	0	-1.042273	-0.871889	-0.571920
40	1	0	-2.527283	2.698106	-0.993399
41	6	0	-0.187689	3.546385	-0.159969
42	8	0	-0.986976	4.389430	0.151194
43	1	0	0.047860	1.726373	-1.202949
44	8	0	1.103958	3.835870	-0.432871
45	6	0	1.452314	5.221524	-0.262579
46	1	0	0.855817	5.836411	-0.932145

Imaginary frequency: none
Electronic energy E = -1490.21797 a.u.
Enthalpy H = -1490.18995 a.u.
Entropy S = 181.560 cal/mol/K
Gibbs free energy G = -1490.276215 a.u.
Total free energy in solution E_{sol}= -1491.10479 a.u.

47	1	0	1.269248	5.524564	0.766383
48	1	0	2.507440	5.290354	-0.507358
49	6	0	-3.628467	-1.809744	0.184125
50	6	0	-5.606024	-1.363361	-1.133581
51	6	0	-6.075472	-2.638998	-0.877342
52	6	0	-5.315156	-3.499550	-0.077804
53	6	0	-4.099844	-3.095389	0.452408
54	1	0	-3.501927	-3.748478	1.073503
55	1	0	-5.675971	-4.498811	0.131360
56	1	0	-7.021344	-2.968362	-1.285714
57	1	0	-6.163858	-0.657248	-1.734904

cis-exo-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.566770	0.303214	0.498642
2	7	0	-0.684141	-0.473879	0.730714
3	6	0	0.155869	0.763388	0.824780
4	6	0	0.060627	1.297284	2.266580
5	6	0	1.969738	-0.987680	0.256715
6	6	0	-0.109047	-1.720223	1.246777
7	6	0	1.046484	-2.158756	0.356739
8	1	0	0.668157	2.194407	2.368595
9	1	0	0.412621	0.553638	2.982554
10	1	0	-0.978496	1.549933	2.485549
11	6	0	3.382955	-0.952704	0.026735
12	6	0	3.778066	0.392755	0.156528
13	7	0	2.657863	1.134172	0.454215
14	1	0	2.603877	2.132122	0.559810
15	1	0	-0.907080	-2.460094	1.286706
16	1	0	0.254829	-1.552675	2.261990
17	1	0	0.667133	-2.476198	-0.619278
18	1	0	1.551664	-3.015014	0.811284
19	6	0	4.337595	-1.944850	-0.265517
20	6	0	5.655199	-1.552625	-0.423350
21	6	0	6.036105	-0.197419	-0.293707
22	6	0	5.111911	0.783005	-0.004809
23	8	0	6.684499	-2.403021	-0.711547
24	6	0	6.363106	-3.769877	-0.860565
25	1	0	7.297289	-4.277925	-1.085413
26	1	0	5.657350	-3.922063	-1.682188
27	1	0	5.938016	-4.178491	0.060715
28	1	0	4.033316	-2.976855	-0.368361
29	1	0	7.081984	0.041725	-0.430230
30	1	0	5.415308	1.817712	0.093324
31	6	0	-3.821651	0.491673	-1.039157
32	6	0	-4.783547	-0.569576	-0.585164
33	6	0	-2.501645	0.581919	-0.403467
34	6	0	-1.919506	-0.486594	0.239754
35	8	0	-4.391666	-0.285918	1.804937
36	8	0	-4.135864	1.249156	-1.945090
37	6	0	-1.637926	1.690868	-0.688095
38	6	0	-0.397838	1.801209	-0.166515
39	1	0	-2.006908	2.464023	-1.349578
40	6	0	0.271431	3.081463	-0.496407
41	8	0	-0.009500	3.783355	-1.437969
42	8	0	1.201909	3.481750	0.417804
43	6	0	1.774558	4.771858	0.144333

Imaginary frequency: none
Electronic energy E = -1490.220554 a.u.
Enthalpy H = -1490.191479 a.u.
Entropy S = 186.163 cal/mol/K
Gibbs free energy G = -1490.279931 a.u.
Total free energy in solution E_{sol}= -1491.11629 a.u.

44	1	0	2.273085	4.764694	-0.822776
45	1	0	0.993768	5.528727	0.137717
46	1	0	2.481191	4.952692	0.949257
47	6	0	-5.018359	-0.895268	0.759642
48	6	0	-5.542480	-1.205561	-1.573959
49	6	0	-6.467770	-2.185438	-1.253569
50	6	0	-6.665490	-2.521388	0.086738
51	6	0	-5.954866	-1.876824	1.087274
52	1	0	-6.116379	-2.098882	2.133662
53	1	0	-7.389030	-3.281203	0.354718
54	1	0	-7.034800	-2.677389	-2.032405
55	1	0	-5.378985	-0.903727	-2.600500
56	1	0	-3.822181	0.420444	1.464613
57	1	0	-2.448532	-1.427361	0.338923

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cis-exo-3a’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.719528	-0.930832	-0.855350
2	6	0	-3.377851	-2.298929	-0.409437
3	6	0	-2.620511	0.063006	-0.712677
4	6	0	-1.248554	-0.441780	-0.364043
5	6	0	-2.190478	-2.532525	0.292784
6	8	0	-1.303783	-1.534871	0.571114
7	8	0	-4.815270	-0.639560	-1.298197
8	6	0	-2.850654	1.352797	-0.950454
9	6	0	-1.763144	2.384440	-0.880606
10	1	0	-0.738512	-0.801297	-1.263384
11	1	0	-3.847585	1.688611	-1.205813
12	6	0	-2.273745	3.509952	0.042887
13	8	0	-3.352855	4.025710	-0.115361
14	8	0	-1.405491	3.882469	0.986180
15	6	0	-1.871796	4.940863	1.839856
16	1	0	-2.780574	4.630691	2.351229
17	1	0	-1.067936	5.118361	2.546918
18	1	0	-2.077662	5.831197	1.249535
19	1	0	-1.738565	2.876084	-1.863465
20	6	0	-4.268053	-3.354375	-0.627395
21	6	0	-3.981118	-4.624942	-0.158930
22	6	0	-2.794849	-4.842246	0.548269
23	6	0	-1.900518	-3.806696	0.777209
24	1	0	-5.182306	-3.135477	-1.163511
25	1	0	-4.668688	-5.441518	-0.332753
26	1	0	-2.563499	-5.831922	0.921401
27	1	0	-0.978199	-3.964976	1.320062
28	7	0	-0.462963	1.801506	-0.658164
29	6	0	-0.384418	0.667266	0.271192
30	6	0	-0.851100	0.975188	1.703670
31	6	0	0.662545	2.737272	-0.650101
32	1	0	-0.708294	0.105274	2.343605
33	1	0	-1.909098	1.241140	1.723908
34	1	0	-0.269897	1.805006	2.102681
35	6	0	1.046726	0.205384	0.274379
36	6	0	1.929547	2.052523	-1.157313
37	6	0	2.097425	0.789553	-0.375675

Imaginary frequency: none

Electronic energy E = -1490.225776 a.u.

Enthalpy H = -1490.197763 a.u.

Entropy S = 178.920 cal/mol/K

Gibbs free energy G = -1490.282774 a.u.

Total free energy in solution E_{sol}= -1491.11629 a.u.

38	7	0	1.472058	-0.916817	0.946493
39	6	0	2.819611	-1.087072	0.707813
40	6	0	3.251115	-0.022340	-0.111664
41	1	0	0.847258	-1.590866	1.353344
42	1	0	0.390737	3.573484	-1.298165
43	1	0	0.847524	3.144113	0.349455
44	1	0	1.840832	1.848326	-2.228473
45	1	0	2.784268	2.720369	-1.016888
46	6	0	4.600935	0.067313	-0.497135
47	6	0	5.471160	-0.916846	-0.060410
48	6	0	5.022872	-1.981063	0.752759
49	6	0	3.704151	-2.077329	1.145157
50	8	0	6.804176	-0.958094	-0.361924
51	6	0	7.309569	0.083946	-1.168617
52	1	0	3.372723	-2.894760	1.773218
53	1	0	5.753297	-2.717602	1.059323
54	1	0	4.930466	0.884544	-1.123122
55	1	0	7.171705	1.057367	-0.689313
56	1	0	8.371671	-0.113801	-1.289523
57	1	0	6.826405	0.094437	-2.150083

trans-endo-TSa

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.035483	-0.766205	-1.386385
2	7	0	1.337472	-0.755782	-1.444802
3	6	0	0.230756	-1.449788	-1.513959
4	6	0	0.246774	-2.907131	-1.881551
5	6	0	-1.150875	0.548519	-0.998675
6	6	0	1.239844	0.715526	-1.517631
7	6	0	0.075602	1.371306	-0.763163
8	1	0	-0.442228	-3.487899	-1.267532
9	1	0	1.248603	-3.327038	-1.815450
10	1	0	-0.068599	-2.983746	-2.926854
11	6	0	-2.539505	0.796754	-0.795668
12	6	0	-3.210341	-0.414118	-1.084151
13	7	0	-2.283360	-1.353140	-1.479738
14	1	0	-2.429409	-2.342970	-1.347452
15	1	0	1.129063	0.934630	-2.583340
16	1	0	2.193160	1.127531	-1.196181
17	1	0	-0.042245	2.388205	-1.146209
18	1	0	0.284419	1.453759	0.307912
19	6	0	-3.265921	1.931040	-0.378912
20	6	0	-4.635583	1.809869	-0.247482
21	6	0	-5.294114	0.587834	-0.532687
22	6	0	-4.601350	-0.524051	-0.956026
23	8	0	-5.466086	2.812624	0.155174
24	6	0	-4.866346	4.054351	0.467104
25	1	0	-4.358316	4.475589	-0.404804
26	1	0	-4.151838	3.950669	1.288189
27	1	0	-2.747945	2.854272	-0.163219
28	1	0	-6.368511	0.563382	-0.409495
29	1	0	-5.115857	-1.450634	-1.175755
30	1	0	-5.675873	4.713108	0.769671
31	6	0	2.738551	0.521433	1.409438
32	6	0	3.990409	0.907422	0.707931
33	6	0	2.150731	-0.720938	0.959606
34	6	0	2.593700	-1.313791	-0.263277

Imaginary frequency: -310.5476 cm^{-1}
Electronic energy E = -1490.186174 a.u.
Enthalpy H = -1490.157544 a.u.
Entropy S = 181.697 cal/mol/K
Gibbs free energy G = -1490.243874 a.u.
Total free energy in solution E_{sol}= -1491.07382 a.u.

35	6	0	4.461787	0.142180	-0.356376
36	8	0	3.798211	-0.974267	-0.804715
37	8	0	2.270254	1.222612	2.305005
38	6	0	0.923174	-1.147152	1.531761
39	6	0	0.242289	-2.265543	1.162412
40	1	0	2.435153	-2.371548	-0.413883
41	1	0	0.471408	-0.455361	2.234757
42	6	0	-1.174229	-2.483869	1.421538
43	8	0	-1.845667	-3.309911	0.816631
44	1	0	0.693415	-3.038381	0.559561
45	8	0	-1.704433	-1.648801	2.328053
46	6	0	-3.120751	-1.755688	2.499504
47	1	0	-3.632706	-1.467524	1.581968
48	1	0	-3.393853	-2.775413	2.763842
49	1	0	-3.368302	-1.068297	3.302682
50	6	0	4.715654	2.034433	1.100620
51	6	0	5.889403	2.378185	0.449022
52	6	0	6.347659	1.591304	-0.611608
53	6	0	5.637325	0.472270	-1.022675
54	1	0	7.264685	1.854057	-1.123272
55	1	0	6.450552	3.249745	0.759043
56	1	0	4.324520	2.612597	1.927508
57	1	0	5.968712	-0.149232	-1.843348

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trans-exo-TS1a

Standard orientation:

Imaginary frequency: -228.1083 cm^{-1}

Electronic energy E = -1490.179742 a.u.

Enthalpy H = -1490.150633 a.u.

Entropy S = 188.148 cal/mol/K

Gibbs free energy G = -1490.240028 a.u.

Total free energy in solution E_{sol}= -1491.07382 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.097144	-1.211753	-0.298609
2	7	0	0.754641	-0.583250	1.009948
3	6	0	0.316147	-0.953307	-0.152214
4	6	0	1.212847	-1.079452	-1.345564
5	6	0	-2.033223	-0.752809	0.604322
6	6	0	-0.170041	-0.588928	2.154285
7	6	0	-1.565421	-0.046306	1.834456
8	1	0	1.343300	-0.102416	-1.816635
9	1	0	0.772239	-1.758809	-2.074291
10	1	0	2.193595	-1.459030	-1.071706
11	6	0	-3.315147	-1.011861	0.048828
12	6	0	-3.091826	-1.654017	-1.191698
13	7	0	-1.739850	-1.748390	-1.395864
14	1	0	-1.305317	-2.201522	-2.179120
15	1	0	0.295724	-0.023654	2.960888
16	1	0	-0.261271	-1.629224	2.481489
17	1	0	-1.563588	1.036795	1.671816
18	1	0	-2.214151	-0.250326	2.688439
19	6	0	-4.630513	-0.764329	0.497703
20	6	0	-5.673630	-1.178087	-0.303878
21	6	0	-5.432832	-1.835025	-1.540050
22	6	0	-4.160496	-2.080672	-1.995452
23	1	0	-4.793484	-0.261766	1.439894
24	1	0	-3.995124	-2.577399	-2.942609
25	1	0	-6.298264	-2.133763	-2.116116
26	8	0	-6.991268	-1.011373	-0.010528
27	6	0	-7.299855	-0.349068	1.201411
28	1	0	-6.916783	-0.906367	2.060689
29	1	0	-8.384138	-0.301973	1.251707
30	1	0	-6.887187	0.663147	1.210186
31	6	0	3.718523	0.726026	-0.698966

32	6	0	4.456815	-0.518238	-0.339392
33	6	0	2.658699	1.068742	0.199434
34	6	0	2.313060	0.210118	1.293941
35	6	0	4.135694	-1.227055	0.816007
36	8	0	3.156015	-0.799645	1.680388
37	8	0	4.021997	1.358132	-1.713745
38	6	0	1.831508	2.196890	-0.068760
39	6	0	0.715652	2.538283	0.624650
40	1	0	1.959197	0.717462	2.186738
41	1	0	2.120685	2.788081	-0.930890
42	6	0	-0.183109	3.630560	0.288898
43	8	0	-1.239714	3.839103	0.859634
44	1	0	0.388182	1.986796	1.494336
45	8	0	0.240799	4.395864	-0.741984
46	6	0	-0.652864	5.447902	-1.103894
47	1	0	-1.621030	5.042936	-1.395636
48	1	0	-0.795511	6.130773	-0.267622
49	1	0	-0.182476	5.958357	-1.939520
50	6	0	5.477226	-1.001613	-1.160326
51	6	0	6.161698	-2.161007	-0.829423
52	6	0	5.826755	-2.852277	0.337864
53	6	0	4.812252	-2.391335	1.166173
54	1	0	5.705068	-0.429909	-2.050568
55	1	0	6.953796	-2.528186	-1.468634
56	1	0	6.358947	-3.756846	0.603493
57	1	0	4.536768	-2.906601	2.076484

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trans-exo-IM1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.080408	-1.239771	-0.222710
2	7	0	0.733868	-0.429150	1.020932
3	6	0	0.320104	-0.946115	-0.104007
4	6	0	1.223711	-1.191626	-1.269276
5	6	0	-2.036022	-0.682024	0.607237
6	6	0	-0.205772	-0.349419	2.159590
7	6	0	-1.591792	0.153274	1.761350
8	1	0	1.392635	-0.252582	-1.800914
9	1	0	0.765353	-1.905184	-1.951701
10	1	0	2.190895	-1.578622	-0.959382
11	6	0	-3.305014	-1.001667	0.061911
12	6	0	-3.059776	-1.779228	-1.094716
13	7	0	-1.706941	-1.893736	-1.266532
14	1	0	-1.262711	-2.448339	-1.975840
15	1	0	0.246180	0.291916	2.912157
16	1	0	-0.291428	-1.359399	2.570874
17	1	0	-1.583198	1.214078	1.488913
18	1	0	-2.254478	0.036504	2.620785
19	6	0	-4.628057	-0.703487	0.458199
20	6	0	-5.656596	-1.205470	-0.309360
21	6	0	-5.393458	-1.999842	-1.459657
22	6	0	-4.115720	-2.295676	-1.863580
23	1	0	-4.805914	-0.096894	1.334149
24	1	0	-3.935211	-2.895999	-2.745680
25	1	0	-6.249806	-2.361776	-2.012683
26	8	0	-6.977668	-1.007703	-0.064414
27	6	0	-7.311237	-0.205162	1.053818
28	1	0	-6.947723	-0.656507	1.980743

Imaginary frequency: none
Electronic energy E = -1490.180065 a.u.
Enthalpy H = -1490.150652 a.u.
Entropy S = 189.232 cal/mol/K
Gibbs free energy G = -1490.240562 a.u.
Total free energy in solution E_{sol}= -1491.07835 a.u.

29	1	0	-8.396105	-0.153754	1.074254
30	1	0	-6.896738	0.800679	0.949809
31	6	0	3.703219	0.695187	-0.698238
32	6	0	4.433399	-0.551481	-0.320104
33	6	0	2.600621	1.024111	0.141047
34	6	0	2.176182	0.149011	1.246360
35	6	0	4.041812	-1.303352	0.785331
36	8	0	2.986297	-0.941767	1.587381
37	8	0	4.064884	1.340332	-1.689160
38	6	0	1.829402	2.180010	-0.115596
39	6	0	0.737780	2.587815	0.594505
40	1	0	2.010794	0.711753	2.166860
41	1	0	2.138161	2.757155	-0.980778
42	6	0	-0.124150	3.698472	0.251586
43	8	0	-1.170114	3.954981	0.828569
44	1	0	0.410175	2.076312	1.487433
45	8	0	0.308253	4.432638	-0.801877
46	6	0	-0.559073	5.501567	-1.172817
47	1	0	-1.542536	5.120393	-1.445743
48	1	0	-0.672922	6.205166	-0.349304
49	1	0	-0.085237	5.982721	-2.024044
50	6	0	5.517428	-0.991189	-1.080067
51	6	0	6.199870	-2.150632	-0.741301
52	6	0	5.794006	-2.886721	0.373367
53	6	0	4.713874	-2.469291	1.140941
54	1	0	5.795241	-0.384509	-1.932159
55	1	0	7.042361	-2.481827	-1.334210
56	1	0	6.321467	-3.791562	0.648008
57	1	0	4.383038	-3.021150	2.010776

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trans-exo-TS2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.059558	-0.491759	0.676446
2	7	0	-1.056351	-1.068304	-0.203298
3	6	0	-0.363509	-0.298686	0.623807
4	6	0	-1.020429	0.524971	1.689702
5	6	0	1.772663	-1.193329	-0.271813
6	6	0	-0.363142	-2.206917	-0.841404
7	6	0	1.035356	-1.885750	-1.372226
8	1	0	-0.554326	1.506563	1.772101
9	1	0	-0.883342	-0.024172	2.628256
10	1	0	-2.085155	0.641739	1.528351
11	6	0	3.151538	-1.021739	0.031239
12	6	0	3.209727	-0.206692	1.192516
13	7	0	1.925265	0.097020	1.572731
14	1	0	1.669157	0.729270	2.309521
15	1	0	-1.024677	-2.586776	-1.617095
16	1	0	-0.274054	-2.976375	-0.071291
17	1	0	1.000746	-1.255105	-2.266824
18	1	0	1.520380	-2.821477	-1.657716
19	6	0	4.335894	-1.482400	-0.560141
20	6	0	5.544672	-1.124000	0.007287
21	6	0	5.589381	-0.313184	1.166093
22	6	0	4.430820	0.146608	1.766263
23	1	0	4.333043	-2.100381	-1.447931
24	1	0	4.481201	0.767581	2.651239
25	1	0	6.539732	-0.039580	1.600244

Imaginary frequency: -37.7539 cm^{-1}

Electronic energy E = -1490.173142 a.u.

Enthalpy H = -1490.144410 a.u.

Entropy S = 184.511 cal/mol/K

Gibbs free energy G = -1490.232077 a.u.

Total free energy in solution E_{sol}= -1491.06641 a.u.

26	8	0	6.661728	-1.599416	-0.614753
27	6	0	7.921710	-1.236129	-0.085759
28	1	0	8.059857	-0.151757	-0.097469
29	1	0	8.661220	-1.700191	-0.732944
30	1	0	8.048437	-1.609868	0.933960
31	6	0	-3.908699	1.121711	-0.179267
32	6	0	-4.712206	-0.092950	0.134330
33	6	0	-2.644117	0.858222	-0.817462
34	6	0	-2.233981	-0.516765	-1.109609
35	6	0	-4.319670	-1.345279	-0.334123
36	8	0	-3.217545	-1.502866	-1.137001
37	8	0	-4.304055	2.238257	0.155085
38	6	0	-1.668943	1.862363	-0.851186
39	6	0	-0.347423	1.675902	-1.187172
40	1	0	-1.729472	-0.576174	-2.075976
41	1	0	-1.975316	2.820594	-0.444661
42	6	0	0.709862	2.633414	-0.915973
43	8	0	1.876555	2.484365	-1.226364
44	1	0	0.000966	0.806314	-1.725396
45	8	0	0.290132	3.712117	-0.200703
46	6	0	1.311730	4.672800	0.061038
47	1	0	2.117474	4.226708	0.643298
48	1	0	1.726804	5.052489	-0.871344
49	1	0	0.829976	5.471356	0.618473
50	6	0	-5.873828	0.006598	0.901364
51	6	0	-6.626635	-1.120575	1.193242
52	6	0	-6.219414	-2.365734	0.708627
53	6	0	-5.067051	-2.485446	-0.056984
54	1	0	-6.156199	0.993380	1.244316
55	1	0	-7.526923	-1.037705	1.787830
56	1	0	-6.803760	-3.250198	0.929277
57	1	0	-4.735873	-3.438399	-0.447360

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trans-endo-TSb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.426605	0.603189	1.140375
2	6	0	1.476422	-0.156706	1.689650
3	6	0	1.858235	-1.004209	2.879490
4	6	0	2.012865	1.855144	0.468735
5	1	0	1.220104	-1.884789	2.980605
6	1	0	1.776727	-0.406518	3.791617
7	1	0	2.897342	-1.326278	2.799342
8	6	0	0.085435	0.241400	1.500692
9	6	0	0.664743	1.883691	-0.269252
10	6	0	-0.338138	1.164574	0.576894
11	7	0	-1.001376	-0.296710	2.153085
12	6	0	-2.147250	0.269223	1.637446
13	6	0	-1.763252	1.194250	0.639078
14	1	0	-0.969811	-1.033089	2.834362
15	1	0	1.964992	2.584151	1.283354
16	1	0	2.818942	2.152346	-0.196994
17	1	0	0.381265	2.931664	-0.407215

Imaginary frequency: -508.0325 cm^{-1}

Electronic energy E = -1490.159438 a.u.

Enthalpy H = -1490.130823 a.u.

Entropy S = 181.217 cal/mol/K

Gibbs free energy G = -1490.216924 a.u.

Total free energy in solution E_{sol}= -1491.04360 a.u.

18	1	0	0.740766	1.442444	-1.265306
19	6	0	-3.491213	0.051660	1.955990
20	6	0	-2.746905	1.917492	-0.063540
21	6	0	-4.073734	1.691791	0.253861
22	6	0	-4.441106	0.765976	1.257556
23	8	0	-5.128790	2.317507	-0.348472
24	6	0	-4.821671	3.260897	-1.353396
25	1	0	-2.452443	2.618650	-0.831161
26	1	0	-3.783456	-0.656348	2.721771
27	1	0	-5.496376	0.639262	1.458030
28	1	0	-4.218557	4.080976	-0.953229
29	1	0	-5.773815	3.648800	-1.706316
30	1	0	-4.286614	2.792916	-2.184513
31	6	0	0.466312	-1.186950	-1.906846
32	6	0	-0.837276	-1.720260	-1.474178
33	6	0	1.560396	-1.360988	-0.925524
34	6	0	1.298384	-2.038319	0.254656
35	6	0	-0.959494	-2.402091	-0.262715
36	8	0	0.112580	-2.641467	0.544399
37	8	0	0.620645	-0.602093	-2.968064
38	6	0	2.731937	-0.605446	-1.072181
39	6	0	3.535564	-0.379078	0.055686
40	1	0	2.079407	-2.439070	0.880003
41	1	0	2.838171	0.004628	-1.958160
42	6	0	4.805786	0.406838	-0.053107
43	8	0	5.744199	0.255919	0.689611
44	8	0	4.795230	1.295391	-1.059603
45	6	0	6.006070	2.052199	-1.194832
46	1	0	6.843422	1.382847	-1.381714
47	1	0	5.842727	2.714485	-2.039013
48	1	0	6.196170	2.617800	-0.284776
49	1	0	3.700556	-1.176933	0.769123
50	6	0	-1.984073	-1.506789	-2.249144
51	6	0	-3.215267	-1.966924	-1.823663
52	6	0	-3.314093	-2.656133	-0.607749
53	6	0	-2.194546	-2.880622	0.173523
54	1	0	-1.863164	-0.966350	-3.178682
55	1	0	-4.100968	-1.791813	-2.419269
56	1	0	-4.278118	-3.012400	-0.268147
57	1	0	-2.249552	-3.408514	1.116302

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trans-exo-TSb

Standard orientation:

Imaginary frequency: -525.4974 cm^{-1}

Electronic energy E = -1490.153885 a.u.

Enthalpy H = -1490.125166 a.u.

Entropy S = 184.625 cal/mol/K

Gibbs free energy G = -1490.212887 a.u.

Total free energy in solution E_{sol}= -1491.03867 a.u. 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	1.322941	-1.846650	0.534007	
2	6	0	0.738861	-0.687436	0.886311
3	6	0	1.504749	0.153306	1.871701
4	6	0	0.442626	-2.943982	0.089240
5	1	0	1.170756	1.193036	1.880735
6	1	0	2.567997	0.121064	1.631192
7	1	0	1.382007	-0.274952	2.870235
8	6	0	-0.718055	-0.616625	0.840002
9	6	0	-0.837854	-2.562596	-0.672649
10	6	0	-1.500262	-1.456202	0.086965
11	7	0	-1.496435	0.350436	1.426874
12	6	0	-2.805516	0.146809	1.046759
13	6	0	-2.844022	-0.985985	0.199067
14	1	0	-1.162789	1.108894	1.993856

15	1	0	1.051466	-3.647181	-0.477256
16	1	0	0.142234	-3.446972	1.013242
17	1	0	-0.613565	-2.266500	-1.704601
18	1	0	-1.475257	-3.448079	-0.739436
19	6	0	-4.072824	-1.419517	-0.335724
20	6	0	-5.214773	-0.711132	-0.007388
21	6	0	-5.159200	0.416503	0.843982
22	6	0	-3.965923	0.852255	1.379358
23	8	0	-6.468031	-1.015869	-0.456355
24	6	0	-6.590092	-2.141343	-1.300513
25	1	0	-3.935069	1.714893	2.033316
26	1	0	-6.089066	0.924262	1.060982
27	1	0	-4.102678	-2.282366	-0.985550
28	1	0	-6.257451	-3.052157	-0.794485
29	1	0	-7.646490	-2.225433	-1.542386
30	1	0	-6.014235	-2.008940	-2.220974
31	6	0	2.774889	2.134136	-0.599206
32	6	0	1.712419	3.142910	-0.426339
33	6	0	2.288171	0.764655	-0.892540
34	6	0	0.912570	0.542416	-0.985393
35	6	0	0.371040	2.796134	-0.601319
36	8	0	-0.011742	1.547102	-0.971237
37	8	0	3.959309	2.399033	-0.481518
38	6	0	3.166518	-0.306736	-0.758029
39	6	0	2.657482	-1.618904	-0.743539
40	1	0	0.501837	-0.322064	-1.479752
41	1	0	4.172584	-0.097955	-0.422451
42	6	0	3.568536	-2.743954	-0.373708
43	8	0	3.430965	-3.880006	-0.766593
44	8	0	4.526795	-2.366305	0.477711
45	6	0	5.399802	-3.422828	0.897594
46	1	0	5.896927	-3.863415	0.035658
47	1	0	6.118745	-2.958355	1.564894
48	1	0	4.829220	-4.191943	1.414567
49	1	0	1.988953	-1.911221	-1.547774
50	6	0	2.029896	4.457635	-0.059878
51	6	0	1.031707	5.394876	0.125207
52	6	0	-0.309263	5.024756	-0.052756
53	6	0	-0.648098	3.732554	-0.413311
54	1	0	3.076572	4.699913	0.069796
55	1	0	1.280210	6.409480	0.406325
56	1	0	-1.093082	5.757315	0.092409
57	1	0	-1.674052	3.420309	-0.558134

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trans-endo-3a

Standard orientation:

Imaginary frequency: none

Electronic energy E = -1490.211023 a.u.

Enthalpy H = -1490.183062 a.u.

Entropy S = 180.930 cal/mol/K

Gibbs free energy G = -1490.269028 a.u.

Total free energy in solution E_{sol} = -1491.10058 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.900357	0.940092	0.640508
2	7	0	1.145304	-1.280993	1.621801
3	6	0	1.883212	-0.132302	1.056546
4	6	0	2.877262	0.405777	2.093637
5	6	0	-0.415133	0.984823	1.021052
6	6	0	0.073934	-0.874080	2.541352
7	6	0	-1.045410	-0.055300	1.889951
8	1	0	3.389080	1.286826	1.699077
9	1	0	3.611664	-0.361261	2.342337
10	1	0	2.358627	0.712160	3.000285
11	6	0	-0.977920	2.167637	0.437120

12	6	0	0.057883	2.792920	-0.285505
13	7	0	1.204061	2.042979	-0.126415
14	1	0	2.033244	2.120974	-0.696072
15	1	0	0.546794	-0.266644	3.314050
16	1	0	-0.315116	-1.764049	3.027552
17	1	0	-1.655780	0.405675	2.673111
18	1	0	-1.714671	-0.699741	1.310570
19	6	0	-2.262739	2.739172	0.468550
20	6	0	-0.160283	3.976160	-0.997935
21	6	0	-2.470848	3.912328	-0.236366
22	6	0	-1.426347	4.522327	-0.965819
23	1	0	-3.054664	2.258930	1.026053
24	8	0	-3.666328	4.574953	-0.296283
25	1	0	-1.655513	5.435592	-1.498010
26	1	0	0.634545	4.452435	-1.558077
27	6	0	-4.746283	4.006453	0.411579
28	1	0	-5.596083	4.665109	0.249586
29	1	0	-4.529958	3.946352	1.482349
30	1	0	-4.982615	3.006462	0.036258
31	6	0	-0.445439	-2.179824	-1.685642
32	6	0	-1.564109	-2.870503	-1.023902
33	6	0	0.684201	-1.838265	-0.790646
34	6	0	0.769874	-2.333710	0.634389
35	6	0	-1.475859	-3.225670	0.325148
36	8	0	-0.386984	-3.006977	1.107602
37	8	0	-0.448036	-1.886917	-2.867781
38	6	0	1.693882	-1.073254	-1.207833
39	6	0	2.695398	-0.708060	-0.160515
40	1	0	1.560850	-3.089848	0.673359
41	1	0	1.724634	-0.665167	-2.210247
42	6	0	3.789340	0.208361	-0.653162
43	8	0	3.633747	1.177013	-1.366123
44	1	0	3.191621	-1.600498	0.235465
45	8	0	4.986682	-0.176435	-0.209788
46	6	0	6.080856	0.667625	-0.605483
47	1	0	6.156611	0.692685	-1.690315
48	1	0	5.924418	1.677243	-0.230742
49	1	0	6.964749	0.221108	-0.162687
50	6	0	-2.732077	-3.160840	-1.738801
51	6	0	-3.797466	-3.792433	-1.125475
52	6	0	-3.696267	-4.142081	0.225953
53	6	0	-2.548749	-3.865595	0.950600
54	1	0	-2.761537	-2.867673	-2.780231
55	1	0	-4.699111	-4.013278	-1.680281
56	1	0	-4.523986	-4.637190	0.718021
57	1	0	-2.453628	-4.133753	1.994077

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trans-endo-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.626839	0.317516	0.580852
2	7	0	0.608812	-0.491769	0.855945
3	6	0	-0.225294	0.745304	0.985729
4	6	0	-0.193987	1.205439	2.455817
5	6	0	-2.031958	-0.962394	0.281574
6	6	0	0.009794	-1.749810	1.309282
7	6	0	-1.123999	-2.146561	0.372275
8	1	0	-0.781342	2.116250	2.557824

Imaginary frequency: none
Electronic energy E = -1490.224292 a.u.
Enthalpy H = -1490.195125 a.u.
Entropy S = 186.579 cal/mol/K
Gibbs free energy G = -1490.283775 a.u.
Total free energy in solution E_{sol}= -1491.10669 a.u.

9	1	0	0.839167	1.411295	2.740518
10	1	0	-0.612186	0.444807	3.116324
11	6	0	-3.435858	-0.904971	0.008463
12	6	0	-3.821347	0.440775	0.172470
13	7	0	-2.706824	1.159776	0.532921
14	1	0	-2.632864	2.157908	0.663862
15	1	0	-0.381602	-1.614672	2.318949
16	1	0	0.800463	-2.498356	1.345138
17	1	0	-1.651684	-3.011590	0.783333
18	1	0	-0.717536	-2.438389	-0.601326
19	6	0	-4.391241	-1.875874	-0.346971
20	6	0	-5.145571	0.850302	-0.019960
21	6	0	-5.698767	-1.463663	-0.533258
22	6	0	-6.070151	-0.109530	-0.371403
23	1	0	-4.094838	-2.907564	-0.474245
24	8	0	-6.727849	-2.294507	-0.881942
25	1	0	-7.108731	0.145745	-0.532910
26	1	0	-5.439795	1.884693	0.104347
27	6	0	-6.415221	-3.659472	-1.055463
28	1	0	-7.346125	-4.152374	-1.324441
29	1	0	-6.024412	-4.096350	-0.131782
30	1	0	-5.683746	-3.799141	-1.856763
31	6	0	3.774120	0.527599	-0.826243
32	6	0	4.670429	-0.662290	-0.586612
33	6	0	2.438932	0.574660	-0.245647
34	6	0	1.838525	-0.506448	0.351146
35	6	0	4.947744	-1.220045	0.667361
36	8	0	4.331283	-0.701507	1.771604
37	8	0	4.176761	1.414275	-1.568108
38	6	0	1.628781	1.737089	-0.418646
39	6	0	0.380865	1.842512	0.094572
40	1	0	2.053294	2.555171	-0.983458
41	6	0	-0.312237	3.132533	-0.024899
42	8	0	-1.296315	3.479693	0.615891
43	8	0	0.262095	3.967151	-0.903744
44	6	0	-0.339096	5.263172	-0.991680
45	1	0	-1.376161	5.176039	-1.309728
46	1	0	-0.301232	5.763828	-0.026000
47	1	0	0.246992	5.801635	-1.729785
48	6	0	5.348550	-1.162729	-1.700193
49	6	0	6.239726	-2.222168	-1.596364
50	6	0	6.488417	-2.779203	-0.345284
51	6	0	5.850988	-2.277314	0.782003
52	1	0	5.161235	-0.686574	-2.653760
53	1	0	6.742845	-2.600748	-2.475773
54	1	0	7.185953	-3.600417	-0.240302
55	1	0	6.058289	-2.697570	1.760755
56	1	0	4.724100	-1.096244	2.560046
57	1	0	2.346377	-1.460832	0.403961

trans-endo-3a’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.391011	2.008734	1.647890
2	6	0	-0.632698	2.922057	1.105951
3	6	0	1.321437	1.453110	0.639946
4	6	0	1.231874	1.805846	-0.817020
5	6	0	-0.696540	3.187488	-0.264948

Imaginary frequency: none
Electronic energy E = -1490.228986 a.u.
Enthalpy H = -1490.201585 a.u.
Entropy S = 175.189 cal/mol/K
Gibbs free energy G = -1490.284823 a.u.
Total free energy in solution E_{sol}= -1491.04360 a.u.

6	8	0	0.131694	2.635845	-1.193917
7	8	0	0.475847	1.737249	2.831295
8	6	0	2.261991	0.563126	0.960203
9	6	0	3.124027	0.097225	-0.175868
10	1	0	2.133790	2.340868	-1.137147
11	1	0	2.393588	0.198548	1.970892
12	6	0	4.099131	-0.984269	0.261480
13	8	0	4.793493	-1.632292	-0.481566
14	8	0	4.075195	-1.147962	1.588688
15	6	0	4.990368	-2.136613	2.084369
16	1	0	6.011259	-1.863734	1.822082
17	1	0	4.855413	-2.144154	3.161039
18	1	0	4.757991	-3.108897	1.654806
19	1	0	3.754646	0.938427	-0.492601
20	6	0	-1.558741	3.521617	1.965760
21	6	0	-2.534034	4.371544	1.476046
22	6	0	-2.586392	4.628935	0.102543
23	6	0	-1.677773	4.045426	-0.766856
24	1	0	-1.479847	3.287746	3.019438
25	1	0	-3.248642	4.831066	2.145220
26	1	0	-3.343205	5.294332	-0.293557
27	1	0	-1.699345	4.243457	-1.830538
28	7	0	2.352462	-0.322162	-1.373240
29	6	0	1.143221	0.491670	-1.648659
30	6	0	1.113656	0.833713	-3.142184
31	6	0	2.114599	-1.766381	-1.483621
32	1	0	0.225668	1.411937	-3.397033
33	1	0	1.109595	-0.084991	-3.728883
34	1	0	2.004046	1.408542	-3.401616
35	6	0	-0.102319	-0.250406	-1.225270
36	6	0	1.092219	-2.314300	-0.484466
37	6	0	-0.146089	-1.495978	-0.658695
38	7	0	-1.382290	0.242030	-1.358212
39	6	0	-2.269196	-0.682840	-0.851341
40	6	0	-1.525361	-1.795422	-0.406926
41	1	0	-1.615617	1.163380	-1.681090
42	1	0	1.745720	-1.949754	-2.495284
43	1	0	3.075468	-2.275298	-1.408240
44	1	0	0.897519	-3.368991	-0.701330
45	1	0	1.488012	-2.262125	0.534970
46	6	0	-3.662949	-0.644066	-0.746539
47	6	0	-2.185770	-2.907523	0.146926
48	6	0	-3.565612	-2.864348	0.245056
49	6	0	-4.296097	-1.738954	-0.197407
50	8	0	-4.334836	-3.869222	0.763160
51	6	0	-3.656987	-5.017893	1.225368
52	1	0	-1.614637	-3.758457	0.490176
53	1	0	-4.231448	0.214340	-1.081861
54	1	0	-5.371897	-1.767469	-0.088694
55	1	0	-3.102085	-5.501760	0.416188
56	1	0	-4.423504	-5.694449	1.594930
57	1	0	-2.966709	-4.769559	2.036582

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trans-exo-3a

Imaginary frequency: none

Standard orientation:

Electronic energy E = -1490.221375 a.u.

Enthalpy H = -1490.194224 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 176.409 cal/mol/K

Gibbs free energy G = -1490.278042 a.u.

1	6	0	1.423999	0.624714	0.463926
2	7	0	-0.817798	0.045494	1.241530
3	6	0	0.067676	1.168294	0.851459
4	6	0	0.155776	2.117383	2.058529
5	6	0	1.842070	-0.673011	0.609320
6	6	0	-0.109185	-0.973208	2.036894
7	6	0	0.986760	-1.711134	1.262534
8	1	0	0.888688	2.906424	1.882625
9	1	0	0.471063	1.570649	2.944856
10	1	0	-0.825679	2.554221	2.246986
11	6	0	3.176483	-0.738763	0.087764
12	6	0	3.502490	0.560137	-0.356153
13	7	0	2.420763	1.377395	-0.110355
14	1	0	2.316050	2.344332	-0.383364
15	1	0	-0.852932	-1.658111	2.432235
16	1	0	0.345882	-0.459985	2.883649
17	1	0	0.546382	-2.400050	0.533684
18	1	0	1.570816	-2.321318	1.957725
19	6	0	4.114635	-1.780999	-0.029767
20	6	0	5.344978	-1.489782	-0.592771
21	6	0	5.655543	-0.185538	-1.038076
22	6	0	4.747596	0.846137	-0.925550
23	8	0	6.348889	-2.401778	-0.768974
24	6	0	6.095321	-3.722118	-0.340104
25	1	0	6.994968	-4.291045	-0.560953
26	1	0	5.247274	-4.156501	-0.877554
27	1	0	5.895733	-3.757583	0.734944
28	1	0	3.863825	-2.774714	0.313540
29	1	0	6.634366	-0.025177	-1.469669
30	1	0	4.996581	1.842976	-1.266743
31	6	0	-3.887188	0.212601	-0.817955
32	6	0	-4.304066	-1.177930	-0.573813
33	6	0	-2.490643	0.522911	-0.420344
34	6	0	-1.586770	-0.535427	0.147640
35	8	0	-2.296462	-1.640489	0.706788
36	8	0	-4.617411	1.046716	-1.323728
37	6	0	-1.983413	1.735526	-0.620288
38	6	0	-0.521591	1.955780	-0.394756
39	1	0	-0.943973	-0.951964	-0.646545
40	1	0	-2.605810	2.520630	-1.029341
41	6	0	-0.134449	3.420854	-0.326277
42	8	0	0.979487	3.842837	-0.559789
43	1	0	0.002354	1.569719	-1.276075
44	8	0	-1.140960	4.209949	0.040573
45	6	0	-0.809293	5.602761	0.170326
46	1	0	-0.037528	5.727414	0.927208
47	1	0	-0.450214	5.989173	-0.780668
48	1	0	-1.730793	6.091208	0.468411
49	6	0	-3.480680	-2.029928	0.167987
50	6	0	-5.535863	-1.643204	-1.046258
51	6	0	-5.942993	-2.939476	-0.789071
52	6	0	-5.111290	-3.781445	-0.042235
53	6	0	-3.888503	-3.337536	0.435673
54	1	0	-3.236046	-3.975874	1.015799
55	1	0	-5.421997	-4.797462	0.166702
56	1	0	-6.894073	-3.299624	-1.157168
57	1	0	-6.148434	-0.951035	-1.609275

Total free energy in solution E_{sol}= -1491.03867 a.u.

trans-exo-4a

Standard orientation:

Imaginary frequency: none

Electronic energy E = -1490.228790 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.614195	0.305930	0.578880
2	7	0	-0.618848	-0.524400	0.814113
3	6	0	0.205146	0.717441	0.974021
4	6	0	0.150770	1.154049	2.450093
5	6	0	2.030016	-0.965906	0.260495
6	6	0	-0.015821	-1.788650	1.251217
7	6	0	1.129646	-2.157775	0.318428
8	1	0	0.731426	2.066328	2.573936
9	1	0	0.563451	0.385364	3.104198
10	1	0	-0.886184	1.352068	2.728038
11	6	0	3.437048	-0.896415	0.007433
12	6	0	3.813462	0.447358	0.201521
13	7	0	2.690858	1.154404	0.561222
14	1	0	2.614475	2.148975	0.711962
15	1	0	-0.802329	-2.541937	1.265946
16	1	0	0.362581	-1.667205	2.267252
17	1	0	0.735984	-2.434210	-0.664773
18	1	0	1.659166	-3.026381	0.718835
19	6	0	4.401271	-1.856835	-0.352681
20	6	0	5.708947	-1.435244	-0.514312
21	6	0	6.071152	-0.081910	-0.323750
22	6	0	5.138070	0.867104	0.033205
23	8	0	6.746354	-2.253883	-0.863657
24	6	0	6.445430	-3.619124	-1.057966
25	1	0	7.383265	-4.102178	-1.320257
26	1	0	5.725911	-3.753635	-1.870844
27	1	0	6.045402	-4.069320	-0.144756
28	1	0	4.111616	-2.887390	-0.502202
29	1	0	7.110446	0.180962	-0.467265
30	1	0	5.425778	1.900348	0.180059
31	6	0	-3.767641	0.484460	-0.914648
32	6	0	-4.685690	-0.663256	-0.602455
33	6	0	-2.460383	0.561368	-0.254519
34	6	0	-1.844703	-0.537133	0.306816
35	8	0	-4.357556	-0.628321	1.813192
36	8	0	-4.106455	1.325273	-1.735655
37	6	0	-1.644079	1.725691	-0.424210
38	6	0	-0.399388	1.822932	0.091929
39	1	0	-2.063490	2.543905	-0.992800
40	6	0	0.296399	3.116870	-0.015391
41	8	0	1.260957	3.464644	0.651324
42	8	0	-0.258756	3.944649	-0.909592
43	6	0	0.338421	5.244706	-0.987185
44	1	0	0.275508	5.746449	-0.023566
45	1	0	1.382643	5.160334	-1.281160
46	1	0	-0.233135	5.777870	-1.740083
47	6	0	-4.932087	-1.146806	0.691245
48	6	0	-5.389616	-1.221429	-1.675206
49	6	0	-6.269000	-2.275697	-1.489771
50	6	0	-6.477695	-2.767413	-0.200252
51	6	0	-5.823296	-2.203625	0.883959
52	1	0	-5.995334	-2.548180	1.894896
53	1	0	-7.166206	-3.586973	-0.036772
54	1	0	-6.792328	-2.705845	-2.333053
55	1	0	-5.219907	-0.799736	-2.657544
56	1	0	-3.828263	0.146180	1.570705
57	1	0	-2.344329	-1.498857	0.325621

Enthalpy H = -1490.19975 a.u.
Entropy S = 186.826 cal/mol/K
Gibbs free energy G = -1490.288518 a.u.
Total free energy in solution E_{sol}=- -1491.12235 a.u.

trans-exo-3a’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.550117	1.128993	-0.865254
2	6	0	3.118016	2.486042	-0.466534
3	6	0	2.520755	0.069270	-0.682745
4	6	0	1.118621	0.492825	-0.346230
5	6	0	1.918989	2.664176	0.232135
6	8	0	1.101989	1.619740	0.549428
7	8	0	4.662109	0.896424	-1.302276
8	6	0	2.836711	-1.209786	-0.875747
9	6	0	1.821233	-2.309023	-0.764729
10	1	0	0.583785	0.785031	-1.255501
11	1	0	3.853481	-1.486736	-1.123395
12	6	0	2.408224	-3.364111	0.195771
13	8	0	1.705425	-4.060589	0.886075
14	8	0	3.742548	-3.399690	0.223143
15	6	0	4.293634	-4.371685	1.127538
16	1	0	3.956319	-5.368173	0.850380
17	1	0	5.370540	-4.282875	1.027443
18	1	0	3.975824	-4.154814	2.145142
19	1	0	1.827876	-2.835870	-1.729467
20	6	0	3.934744	3.590487	-0.725553
21	6	0	3.563869	4.854768	-0.301082
22	6	0	2.367049	5.016908	0.403133
23	6	0	1.544884	3.932416	0.672441
24	1	0	4.860606	3.414570	-1.257556
25	1	0	4.194585	5.708991	-0.506665
26	1	0	2.070350	6.001454	0.742025
27	1	0	0.615067	4.047588	1.213356
28	7	0	0.485206	-1.807215	-0.557402
29	6	0	0.332323	-0.648464	0.331584
30	6	0	0.821467	-0.873167	1.772017
31	6	0	-0.574757	-2.815604	-0.511356
32	1	0	0.621692	0.007406	2.381395
33	1	0	1.895002	-1.066547	1.797055
34	1	0	0.298207	-1.725433	2.202651
35	6	0	-1.126651	-0.283958	0.324646
36	6	0	-1.885958	-2.236010	-1.036965
37	6	0	-2.136923	-0.960161	-0.299769
38	7	0	-1.625226	0.830335	0.958485
39	6	0	-2.981646	0.901067	0.719787
40	6	0	-3.342118	-0.218734	-0.059634
41	1	0	-1.046411	1.558888	1.338522
42	1	0	-0.248557	-3.654195	-1.130610
43	1	0	-0.729984	-3.198127	0.502759
44	1	0	-1.813279	-2.064560	-2.115053
45	1	0	-2.693520	-2.954351	-0.869294
46	6	0	-4.683595	-0.412533	-0.435827
47	6	0	-5.617224	0.525851	-0.030412
48	6	0	-5.239983	1.646042	0.742650
49	6	0	-3.929966	1.844592	1.125667
50	8	0	-6.950580	0.466690	-0.327404
51	6	0	-7.386275	-0.634994	-1.094531
52	1	0	-3.653075	2.704274	1.722975
53	1	0	-6.017720	2.342284	1.026138
54	1	0	-4.958603	-1.271814	-1.031078
55	1	0	-7.182279	-1.579280	-0.581698

Imaginary frequency: none
Electronic energy E = -1490.213372 a.u.
Enthalpy H = -1490.185297 a.u.
Entropy S = 179.937 cal/mol/K
Gibbs free energy G = -1490.270790 a.u.
Total free energy in solution E_{sol}= -1491.03867 a.u.

56	1	0	-8.459512	-0.513480	-1.217742
57	1	0	-6.905419	-0.647918	-2.077101

5.2 $ZnCl_2$-catalyzed reaction

5.2.1 cis-2a as diene

$ZnCl_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
30	0	0.000000	0.000000	0.000012	
2	17	0	0.000000	0.000000	-2.090318
3	17	0	0.000000	0.000000	2.090296

Imaginary frequency: none
Electronic energy E = -2699.445954 a.u.
Enthalpy H = -2699.440847 a.u.
Entropy S = 58.864 cal/mol/K
Gibbs free energy G = -2699.468815 a.u.
Total free energy in solution E_{sol}= -2699.76669 a.u. 1

COM-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.696940	-0.689024	-0.745523	
2	7	0	3.550569	0.610056	-1.476213
3	6	0	3.133981	-0.375865	-0.784574
4	6	0	4.075667	-1.204863	0.038386
5	6	0	0.741724	0.254306	-1.073836
6	6	0	2.574138	1.332452	-2.301150
7	6	0	1.195187	1.563370	-1.663326
8	1	0	3.774540	-1.187940	1.089072
9	1	0	5.081523	-0.805037	-0.064889
10	1	0	4.071943	-2.245441	-0.300410
11	6	0	-0.541821	-0.391572	-0.882294
12	6	0	-0.262303	-1.709863	-0.444708
13	7	0	1.103573	-1.868221	-0.407389
14	1	0	1.570545	-2.619258	0.074958
15	1	0	2.451708	0.755535	-3.225008
16	1	0	3.018898	2.288342	-2.572775
17	1	0	0.493543	1.905681	-2.426077
18	1	0	1.244387	2.350744	-0.906959
19	6	0	-1.880912	0.048616	-1.013278
20	6	0	-2.885595	-0.842984	-0.687714
21	6	0	-2.585625	-2.162092	-0.254527
22	6	0	-1.292176	-2.607372	-0.128569
23	8	0	-4.206752	-0.554730	-0.736089
24	6	0	-4.563109	0.790335	-1.019645
25	1	0	-2.081928	1.064016	-1.320176

Imaginary frequency: none
Electronic energy E = -3387.696737 a.u.
Enthalpy H = -3387.676466 a.u.
Entropy S = 146.107 cal/mol/K
Gibbs free energy G = -3387.745886 a.u.
Total free energy in solution E_{sol}= -3388.43909 a.u. 1

26	1	0	-3.421392	-2.802271	-0.007491
27	1	0	-1.078140	-3.608747	0.219887
28	1	0	-4.261324	1.067737	-2.032635
29	1	0	-5.645046	0.835637	-0.937060
30	1	0	-4.104728	1.471292	-0.298458
31	30	0	0.051204	0.618550	1.125308
32	17	0	0.911216	-0.725715	2.603763
33	17	0	-0.794288	2.618981	1.148428

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cis-endo-TS-I

Imaginary frequency: -345.1806 cm^{-1}

Standard orientation:

Electronic energy E = -4189.677372 a.u.

Enthalpy H = -4189.643037 a.u.

Entropy S = 213.128 cal/mol/K

Gibbs free energy G = -4189.744300 a.u.

Total free energy in solution E_{sol}= -4190.86086 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.668036	0.720044	-0.813622
2	7	0	-1.624432	0.238883	-1.216954
3	6	0	-0.596054	1.007892	-1.472976
4	6	0	-0.600750	1.968380	-2.628769
5	6	0	0.814515	-0.238262	0.180261
6	6	0	-1.420816	-0.994891	-0.428830
7	6	0	-0.411039	-0.913802	0.721729
8	1	0	-0.075351	2.893305	-2.390475
9	1	0	-1.611144	2.198322	-2.960767
10	1	0	-0.090520	1.472919	-3.461746
11	6	0	2.189007	-0.151637	0.619464
12	6	0	2.796357	0.861103	-0.162434
13	7	0	1.837493	1.396807	-0.988607
14	1	0	2.034618	2.007724	-1.764359
15	1	0	-1.068892	-1.742423	-1.149037
16	1	0	-2.392762	-1.325795	-0.073684
17	1	0	-0.195342	-1.929006	1.057455
18	1	0	-0.807606	-0.350563	1.570454
19	6	0	2.949468	-0.884011	1.560540
20	6	0	4.292449	-0.577620	1.675745
21	6	0	4.884359	0.442575	0.883371
22	6	0	4.159097	1.163349	-0.034351
23	8	0	5.149415	-1.201170	2.515145
24	6	0	4.639201	-2.294669	3.264181
25	1	0	2.478509	-1.665409	2.137819
26	1	0	5.942002	0.621063	1.020767
27	1	0	4.627990	1.923416	-0.644975
28	1	0	4.245425	-3.067548	2.599719
29	1	0	5.479875	-2.685923	3.829445
30	1	0	3.856960	-1.963484	3.951248
31	30	0	1.969858	-1.697266	-1.147879
32	17	0	1.577094	-3.668713	-0.319236
33	17	0	2.610563	-0.943582	-3.088157
34	6	0	-3.613667	0.423240	1.554100
35	6	0	-4.637962	-0.480195	0.976400
36	6	0	-2.972175	1.310729	0.596293
37	6	0	-3.142070	1.084766	-0.807200
38	6	0	-4.864569	-0.495190	-0.398297
39	8	0	-4.164498	0.309483	-1.267125
40	8	0	-3.347288	0.410750	2.751270
41	6	0	-1.929075	2.149118	1.039501
42	6	0	-1.184122	2.965498	0.237519
43	1	0	-3.012950	1.920438	-1.480379
44	1	0	-1.631445	2.037676	2.077951
45	6	0	0.067178	3.533546	0.735931
46	8	0	0.557425	3.354457	1.828527

47	1	0	-1.515038	3.292728	-0.736050
48	8	0	0.687790	4.266806	-0.228187
49	6	0	1.951115	4.803116	0.175649
50	1	0	1.826729	5.456898	1.036793
51	1	0	2.634762	3.997619	0.445178
52	1	0	2.322516	5.362058	-0.679013
53	6	0	-5.387049	-1.330113	1.793959
54	6	0	-6.347349	-2.164594	1.246370
55	6	0	-6.562563	-2.157983	-0.135157
56	6	0	-5.823668	-1.327190	-0.965453
57	1	0	-5.186472	-1.302033	2.856906
58	1	0	-6.928249	-2.819141	1.882215
59	1	0	-7.311322	-2.808696	-0.568274
60	1	0	-5.969484	-1.308778	-2.036798

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cis-exo-TS-I

Imaginary frequency: -378.6187 cm^{-1}

Standard orientation:

Electronic energy E = -4189.673193 a.u.

Enthalpy H = -4189.638959 a.u.

Entropy S = 212.491 cal/mol/K

Gibbs free energy G = -4189.739920 a.u.

Total free energy in solution E_{sol}= -4190.85671 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.494920	0.367693	0.425712
2	7	0	-1.555759	-0.563056	-0.363485
3	6	0	-0.956688	0.262063	0.476182
4	6	0	-1.663137	0.737558	1.709279
5	6	0	1.270201	-0.168150	-0.593162
6	6	0	-0.724108	-1.406105	-1.243353
7	6	0	0.566536	-0.768592	-1.774464
8	1	0	-1.397364	1.765346	1.961051
9	1	0	-1.358597	0.067029	2.521353
10	1	0	-2.740779	0.653410	1.602522
11	6	0	2.627152	0.255166	-0.328173
12	6	0	2.583627	1.002796	0.874301
13	7	0	1.273640	1.083597	1.281153
14	1	0	0.970240	1.442704	2.172201
15	1	0	-1.361690	-1.756763	-2.053869
16	1	0	-0.453518	-2.287766	-0.652553
17	1	0	0.365088	0.008954	-2.518503
18	1	0	1.163447	-1.543781	-2.255637
19	6	0	3.863788	-0.001277	-0.965853
20	6	0	5.008169	0.501131	-0.373070
21	6	0	4.943010	1.255924	0.828649
22	6	0	3.750267	1.509335	1.462543
23	1	0	3.889024	-0.594321	-1.867708
24	1	0	3.717136	2.065171	2.390008
25	1	0	5.878517	1.608619	1.240770
26	8	0	6.258499	0.320693	-0.855178
27	6	0	6.400539	-0.536078	-1.978925
28	1	0	5.991928	-1.526326	-1.763461
29	1	0	5.903575	-0.113818	-2.855673
30	1	0	7.467911	-0.608476	-2.164950
31	30	0	2.220611	-1.842945	0.644593
32	17	0	2.692500	-3.400264	-0.802080
33	17	0	1.903429	-1.757660	2.790385
34	6	0	-4.719600	1.267901	-0.061927
35	6	0	-5.376446	-0.061577	-0.029470
36	6	0	-3.430886	1.285938	-0.743562
37	6	0	-2.909735	0.079763	-1.315606
38	6	0	-4.842654	-1.132953	-0.743002
39	8	0	-3.727486	-0.990317	-1.533877

40	8	0	-5.210663	2.245236	0.487537
41	6	0	-2.551006	2.347841	-0.514468
42	6	0	-1.221832	2.334258	-0.876608
43	1	0	-2.287748	0.214856	-2.196026
44	1	0	-2.906358	3.141512	0.135454
45	6	0	-0.283479	3.296332	-0.308302
46	8	0	-0.478928	3.983842	0.675472
47	1	0	-0.845494	1.724342	-1.685038
48	8	0	0.899123	3.271324	-0.961374
49	6	0	1.898296	4.143471	-0.426989
50	1	0	1.606375	5.182584	-0.572456
51	1	0	2.032800	3.959274	0.637282
52	1	0	2.809533	3.916624	-0.972794
53	6	0	-6.540602	-0.261075	0.717376
54	6	0	-7.151206	-1.503503	0.746835
55	6	0	-6.600596	-2.563049	0.018964
56	6	0	-5.447007	-2.385368	-0.730753
57	1	0	-6.936635	0.588070	1.258853
58	1	0	-8.051379	-1.655652	1.327243
59	1	0	-7.075119	-3.535740	0.038594
60	1	0	-5.004694	-3.189465	-1.302900

COM-II

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3387.715512 a.u.

Enthalpy H = -3387.695121 a.u.

Entropy S = 151.649 cal/mol/K

Gibbs free energy G = -3387.767174 a.u.

Total free energy in solution E_{sol}= -3388.20813 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.632023	0.840654	-0.321293
2	7	0	-1.523571	-0.110000	-0.105344
3	6	0	-0.804018	0.958087	-0.234179
4	6	0	-1.423780	2.320220	-0.285470
5	6	0	1.303138	-0.302238	0.051516
6	6	0	-0.848132	-1.422633	-0.211638
7	6	0	0.504770	-1.485385	0.494277
8	1	0	-0.950982	2.976770	0.447127
9	1	0	-2.490668	2.280129	-0.078417
10	1	0	-1.268096	2.749706	-1.279577
11	6	0	2.693814	-0.004328	0.001560
12	6	0	2.800703	1.340746	-0.423923
13	7	0	1.535421	1.846430	-0.591419
14	1	0	1.315990	2.757430	-0.953384
15	1	0	-0.711756	-1.619303	-1.279860
16	1	0	-1.531602	-2.177363	0.170236
17	1	0	0.989786	-2.426986	0.231401
18	1	0	0.380568	-1.474764	1.582795
19	6	0	3.854850	-0.760748	0.270309
20	6	0	5.078852	-0.149329	0.094245
21	6	0	5.169095	1.198065	-0.344282
22	6	0	4.050735	1.951271	-0.607244
23	8	0	6.281981	-0.745247	0.310353
24	6	0	6.264469	-2.093486	0.739365
25	1	0	3.767281	-1.785872	0.599590
26	1	0	6.160946	1.612876	-0.463007
27	1	0	4.137559	2.977882	-0.938461
28	1	0	5.780726	-2.734077	-0.002909
29	1	0	7.304307	-2.387166	0.852317
30	1	0	5.749068	-2.192928	1.698346
31	30	0	-3.516656	-0.222685	0.059417
32	17	0	-4.214341	-2.021359	-0.950861
33	17	0	-4.558092	1.291112	1.226528

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cis-endo-TS-II

Standard orientation:

Imaginary frequency: -467.1111 cm^{-1}

Electronic energy E = -4189.683011 a.u.

Enthalpy H = -4189.648815 a.u.

Entropy S = 210.433 cal/mol/K

Gibbs free energy G = -4189.748799 a.u.

Total free energy in solution E_{sol}= -4190.39191 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.574882	-0.824677	-0.507375
2	7	0	0.815672	-0.586879	-0.386462
3	6	0	-0.281233	-1.377893	-0.193153
4	6	0	-0.105765	-2.871498	-0.238799
5	6	0	-1.847907	0.520676	-0.600324
6	6	0	0.553167	0.793111	-0.911669
7	6	0	-0.727797	1.496167	-0.448948
8	1	0	-0.913965	-3.374166	0.290602
9	1	0	0.845566	-3.190141	0.181104
10	1	0	-0.105645	-3.188392	-1.287354
11	6	0	-3.250627	0.650513	-0.798725
12	6	0	-3.777101	-0.662344	-0.821956
13	7	0	-2.743516	-1.546390	-0.624613
14	1	0	-2.818806	-2.547764	-0.641351
15	1	0	0.502270	0.674513	-1.995205
16	1	0	1.437974	1.393222	-0.708517
17	1	0	-0.868529	2.363473	-1.098676
18	1	0	-0.659835	1.873041	0.574124
19	6	0	-4.105471	1.759843	-0.961473
20	6	0	-5.451800	1.517602	-1.149243
21	6	0	-5.961179	0.194650	-1.184381
22	6	0	-5.142638	-0.899508	-1.025458
23	8	0	-6.396497	2.483195	-1.315233
24	6	0	-5.958027	3.826958	-1.261685
25	1	0	-3.701755	2.761304	-0.931645
26	1	0	-7.025186	0.077743	-1.339541
27	1	0	-5.545716	-1.903904	-1.055433
28	1	0	-5.241620	4.038662	-2.060129
29	1	0	-6.845561	4.438957	-1.397721
30	1	0	-5.501682	4.051528	-0.293969
31	6	0	1.671250	1.738030	2.150819
32	6	0	2.931088	2.092855	1.455635
33	6	0	1.249738	0.345935	1.995616
34	6	0	1.902603	-0.506425	1.066136
35	6	0	3.583751	1.167333	0.647187
36	8	0	3.101555	-0.129468	0.494775
37	8	0	1.031855	2.557085	2.793721
38	6	0	-0.006807	-0.061131	2.436818
39	6	0	-0.527053	-1.316002	2.180064
40	1	0	1.938133	-1.573442	1.251463
41	1	0	-0.659123	0.697466	2.857897
42	6	0	-1.966568	-1.515861	2.407447
43	8	0	-2.761026	-0.635704	2.644396
44	1	0	0.093020	-2.198327	2.118301
45	8	0	-2.325034	-2.811737	2.259864
46	6	0	-3.729253	-3.048950	2.427075
47	1	0	-4.038201	-2.771434	3.432835
48	1	0	-4.297474	-2.457811	1.709323
49	1	0	-3.869206	-4.113295	2.262406
50	6	0	3.471697	3.376348	1.569447
51	6	0	4.635570	3.708032	0.895738
52	6	0	5.267026	2.756771	0.089885
53	6	0	4.746516	1.476274	-0.042418
54	1	0	2.947087	4.085385	2.196043

55	1	0	5.052831	4.701671	0.987443
56	1	0	6.171634	3.014335	-0.444691
57	1	0	5.211223	0.730546	-0.673121
58	30	0	2.604284	-1.226695	-1.383286
59	17	0	3.073656	0.054447	-3.078007
60	17	0	3.306480	-3.206050	-0.771158

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cis-exo-TS-II

Imaginary frequency: -467.0666 cm^{-1}

Standard orientation:

Electronic energy E = -4189.677784 a.u.

Enthalpy H = -4189.643901 a.u.

Entropy S = 207.348 cal/mol/K

Gibbs free energy G = -4189.742418 a.u.

Total free energy in solution E_{sol}= -4190.85753 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.628265	0.035372	0.562969
2	7	0	-0.594608	-0.408179	-0.289690
3	6	0	0.222653	0.407588	0.470043
4	6	0	-0.388884	1.112795	1.647089
5	6	0	2.296851	-0.699621	-0.382522
6	6	0	0.098412	-1.520639	-1.017242
7	6	0	1.511281	-1.235623	-1.533755
8	1	0	0.196143	1.991690	1.920179
9	1	0	-0.436979	0.418049	2.490776
10	1	0	-1.411910	1.418690	1.440930
11	6	0	3.672871	-0.710714	-0.008573
12	6	0	3.767191	0.038111	1.187884
13	7	0	2.510779	0.500475	1.508908
14	1	0	2.269974	1.034455	2.325895
15	1	0	-0.571572	-1.845011	-1.812785
16	1	0	0.164847	-2.350910	-0.314307
17	1	0	1.518366	-0.542224	-2.382912
18	1	0	1.920066	-2.178957	-1.901973
19	6	0	4.828272	-1.286603	-0.574617
20	6	0	6.032835	-1.099626	0.076721
21	6	0	6.108283	-0.354287	1.279420
22	6	0	4.990261	0.213619	1.846945
23	1	0	4.755533	-1.856159	-1.489922
24	1	0	5.060847	0.776407	2.769206
25	1	0	7.081631	-0.251699	1.739630
26	8	0	7.227852	-1.593315	-0.350537
27	6	0	7.218568	-2.369841	-1.532447
28	1	0	6.588150	-3.255502	-1.414918
29	1	0	6.866187	-1.783425	-2.385516
30	1	0	8.247702	-2.674907	-1.701097
31	30	0	-2.272229	-1.340394	0.608682
32	17	0	-2.233089	-3.498621	0.130340
33	17	0	-3.184943	-0.547369	2.436975
34	6	0	-3.146035	2.213903	-0.775467
35	6	0	-4.070047	1.060099	-0.696497
36	6	0	-1.791769	1.850133	-1.214451
37	6	0	-1.526230	0.536501	-1.689166
38	6	0	-3.697318	-0.175736	-1.232742
39	8	0	-2.540013	-0.313163	-1.980130
40	8	0	-3.458312	3.337956	-0.425793
41	6	0	-0.713401	2.617241	-0.803615
42	6	0	0.583086	2.116347	-0.856731
43	1	0	-0.720892	0.387101	-2.394612
44	1	0	-0.915668	3.523629	-0.242679
45	6	0	1.681379	2.873809	-0.225264
46	8	0	1.547157	3.645713	0.701302
47	1	0	0.892789	1.446767	-1.645607
48	8	0	2.861970	2.559297	-0.771341

49	6	0	3.999666	3.186018	-0.164455
50	1	0	3.974721	4.258614	-0.349607
51	1	0	3.997393	3.003679	0.907940
52	1	0	4.866883	2.726655	-0.627904
53	6	0	-5.273070	1.153332	-0.000048
54	6	0	-6.083641	0.036739	0.147019
55	6	0	-5.698973	-1.184345	-0.405163
56	6	0	-4.507197	-1.300832	-1.114565
57	1	0	-5.530956	2.111170	0.431597
58	1	0	-7.006524	0.108272	0.705999
59	1	0	-6.323063	-2.058928	-0.280659
60	1	0	-4.192536	-2.234228	-1.559653

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cis-COM-III

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.458767 a.u.

Enthalpy H = -3501.437441 a.u.

Entropy S = 159.056 cal/mol/K

Gibbs free energy G = -3501.513014 a.u.

Total free energy in solution E_{sol}= -3502.20236 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.466995	2.434093	-0.082951
2	6	0	-1.010145	2.429181	-0.087766
3	6	0	1.089015	1.094794	-0.143131
4	6	0	0.317027	0.001729	-0.231507
5	6	0	-1.726002	1.238467	-0.137740
6	8	0	-1.056275	0.017384	-0.199234
7	8	0	1.121536	3.458305	-0.047835
8	6	0	2.552043	1.014272	-0.156831
9	6	0	3.266623	-0.036020	0.254583
10	1	0	0.688946	-1.002551	-0.374614
11	1	0	3.073124	1.896940	-0.509934
12	6	0	4.745002	0.008692	0.153880
13	8	0	5.389127	0.932182	-0.284215
14	1	0	2.829637	-0.929075	0.683265
15	8	0	5.289727	-1.125576	0.620627
16	6	0	6.721257	-1.166028	0.559126
17	1	0	7.053924	-1.064434	-0.472197
18	1	0	7.143597	-0.356757	1.151886
19	1	0	7.003875	-2.132355	0.964512
20	30	0	-1.927648	-1.915496	-0.041859
21	17	0	-0.765068	-3.032911	-1.444265
22	17	0	-3.395411	-1.934111	1.502290
23	6	0	-1.720343	3.633578	-0.050422
24	6	0	-3.103444	3.630181	-0.064117
25	6	0	-3.795322	2.415829	-0.115673
26	6	0	-3.114009	1.208860	-0.155011
27	1	0	-1.146599	4.549911	-0.012431
28	1	0	-3.650438	4.562597	-0.034664
29	1	0	-4.877044	2.407561	-0.123523
30	1	0	-3.646545	0.268317	-0.172367

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cis-endo-TS-III

Imaginary frequency: -273.0813 cm^{-1}

Standard orientation:

Electronic energy E = -4189.659803 a.u.

Enthalpy H = -4189.624987 a.u.

Entropy S = 216.177 cal/mol/K

Gibbs free energy G = -4189.727699 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Total free energy in solution E_{sol}= -4190.84757 a.u.

1	6	0	-1.919194	-0.717674	-1.380907
2	7	0	0.307477	0.037212	-1.039194
3	6	0	-0.504871	-0.958904	-1.236776
4	6	0	-0.006757	-2.372850	-1.303781
5	6	0	-2.509473	0.474397	-1.021097
6	6	0	-0.240097	1.398776	-1.181564
7	6	0	-1.649158	1.623159	-0.612515
8	1	0	-0.378603	-2.965353	-0.463969
9	1	0	1.077814	-2.427326	-1.325431
10	1	0	-0.381223	-2.827918	-2.224860
11	6	0	-3.913124	0.249066	-0.993047
12	6	0	-4.114306	-1.099247	-1.373114
13	7	0	-2.890119	-1.670111	-1.608840
14	1	0	-2.733022	-2.637563	-1.826874
15	1	0	-0.264032	1.586668	-2.258592
16	1	0	0.467996	2.091194	-0.734428
17	1	0	-2.021433	2.567817	-1.015055
18	1	0	-1.645819	1.711924	0.477089
19	6	0	-5.013696	1.067732	-0.659711
20	6	0	-6.275366	0.511705	-0.723698
21	6	0	-6.461048	-0.839160	-1.120057
22	6	0	-5.401811	-1.651109	-1.448966
23	8	0	-7.428598	1.169306	-0.429296
24	6	0	-7.308657	2.514071	-0.003136
25	1	0	-4.850642	2.091284	-0.355599
26	1	0	-7.477073	-1.208979	-1.151434
27	1	0	-5.561535	-2.679939	-1.744907
28	1	0	-6.856116	3.132623	-0.782847
29	1	0	-8.319946	2.858582	0.194004
30	1	0	-6.711737	2.583184	0.909891
31	6	0	1.763987	1.973653	1.506016
32	6	0	2.801679	2.306443	0.485231
33	6	0	1.171939	0.662518	1.362062
34	6	0	1.568765	-0.186576	0.312218
35	6	0	3.245861	1.357212	-0.425712
36	8	0	2.804648	0.025298	-0.311928
37	8	0	1.428357	2.799542	2.347258
38	6	0	-0.064483	0.381587	2.036421
39	6	0	-0.832015	-0.719343	1.883113
40	1	0	1.424598	-1.251229	0.415556
41	1	0	-0.462253	1.198050	2.632043
42	6	0	-2.231210	-0.691459	2.319420
43	8	0	-2.787508	0.223927	2.888090
44	1	0	-0.507572	-1.609449	1.362682
45	8	0	-2.881163	-1.812265	1.929971
46	6	0	-4.284934	-1.804291	2.209094
47	1	0	-4.456907	-1.708248	3.279743
48	1	0	-4.766609	-0.975278	1.691692
49	1	0	-4.663331	-2.753846	1.841296
50	6	0	3.296045	3.606363	0.373113
51	6	0	4.204354	3.927850	-0.625078
52	6	0	4.620909	2.951942	-1.531590
53	6	0	4.139706	1.650963	-1.441319
54	1	0	2.940943	4.335819	1.089050
55	1	0	4.588908	4.935906	-0.704253
56	1	0	5.326386	3.200263	-2.313215
57	1	0	4.461953	0.880279	-2.127570
58	30	0	4.236224	-1.445676	-0.027480
59	17	0	3.124701	-3.256096	0.342822
60	17	0	6.238644	-0.760099	-0.303048

cis-exo-TS-III

Imaginary frequency: -298.8885 cm^{-1}

Standard orientation:

Electronic energy E = -4189.658685 a.u.

Enthalpy H = -4189.623936 a.u.

Entropy S = 216.919 cal/mol/K

Gibbs free energy G = -4189.727001 a.u.

Total free energy in solution E_{sol} = -4190.85166 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.909432	-0.672498	-1.200314
2	7	0	-0.393361	-0.154223	-0.966068
3	6	0	0.530865	-1.074995	-1.075677
4	6	0	0.177358	-2.524840	-1.203478
5	6	0	2.349311	0.601820	-0.909229
6	6	0	0.012380	1.243165	-1.202632
7	6	0	1.346221	1.659464	-0.575110
8	1	0	0.776361	-3.143596	-0.533241
9	1	0	0.387518	-2.814253	-2.239302
10	1	0	-0.878622	-2.697520	-1.024192
11	6	0	3.770082	0.558399	-0.902224
12	6	0	4.134679	-0.771905	-1.221109
13	7	0	2.988563	-1.505505	-1.398125
14	1	0	2.946657	-2.498467	-1.547498
15	1	0	-0.793382	1.886943	-0.855210
16	1	0	0.085634	1.351656	-2.288108
17	1	0	1.259809	1.788714	0.509462
18	1	0	1.626168	2.632636	-0.983709
19	6	0	4.764815	1.525379	-0.642701
20	6	0	6.085112	1.130307	-0.715149
21	6	0	6.434123	-0.204499	-1.050007
22	6	0	5.479768	-1.159409	-1.308843
23	1	0	4.480930	2.537155	-0.391861
24	1	0	5.761941	-2.173621	-1.560897
25	1	0	7.488353	-0.442580	-1.095152
26	8	0	7.151873	1.942906	-0.485373
27	6	0	6.873999	3.282488	-0.124041
28	1	0	6.332327	3.799337	-0.920635
29	1	0	6.291395	3.326020	0.799962
30	1	0	7.837906	3.759441	0.029461
31	6	0	-2.668979	-2.398482	0.779627
32	6	0	-3.632275	-1.901043	-0.245446
33	6	0	-1.596855	-1.479181	1.090266
34	6	0	-1.544887	-0.218724	0.459873
35	6	0	-3.601000	-0.585661	-0.690383
36	8	0	-2.719254	0.323456	-0.078108
37	8	0	-2.765260	-3.533359	1.231474
38	6	0	-0.391187	-1.987835	1.660818
39	6	0	0.774893	-1.304979	1.771948
40	1	0	-1.012259	0.578046	0.963098
41	1	0	-0.387327	-3.051978	1.876387
42	6	0	2.035742	-2.021395	1.960716
43	8	0	2.185329	-3.227653	1.923284
44	1	0	0.851782	-0.232627	1.655836
45	8	0	3.066708	-1.160736	2.090486
46	6	0	4.356817	-1.770764	2.159949
47	1	0	4.455385	-2.342045	3.082032
48	1	0	4.505747	-2.436239	1.311238
49	1	0	5.070653	-0.952495	2.129431
50	6	0	-4.550972	-2.771968	-0.832416
51	6	0	-5.400469	-2.325532	-1.833861
52	6	0	-5.332518	-1.000587	-2.267080
53	6	0	-4.425149	-0.114303	-1.698231
54	1	0	-4.566358	-3.792682	-0.473736
55	1	0	-6.113777	-3.003929	-2.282720

56	1	0	-5.989214	-0.650294	-3.052130
57	1	0	-4.369114	0.916354	-2.018094
58	30	0	-3.321390	2.164442	0.629035
59	17	0	-1.585768	3.025574	1.584543
60	17	0	-5.312833	2.698508	0.063821

cis-COM-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.485318 a.u.

Enthalpy H = -3501.464202 a.u.

Entropy S = 158.894 cal/mol/K

Gibbs free energy G = -3501.539698 a.u.

Total free energy in solution E_{sol}= -3502.22713 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.447959	2.875415	0.327282
2	17	0	-1.896629	4.334825	-1.199280
3	17	0	-1.684879	2.582882	2.459182
4	6	0	-1.390530	0.039619	-0.180145
5	6	0	-2.836071	-0.112854	-0.185880
6	6	0	-0.620386	-1.159518	0.061173
7	6	0	-1.284057	-2.285248	0.431873
8	6	0	-3.396020	-1.337926	0.182273
9	8	0	-2.608487	-2.401619	0.512756
10	8	0	-0.827450	1.136729	-0.388983
11	6	0	0.842533	-1.107467	0.005611
12	6	0	1.626507	-2.148154	-0.286506
13	1	0	-0.784687	-3.196307	0.728838
14	1	0	1.304304	-0.147448	0.205706
15	6	0	3.098794	-1.971491	-0.269437
16	8	0	3.674166	-0.939648	-0.018896
17	1	0	1.248723	-3.125567	-0.559617
18	8	0	3.722217	-3.120259	-0.573037
19	6	0	5.154021	-3.033858	-0.578630
20	1	0	5.480986	-2.306446	-1.319018
21	1	0	5.513483	-2.730768	0.402832
22	1	0	5.505742	-4.029174	-0.830840
23	6	0	-3.697304	0.937720	-0.548455
24	6	0	-5.063251	0.756822	-0.510040
25	6	0	-5.599034	-0.477256	-0.107981
26	6	0	-4.774602	-1.532374	0.233948
27	1	0	-3.283396	1.873767	-0.904491
28	1	0	-5.721149	1.566012	-0.794654
29	1	0	-6.672258	-0.609776	-0.073624
30	1	0	-5.161625	-2.495134	0.537240

cis-endo-TS1-IV

Imaginary frequency: -236.6538 cm^{-1}

Standard orientation:

Electronic energy E = -4189.691966 a.u.

Enthalpy H = -4189.657845 a.u.

Entropy S = 213.130 cal/mol/K

Gibbs free energy G = -4189.759110 a.u.

Total free energy in solution E_{sol}= -4190.87491 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.220958	-2.412426	-0.906435
2	7	0	1.148676	-2.496285	-0.776299
3	6	0	0.001759	-3.005041	-0.428689
4	6	0	-0.074448	-4.211298	0.464641
5	6	0	-1.244771	-1.134121	-1.428713
6	6	0	1.132460	-1.503522	-1.864398
7	6	0	0.028897	-0.443495	-1.781074
8	1	0	-0.793972	-4.063843	1.271355
9	1	0	0.899385	-4.475001	0.872041
10	1	0	-0.408972	-5.058602	-0.141829

11	6	0	-2.593020	-0.693862	-1.397023
12	6	0	-3.358589	-1.766119	-0.882550
13	7	0	-2.507764	-2.802949	-0.585199
14	1	0	-2.776401	-3.673748	-0.164302
15	1	0	0.989710	-2.080232	-2.783179
16	1	0	2.117081	-1.044370	-1.916842
17	1	0	-0.045394	0.054196	-2.750622
18	1	0	0.249797	0.345384	-1.060350
19	6	0	-3.197566	0.536261	-1.725053
20	6	0	-4.558414	0.650836	-1.534178
21	6	0	-5.324274	-0.445873	-1.055259
22	6	0	-4.749006	-1.652367	-0.728804
23	8	0	-5.276416	1.778525	-1.768690
24	6	0	-4.539661	2.934166	-2.142504
25	1	0	-2.585164	1.358402	-2.066035
26	1	0	-6.388713	-0.289556	-0.940757
27	1	0	-5.349668	-2.471388	-0.353935
28	1	0	-4.052637	2.789204	-3.110196
29	1	0	-5.265291	3.739312	-2.216389
30	1	0	-3.785063	3.177666	-1.391091
31	6	0	2.677326	0.411230	0.313311
32	6	0	3.949756	0.089747	-0.339789
33	6	0	1.980289	-0.661563	0.910138
34	6	0	2.390960	-1.992535	0.621570
35	6	0	4.367111	-1.238658	-0.409341
36	8	0	3.611407	-2.255156	0.119489
37	8	0	2.284629	1.614214	0.306762
38	6	0	0.714342	-0.436815	1.557614
39	6	0	-0.082681	-1.356632	2.124685
40	1	0	2.080866	-2.794437	1.272124
41	1	0	0.323061	0.572781	1.537040
42	6	0	-1.460502	-0.983359	2.484478
43	8	0	-1.935903	0.124929	2.424639
44	1	0	0.205821	-2.384384	2.286431
45	8	0	-2.172728	-2.076150	2.844612
46	6	0	-3.550107	-1.799802	3.131794
47	1	0	-3.626913	-1.080583	3.944676
48	1	0	-4.039861	-1.391395	2.248576
49	1	0	-3.987668	-2.752101	3.417981
50	6	0	4.762500	1.082031	-0.899954
51	6	0	5.962770	0.742188	-1.499220
52	6	0	6.362940	-0.597621	-1.550329
53	6	0	5.568290	-1.597100	-1.009086
54	1	0	4.423967	2.107341	-0.843411
55	1	0	6.591353	1.510871	-1.927769
56	1	0	7.301522	-0.862622	-2.019275
57	1	0	5.852567	-2.639959	-1.039416
58	30	0	0.738546	2.736129	0.657713
59	17	0	0.625847	3.443781	2.698574
60	17	0	-0.410112	3.135127	-1.162998

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cis-endo-IM1-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.698674 a.u.

Enthalpy H = -4189.663691 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 220.050 cal/mol/K

Gibbs free energy G = -4189.768244 a.u.

Total free energy in solution E_{sol}= -4190.88867 a.u.

1	6	0	-1.588000	-2.481270	-0.447635
2	7	0	0.752657	-2.535502	-0.221078
3	6	0	-0.422665	-2.950863	0.217642
4	6	0	-0.583806	-3.907738	1.363363
5	6	0	-1.551476	-1.328818	-1.224991
6	6	0	0.794497	-1.900454	-1.554150
7	6	0	-0.255830	-0.805913	-1.735620
8	1	0	-1.298683	-3.519067	2.088910
9	1	0	0.350873	-4.151215	1.859058
10	1	0	-0.983070	-4.837570	0.946755
11	6	0	-2.864430	-0.810594	-1.262516
12	6	0	-3.680585	-1.715258	-0.540307
13	7	0	-2.895747	-2.730853	-0.062780
14	1	0	-3.198443	-3.437366	0.583460
15	1	0	0.606728	-2.703277	-2.270483
16	1	0	1.800078	-1.522922	-1.711989
17	1	0	-0.321036	-0.576235	-2.802076
18	1	0	0.000763	0.127761	-1.232464
19	6	0	-3.396551	0.380262	-1.802972
20	6	0	-4.737498	0.623556	-1.607142
21	6	0	-5.557943	-0.316488	-0.920334
22	6	0	-5.057049	-1.479199	-0.386672
23	8	0	-5.388953	1.737486	-2.018245
24	6	0	-4.589262	2.772904	-2.574182
25	1	0	-2.741132	1.083250	-2.296154
26	1	0	-6.605441	-0.066516	-0.816056
27	1	0	-5.697629	-2.168806	0.147391
28	1	0	-4.134856	2.449909	-3.514086
29	1	0	-5.264438	3.602520	-2.762119
30	1	0	-3.807389	3.077551	-1.874615
31	6	0	2.752933	0.128534	0.242000
32	6	0	3.878666	-0.535331	-0.437913
33	6	0	1.833601	-0.682625	0.898006
34	6	0	1.882538	-2.167861	0.732732
35	6	0	3.989599	-1.925774	-0.396717
36	8	0	3.074834	-2.716315	0.252925
37	8	0	2.721458	1.406653	0.209761
38	6	0	0.674770	-0.126124	1.522788
39	6	0	-0.240600	-0.788411	2.262766
40	1	0	1.660930	-2.689303	1.657938
41	1	0	0.443200	0.910731	1.305943
42	6	0	-1.522619	-0.155011	2.579856
43	8	0	-1.815781	1.006330	2.423152
44	1	0	-0.101968	-1.800828	2.607828
45	8	0	-2.409660	-1.081495	3.034950
46	6	0	-3.716218	-0.553902	3.289804
47	1	0	-3.664267	0.248284	4.023285
48	1	0	-4.150171	-0.165580	2.368908
49	1	0	-4.301205	-1.385937	3.673172
50	6	0	4.858465	0.200746	-1.108951
51	6	0	5.924554	-0.439667	-1.721980
52	6	0	6.018992	-1.831074	-1.664821
53	6	0	5.053845	-2.580804	-1.004063
54	1	0	4.758885	1.277339	-1.121744
55	1	0	6.680967	0.136514	-2.237416
56	1	0	6.850643	-2.337283	-2.137929
57	1	0	5.107245	-3.659433	-0.944965
58	30	0	1.489369	2.862784	0.322151
59	17	0	2.107708	4.526639	1.565844
60	17	0	-0.255518	2.681022	-1.021513

cis-endo-TS2-IV

Imaginary frequency: -281.4027 cm^{-1}

Standard orientation:

Electronic energy E = -4189.690362 a.u.

Enthalpy H = -4189.656292 a.u.

Entropy S = 213.296 cal/mol/K

Gibbs free energy G = -4189.757636 a.u.

Total free energy in solution E_{sol}= -4190.87314 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.385278	-2.043148	-0.558806	
2	7	0	0.974649	-2.322779	-0.708251
3	6	0	-0.178456	-2.661076	-0.052260
4	6	0	-0.271880	-4.050931	0.535754
5	6	0	-1.398742	-0.871247	-1.279317
6	6	0	0.886542	-1.439151	-1.894491
7	6	0	-0.122247	-0.292287	-1.795227
8	1	0	-1.008816	-4.092255	1.336792
9	1	0	0.685986	-4.393884	0.923228
10	1	0	-0.564542	-4.731958	-0.267900
11	6	0	-2.752486	-0.440295	-1.349663
12	6	0	-3.523196	-1.410825	-0.669814
13	7	0	-2.672514	-2.384228	-0.197984
14	1	0	-2.931644	-3.140550	0.409680
15	1	0	0.590970	-2.087010	-2.722276
16	1	0	1.888951	-1.074944	-2.106877
17	1	0	-0.259093	0.127916	-2.794669
18	1	0	0.224425	0.528534	-1.165166
19	6	0	-3.364223	0.700522	-1.904296
20	6	0	-4.731256	0.830087	-1.763275
21	6	0	-5.497339	-0.166612	-1.106511
22	6	0	-4.914310	-1.286918	-0.559009
23	8	0	-5.456172	1.888342	-2.216005
24	6	0	-4.726106	2.972587	-2.763280
25	1	0	-2.757458	1.455958	-2.382217
26	1	0	-6.564625	-0.004416	-1.038384
27	1	0	-5.513311	-2.033498	-0.052774
28	1	0	-4.205163	2.673105	-3.676732
29	1	0	-5.458920	3.739607	-2.998714
30	1	0	-4.002136	3.359322	-2.041895
31	6	0	2.776340	0.338201	0.244277
32	6	0	3.918935	0.001752	-0.603046
33	6	0	2.012843	-0.758055	0.752085
34	6	0	2.171435	-2.126169	0.164992
35	6	0	4.153223	-1.333442	-0.951803
36	8	0	3.347494	-2.362328	-0.569060
37	8	0	2.529123	1.544939	0.490779
38	6	0	0.870036	-0.560377	1.496631
39	6	0	0.037753	-1.615911	1.884750
40	1	0	2.133360	-2.908788	0.918817
41	1	0	0.502696	0.441898	1.682673
42	6	0	-1.309247	-1.249535	2.342847
43	8	0	-1.809801	-0.157166	2.211092
44	1	0	0.455782	-2.536526	2.265099
45	8	0	-1.973156	-2.305428	2.872739
46	6	0	-3.305767	-1.989742	3.302241
47	1	0	-3.276612	-1.227887	4.078524
48	1	0	-3.892039	-1.613081	2.464344
49	1	0	-3.717693	-2.917497	3.688678
50	6	0	4.790855	0.996730	-1.065241
51	6	0	5.881957	0.665801	-1.846584
52	6	0	6.106528	-0.674702	-2.178110
53	6	0	5.250278	-1.673375	-1.740094
54	1	0	4.582614	2.020368	-0.785422
55	1	0	6.555931	1.434784	-2.197916

56	1	0	6.959132	-0.942445	-2.789015
57	1	0	5.405706	-2.712949	-1.993283
58	30	0	1.014573	2.645520	1.073938
59	17	0	0.982515	2.988494	3.207491
60	17	0	-0.143849	3.257477	-0.666429

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cis-endo-IM2-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.721766 a.u.

Enthalpy H = -4189.688506 a.u.

Entropy S = 205.941 cal/mol/K

Gibbs free energy G = -4189.786355 a.u.

Total free energy in solution E_{sol}= -4190.89655 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.344306	0.156578	1.367355	
2	7	0	-2.250410	2.302088	0.707344
3	6	0	-2.615917	0.900492	1.003796
4	6	0	-3.680724	0.841227	2.100880
5	6	0	-0.174249	0.780619	1.732097
6	6	0	-1.434095	2.912237	1.763750
7	6	0	-0.067141	2.243886	2.011112
8	1	0	-3.928774	-0.199667	2.316627
9	1	0	-4.575915	1.373285	1.775100
10	1	0	-3.319011	1.284934	3.026349
11	6	0	0.850575	-0.221684	1.724240
12	6	0	0.224326	-1.433120	1.347138
13	7	0	-1.116850	-1.178846	1.157297
14	1	0	-1.802860	-1.834418	0.799045
15	1	0	-2.030081	2.864152	2.674425
16	1	0	-1.309181	3.965772	1.526836
17	1	0	0.229526	2.422711	3.049321
18	1	0	0.712763	2.692037	1.389415
19	6	0	2.227508	-0.197235	2.006932
20	6	0	2.935332	-1.387663	1.940940
21	6	0	2.288612	-2.601921	1.623034
22	6	0	0.938888	-2.648145	1.321641
23	8	0	4.268785	-1.497957	2.160630
24	6	0	5.024555	-0.301409	2.124937
25	1	0	2.709201	0.735462	2.264068
26	1	0	2.896995	-3.494264	1.577443
27	1	0	0.446455	-3.584895	1.098324
28	1	0	4.810198	0.331361	2.990763
29	1	0	6.067692	-0.604410	2.151447
30	1	0	4.820935	0.248910	1.202635
31	6	0	0.191000	0.968032	-1.563198
32	6	0	1.068707	2.109676	-1.379593
33	6	0	-1.226130	1.186183	-1.288732
34	6	0	-1.722475	2.477322	-0.683548
35	6	0	0.526971	3.341413	-0.987001
36	8	0	-0.791140	3.546930	-0.737154
37	8	0	0.624890	-0.153779	-1.860770
38	6	0	-2.069544	0.145775	-1.244197
39	6	0	-3.245598	0.350463	-0.343519
40	1	0	-2.559208	2.835637	-1.285023
41	1	0	-1.792177	-0.838290	-1.610278
42	6	0	-4.082076	-0.892679	-0.148763
43	8	0	-3.655763	-1.969712	0.206887
44	1	0	-3.908414	1.147622	-0.691658
45	8	0	-5.368588	-0.665389	-0.401245
46	6	0	-6.229579	-1.806752	-0.232097
47	1	0	-5.911424	-2.609443	-0.893234
48	1	0	-6.188974	-2.149325	0.799794
49	1	0	-7.223788	-1.457462	-0.489003

50	6	0	2.455087	1.976331	-1.562550
51	6	0	3.283024	3.068040	-1.387930
52	6	0	2.726057	4.302158	-1.028146
53	6	0	1.362803	4.446498	-0.823473
54	1	0	2.842164	1.001244	-1.836567
55	1	0	4.350216	2.972409	-1.533384
56	1	0	3.369808	5.163036	-0.897459
57	1	0	0.924686	5.390544	-0.529719
58	30	0	1.185618	-1.929458	-1.044764
59	17	0	-0.500038	-3.257362	-1.617045
60	17	0	3.351586	-1.802319	-1.436026

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cis-exo-TS1-IV

Imaginary frequency: -215.6361 cm^{-1}

Standard orientation:

Electronic energy E = -4189.692478 a.u.

Enthalpy H = -4189.657788 a.u.

Entropy S = 179.937 cal/mol/K

Gibbs free energy G = -4189.761774 a.u.

Total free energy in solution E_{sol}= -4190.87599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.384270	-1.411504	-1.158656
2	7	0	0.283840	-2.558374	0.074040
3	6	0	-0.012918	-1.759379	-0.904987
4	6	0	1.057578	-1.167863	-1.761498
5	6	0	-2.424205	-1.808943	-0.348079
6	6	0	-0.783293	-3.370309	0.675711
7	6	0	-2.188867	-2.738464	0.794595
8	1	0	1.176047	-0.098565	-1.576253
9	1	0	0.751610	-1.281924	-2.805103
10	1	0	2.001275	-1.687916	-1.621590
11	6	0	-3.556540	-1.034637	-0.721786
12	6	0	-3.130412	-0.180963	-1.765906
13	7	0	-1.813189	-0.447314	-2.049073
14	1	0	-1.194419	0.221759	-2.485727
15	1	0	-0.436364	-3.710770	1.653262
16	1	0	-0.859422	-4.257690	0.042485
17	1	0	-2.332079	-2.184471	1.726060
18	1	0	-2.911021	-3.558325	0.806448
19	6	0	-4.881410	-0.971869	-0.238688
20	6	0	-5.728229	-0.042379	-0.806045
21	6	0	-5.283039	0.818619	-1.844108
22	6	0	-4.000666	0.761834	-2.334278
23	1	0	-5.199720	-1.632487	0.554833
24	1	0	-3.673342	1.428608	-3.120734
25	1	0	-5.998537	1.527875	-2.237828
26	8	0	-7.027807	0.144467	-0.445679
27	6	0	-7.527615	-0.670253	0.595536
28	1	0	-7.479453	-1.728507	0.324630
29	1	0	-6.970435	-0.508041	1.523072
30	1	0	-8.564096	-0.377144	0.738172
31	6	0	3.017010	-0.131971	0.438056
32	6	0	4.030231	-1.113962	0.043425
33	6	0	1.888447	-0.622545	1.112925
34	6	0	1.710914	-2.031584	1.255539
35	6	0	3.836688	-2.460615	0.349372
36	8	0	2.727711	-2.885051	1.034884
37	8	0	3.222232	1.090944	0.152720
38	6	0	0.823375	0.269199	1.495582
39	6	0	-0.371148	-0.067293	2.004756
40	1	0	1.108893	-2.385741	2.082629
41	1	0	0.972329	1.323040	1.302258
42	6	0	-1.406708	0.967083	2.159610

43	8	0	-1.247097	2.157310	2.025075
44	1	0	-0.654114	-1.083412	2.235241
45	8	0	-2.604787	0.404643	2.429558
46	6	0	-3.696646	1.332608	2.450346
47	1	0	-3.523268	2.101981	3.199980
48	1	0	-3.805048	1.797833	1.471785
49	1	0	-4.577049	0.744293	2.692467
50	6	0	5.195867	-0.739398	-0.636263
51	6	0	6.133011	-1.693917	-0.989855
52	6	0	5.916625	-3.039030	-0.669249
53	6	0	4.768180	-3.431914	0.000556
54	1	0	5.336394	0.308476	-0.862885
55	1	0	7.034117	-1.401106	-1.511417
56	1	0	6.650872	-3.784470	-0.945825
57	1	0	4.577315	-4.463540	0.262352
58	30	0	2.204192	2.677745	-0.245539
59	17	0	3.069177	4.517714	0.483917
60	17	0	0.494082	2.313812	-1.602096

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cis-exo-IM1-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.702486 a.u.

Enthalpy H = -4189.667319 a.u.

Entropy S = 224.670 cal/mol/K

Gibbs free energy G = -4189.774067 a.u.

Total free energy in solution E_{sol}= -4190.89611 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.008292	-1.450788	-0.416930	
2	7	0	-0.369727	-1.464856	1.257060
3	6	0	-0.641227	-1.574723	-0.024222
4	6	0	0.394318	-1.792929	-1.070484
5	6	0	-3.006853	-0.978002	0.419231
6	6	0	-1.481884	-1.528946	2.231933
7	6	0	-2.676483	-0.664258	1.840169
8	1	0	0.694438	-0.824973	-1.490521
9	1	0	-0.036280	-2.398390	-1.868997
10	1	0	1.268579	-2.309471	-0.692311
11	6	0	-4.167014	-0.800889	-0.370591
12	6	0	-3.816634	-1.189426	-1.687240
13	7	0	-2.508692	-1.584344	-1.696547
14	1	0	-1.973617	-1.784042	-2.523631
15	1	0	-1.087732	-1.240897	3.203079
16	1	0	-1.795549	-2.575589	2.283389
17	1	0	-2.456925	0.402800	1.948001
18	1	0	-3.502242	-0.902940	2.512685
19	6	0	-5.475107	-0.348620	-0.079678
20	6	0	-6.380881	-0.300672	-1.115571
21	6	0	-6.012070	-0.693787	-2.433934
22	6	0	-4.750734	-1.137736	-2.736399
23	1	0	-5.735328	-0.051641	0.925780
24	1	0	-4.487961	-1.428872	-3.744627
25	1	0	-6.775825	-0.625738	-3.196951
26	8	0	-7.670216	0.106710	-1.003661
27	6	0	-8.106009	0.524128	0.277608
28	1	0	-8.030246	-0.292319	1.000639
29	1	0	-7.523187	1.379816	0.627925
30	1	0	-9.146387	0.813533	0.161480
31	6	0	2.961569	-0.471673	0.451824
32	6	0	3.493911	-1.844660	0.444059
33	6	0	1.794872	-0.238354	1.156869
34	6	0	1.045289	-1.352229	1.805263
35	6	0	2.806203	-2.858271	1.111419
36	8	0	1.618825	-2.635110	1.762518

37	8	0	3.646180	0.425894	-0.165368
38	6	0	1.312978	1.092064	1.363838
39	6	0	0.254693	1.472926	2.109131
40	1	0	0.865267	-1.123749	2.857432
41	1	0	1.869731	1.889876	0.888120
42	6	0	-0.094821	2.891253	2.207540
43	8	0	0.515850	3.820858	1.731474
44	1	0	-0.373058	0.789361	2.660069
45	8	0	-1.242355	3.054614	2.914731
46	6	0	-1.649596	4.418571	3.056383
47	1	0	-0.880303	4.990810	3.572082
48	1	0	-1.824089	4.864938	2.078947
49	1	0	-2.566027	4.394277	3.639388
50	6	0	4.691642	-2.156949	-0.204585
51	6	0	5.187638	-3.451884	-0.184328
52	6	0	4.482535	-4.451177	0.488259
53	6	0	3.288515	-4.161542	1.137024
54	1	0	5.215034	-1.355304	-0.707602
55	1	0	6.117636	-3.684656	-0.684975
56	1	0	4.865096	-5.463533	0.510173
57	1	0	2.726539	-4.918504	1.667167
58	30	0	3.125088	1.778598	-1.398781
59	17	0	4.644206	3.201973	-1.991215
60	17	0	1.081858	1.477403	-2.194901

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cis-exo-TS2-IV

Imaginary frequency: -247.4276 cm^{-1}

Standard orientation:

Electronic energy E = -4189.684557 a.u.

Enthalpy H = -4189.650471 a.u.

Entropy S = 215.552 cal/mol/K

Gibbs free energy G = -4189.752887 a.u.

Total free energy in solution E_{sol}= -4190.87034 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.074173	0.652169	0.619372
2	7	0	-0.209606	1.964167	-0.080050
3	6	0	-0.639992	0.819742	0.523788
4	6	0	0.206055	0.170826	1.584045
5	6	0	-2.987899	1.322869	-0.158605
6	6	0	-1.220973	2.968008	-0.475037
7	6	0	-2.504617	2.393995	-1.082865
8	1	0	0.097150	-0.914021	1.594176
9	1	0	-0.130380	0.583641	2.541148
10	1	0	1.258569	0.410143	1.481603
11	6	0	-4.261475	0.736024	0.099921
12	6	0	-4.044355	-0.290394	1.057577
13	7	0	-2.703864	-0.317786	1.365752
14	1	0	-2.242031	-1.013229	1.927178
15	1	0	-0.727098	3.667419	-1.147107
16	1	0	-1.484892	3.513126	0.433026
17	1	0	-2.334426	1.992835	-2.088546
18	1	0	-3.232654	3.201818	-1.182915
19	6	0	-5.555379	0.975101	-0.381408
20	6	0	-6.596787	0.193308	0.088235
21	6	0	-6.366605	-0.826350	1.040710
22	6	0	-5.096520	-1.071551	1.534222
23	1	0	-5.765190	1.746698	-1.110131
24	1	0	-4.933404	-1.851603	2.266878
25	1	0	-7.186989	-1.429632	1.400550
26	8	0	-7.829357	0.472950	-0.423621
27	6	0	-8.929796	-0.282005	0.045711
28	1	0	-8.814321	-1.342952	-0.191554
29	1	0	-9.063676	-0.160863	1.123913
30	1	0	-9.801521	0.109211	-0.471858

31	6	0	3.100414	0.680763	-0.542836
32	6	0	3.627471	1.971162	-0.096418
33	6	0	1.751063	0.655000	-0.981177
34	6	0	0.954822	1.912434	-1.050904
35	6	0	2.867522	3.128617	-0.284043
36	8	0	1.678420	3.112618	-0.950748
37	8	0	3.842938	-0.337225	-0.491309
38	6	0	1.041416	-0.537751	-1.032338
39	6	0	-0.335729	-0.573897	-1.216507
40	1	0	0.461621	1.975038	-2.024649
41	1	0	1.530154	-1.448535	-0.705194
42	6	0	-1.090058	-1.792411	-0.909589
43	8	0	-0.709612	-2.679861	-0.173261
44	1	0	-0.842229	0.152879	-1.835779
45	8	0	-2.309441	-1.766010	-1.475028
46	6	0	-3.150988	-2.876701	-1.146046
47	1	0	-2.747021	-3.791441	-1.576586
48	1	0	-3.220296	-2.989874	-0.065885
49	1	0	-4.123272	-2.641235	-1.568071
50	6	0	4.875568	2.065793	0.530644
51	6	0	5.350862	3.291559	0.961375
52	6	0	4.578566	4.439562	0.760221
53	6	0	3.340723	4.366969	0.137633
54	1	0	5.448854	1.158529	0.662920
55	1	0	6.313715	3.362124	1.448445
56	1	0	4.946790	5.401455	1.093284
57	1	0	2.732708	5.244706	-0.033166
58	30	0	3.841573	-2.168536	0.130112
59	17	0	4.959107	-3.552824	-1.089368
60	17	0	2.722572	-2.257860	2.000113

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cis-exo-IM2-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.710157 a.u.

Enthalpy H = -4189.676195 a.u.

Entropy S = 215.741 cal/mol/K

Gibbs free energy G = -4189.778700 a.u.

Total free energy in solution E_{sol} = -4190.89435 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.271246	-0.428639	0.603285	
2	7	0	-0.248213	0.739774	1.301244
3	6	0	-0.820464	-0.596782	0.992208
4	6	0	-0.650319	-1.464484	2.249051
5	6	0	-3.000080	0.727044	0.695904
6	6	0	-1.179421	1.587788	2.067842
7	6	0	-2.438409	1.979010	1.289447
8	1	0	-1.152488	-2.425558	2.127253
9	1	0	-1.096167	-0.972340	3.110645
10	1	0	0.411536	-1.621636	2.442935
11	6	0	-4.312029	0.434222	0.188391
12	6	0	-4.305678	-0.929223	-0.191160
13	7	0	-3.049145	-1.434196	0.074875
14	1	0	-2.724221	-2.367336	-0.115640
15	1	0	-0.627033	2.459447	2.406307
16	1	0	-1.469508	1.022699	2.952362
17	1	0	-2.203693	2.726081	0.523369
18	1	0	-3.155983	2.444404	1.970827
19	6	0	-5.474258	1.192484	0.026037
20	6	0	-6.600685	0.585230	-0.510353
21	6	0	-6.582543	-0.772709	-0.885970
22	6	0	-5.435732	-1.538480	-0.727768

1

23	1	0	-5.524307	2.237710	0.302352
24	1	0	-5.431584	-2.581651	-1.018291
25	1	0	-7.464027	-1.237066	-1.302633
26	8	0	-7.700650	1.387496	-0.643168
27	6	0	-8.865866	0.815150	-1.199585
28	1	0	-8.686188	0.455046	-2.216546
29	1	0	-9.238549	-0.008537	-0.584121
30	1	0	-9.607696	1.609441	-1.224805
31	6	0	2.761988	1.245488	-0.636908
32	6	0	2.782541	2.691728	-0.610885
33	6	0	1.474113	0.616659	-0.345807
34	6	0	0.299258	1.421237	0.138556
35	6	0	1.706632	3.370078	-0.017522
36	8	0	0.644931	2.745130	0.538304
37	8	0	3.780564	0.580231	-0.898071
38	6	0	1.279871	-0.690708	-0.510371
39	6	0	-0.056825	-1.285009	-0.222628
40	1	0	-0.439269	1.533074	-0.671902
41	1	0	2.032156	-1.345228	-0.934564
42	6	0	0.139507	-2.778952	-0.013541
43	8	0	1.187793	-3.286875	0.284301
44	1	0	-0.682177	-1.155322	-1.113807
45	8	0	-0.989381	-3.484232	-0.211584
46	6	0	-0.846971	-4.903753	0.003561
47	1	0	-0.093930	-5.301263	-0.671987
48	1	0	-0.547459	-5.090140	1.032607
49	1	0	-1.823718	-5.328364	-0.203558
50	6	0	3.886667	3.413347	-1.092752
51	6	0	3.908543	4.789466	-1.007803
52	6	0	2.826616	5.455873	-0.414593
53	6	0	1.736417	4.761886	0.081882
54	1	0	4.705117	2.856662	-1.529360
55	1	0	4.751744	5.349601	-1.387214
56	1	0	2.840464	6.535755	-0.338772
57	1	0	0.902220	5.265716	0.549843
58	30	0	4.207926	-1.255681	-0.224148
59	17	0	4.335094	-2.640778	-1.881119
60	17	0	4.371536	-1.138724	1.924468

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cis-COM-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.466988 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.583419	-1.307477	-0.252127	
2	6	0	-2.951906	-0.758461	-0.265268
3	6	0	-0.563012	-0.391841	-0.809635
4	6	0	-0.949928	0.790175	-1.367529
5	6	0	-3.206348	0.484722	-0.837377
6	8	0	-2.196760	1.234477	-1.404649
7	8	0	-1.311118	-2.414448	0.170378
8	6	0	0.820350	-0.850316	-0.775519
9	6	0	1.937934	-0.156139	-1.103385
10	1	0	-0.269845	1.490904	-1.831399
11	1	0	0.949626	-1.855802	-0.381854
12	6	0	3.255896	-0.842674	-0.984937
13	8	0	3.410639	-1.971616	-0.590380
14	1	0	1.936852	0.833031	-1.546214
15	8	0	4.244161	-0.028945	-1.368474
16	6	0	5.558158	-0.603956	-1.276711

Enthalpy H = -3501.445926 a.u.

Entropy S = 156.386 cal/mol/K

Gibbs free energy G = -3501.520230 a.u.

Total free energy in solution E_{sol}= -3502.20823 a.u. 1

17	1	0	5.766432	-0.886774	-0.246961
18	1	0	5.622011	-1.484453	-1.912783
19	1	0	6.237816	0.171454	-1.613514
20	6	0	-4.018276	-1.474815	0.287670
21	6	0	-5.295864	-0.944977	0.264229
22	6	0	-5.524315	0.307955	-0.318486
23	6	0	-4.482869	1.033354	-0.874849
24	1	0	-3.802070	-2.438536	0.729282
25	1	0	-6.120062	-1.495975	0.696596
26	1	0	-6.524720	0.719838	-0.335039
27	1	0	-4.631393	2.003094	-1.329222
28	30	0	1.144224	0.675617	0.991442
29	17	0	1.044329	2.775642	0.463715
30	17	0	1.035366	-0.634133	2.680779

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cis-endo-TS1-V

Imaginary frequency: -171.0069 cm^{-1}

Standard orientation:

Electronic energy E = -4189.678900 a.u.

Enthalpy H = -4189.643782 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.908718	-1.289550	1.496142	
2	7	0	0.396880	-1.688228	1.094549
3	6	0	-0.519945	-1.274226	1.902854
4	6	0	-0.152754	-0.714798	3.250277
5	6	0	-2.287093	-1.474892	0.184823
6	6	0	-0.011928	-2.367366	-0.142992
7	6	0	-1.265770	-1.820546	-0.847642
8	1	0	-0.272453	0.371957	3.280583
9	1	0	0.871479	-0.973416	3.509788
10	1	0	-0.807717	-1.144659	4.011788
11	6	0	-3.667463	-1.136629	0.100846
12	6	0	-4.075611	-0.773220	1.405506
13	7	0	-2.991773	-0.873987	2.241134
14	1	0	-2.985457	-0.632223	3.215763
15	1	0	-0.196594	-3.406712	0.144394
16	1	0	0.838981	-2.361318	-0.822524
17	1	0	-1.630267	-2.597344	-1.523537
18	1	0	-1.051844	-0.941987	-1.461947
19	6	0	-4.582326	-1.090140	-0.972006
20	6	0	-5.876094	-0.690424	-0.701302
21	6	0	-6.274371	-0.343136	0.616497
22	6	0	-5.395441	-0.380651	1.673351
23	8	0	-6.865780	-0.590762	-1.628348
24	6	0	-6.516368	-0.869465	-2.972065
25	1	0	-4.257111	-1.350777	-1.968540
26	1	0	-7.303493	-0.041717	0.758105
27	1	0	-5.714938	-0.106938	2.670585
28	1	0	-6.187739	-1.906022	-3.084765
29	1	0	-7.417820	-0.708201	-3.556584
30	1	0	-5.727210	-0.196655	-3.317475
31	6	0	2.676904	-0.610271	-1.403594
32	6	0	3.704298	-1.572144	-0.941682
33	6	0	1.925923	0.039427	-0.321673
34	6	0	2.026081	-0.489967	0.990873
35	6	0	3.846056	-1.857363	0.413097
36	8	0	3.057589	-1.249310	1.368647
37	8	0	2.468599	-0.401301	-2.587199
38	6	0	0.718304	0.754097	-0.717244
39	6	0	-0.196305	1.328498	0.095684
40	1	0	1.655284	0.081342	1.824787

Gibbs free energy G = -4189.747536 a.u.

Total free energy in solution E_{sol}= -4190.86312 a.u. 1

41	1	0	0.545520	0.784575	-1.789988
42	6	0	-1.488502	1.759312	-0.479153
43	8	0	-1.810732	1.638642	-1.639909
44	1	0	-0.088135	1.408077	1.168897
45	8	0	-2.297798	2.245348	0.473402
46	6	0	-3.607323	2.608928	0.012551
47	1	0	-3.532556	3.391188	-0.740386
48	1	0	-4.106128	1.739551	-0.412351
49	1	0	-4.135816	2.966109	0.890979
50	6	0	4.538376	-2.218612	-1.857042
51	6	0	5.494725	-3.117821	-1.415728
52	6	0	5.622523	-3.382060	-0.048394
53	6	0	4.799385	-2.755343	0.876246
54	1	0	4.409303	-1.981861	-2.904858
55	1	0	6.144910	-3.612066	-2.124920
56	1	0	6.371231	-4.082410	0.298361
57	1	0	4.879032	-2.942010	1.938280
58	30	0	2.412167	2.214731	0.007483
59	17	0	2.315136	2.624577	2.163856
60	17	0	3.209826	3.200503	-1.732139

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cis-endo-IM1-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.689428 a.u.

Enthalpy H = -4189.654397 a.u.

Entropy S = 220.689 cal/mol/K

Gibbs free energy G = -4189.759254 a.u.

Total free energy in solution E_{sol}= -4190.88243 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.949445	0.817898	1.656318	
2	7	0	-0.330479	1.097779	1.178603
3	6	0	0.579615	0.586067	1.975632
4	6	0	0.198243	-0.265534	3.151933
5	6	0	2.347802	1.242258	0.394366
6	6	0	0.074708	2.114686	0.188178
7	6	0	1.340260	1.736536	-0.585946
8	1	0	0.042238	-1.308322	2.863829
9	1	0	-0.720959	0.098990	3.607297
10	1	0	0.987395	-0.231051	3.901259
11	6	0	3.730139	0.964278	0.280132
12	6	0	4.133388	0.398038	1.513680
13	7	0	3.045222	0.319384	2.336619
14	1	0	3.045281	-0.088267	3.254144
15	1	0	0.264515	3.028975	0.755148
16	1	0	-0.766139	2.289105	-0.475646
17	1	0	1.692117	2.635634	-1.096193
18	1	0	1.164929	0.973526	-1.348653
19	6	0	4.654217	1.121445	-0.778220
20	6	0	5.952267	0.714595	-0.559947
21	6	0	6.347203	0.165648	0.693951
22	6	0	5.464890	0.003570	1.732032
23	8	0	6.952711	0.783951	-1.472077
24	6	0	6.616577	1.276286	-2.758700
25	1	0	4.326964	1.530157	-1.722828
26	1	0	7.383391	-0.128247	0.795137
27	1	0	5.784301	-0.423996	2.673242
28	1	0	6.263992	2.309142	-2.700196
29	1	0	7.530614	1.235008	-3.343632
30	1	0	5.850289	0.652288	-3.225169
31	6	0	-2.518807	0.746899	-1.328539
32	6	0	-3.369887	1.817595	-0.749334
33	6	0	-1.833403	-0.119341	-0.357874
34	6	0	-1.667431	0.414617	1.047488

35	6	0	-3.397165	2.034625	0.626685
36	8	0	-2.681506	1.265607	1.510297
37	8	0	-2.407204	0.616451	-2.539014
38	6	0	-0.666998	-0.800277	-0.917350
39	6	0	0.260139	-1.532346	-0.262924
40	1	0	-1.633349	-0.399597	1.759423
41	1	0	-0.514460	-0.625290	-1.979865
42	6	0	1.539097	-1.816294	-0.925799
43	8	0	1.880761	-1.410608	-2.018690
44	1	0	0.144909	-1.877020	0.755040
45	8	0	2.359529	-2.525243	-0.124233
46	6	0	3.658399	-2.770170	-0.672974
47	1	0	3.575821	-3.338649	-1.597493
48	1	0	4.164401	-1.827064	-0.876379
49	1	0	4.193077	-3.339425	0.081890
50	6	0	-4.136527	2.634850	-1.582931
51	6	0	-4.925037	3.641619	-1.049462
52	6	0	-4.946360	3.837806	0.333597
53	6	0	-4.185097	3.040391	1.177417
54	1	0	-4.092975	2.439543	-2.646275
55	1	0	-5.524562	4.267160	-1.696984
56	1	0	-5.562968	4.619371	0.759072
57	1	0	-4.189569	3.174800	2.250535
58	30	0	-2.965171	-1.880150	-0.157064
59	17	0	-2.430553	-2.758789	1.822892
60	17	0	-4.362958	-2.597572	-1.642897

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cis-endo-TS2-V

Imaginary frequency: -313.0444 cm^{-1}

Standard orientation:

Electronic energy E = -4189.678521 a.u.

Enthalpy H = -4189.644605 a.u.

Entropy S = 211.708 cal/mol/K

Gibbs free energy G = -4189.745194 a.u.

Total free energy in solution E_{sol}= -4190.86184 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.968950	-0.088027	-1.299221	
2	7	0	0.269595	0.652991	-1.642344
3	6	0	-0.601347	-0.410001	-1.684745
4	6	0	-0.425588	-1.411817	-2.808887
5	6	0	-2.310503	0.947744	-0.465921
6	6	0	-0.207441	1.963341	-1.140813
7	6	0	-1.244075	1.892454	-0.014402
8	1	0	-0.945354	-2.340824	-2.575933
9	1	0	0.619721	-1.649804	-2.997438
10	1	0	-0.844102	-0.972943	-3.717838
11	6	0	-3.707644	0.830877	-0.206296
12	6	0	-4.154395	-0.307978	-0.914968
13	7	0	-3.077029	-0.857709	-1.570753
14	1	0	-3.093202	-1.690273	-2.132213
15	1	0	-0.664051	2.467312	-1.994908
16	1	0	0.664876	2.542311	-0.847103
17	1	0	-1.639478	2.897498	0.147260
18	1	0	-0.798514	1.565497	0.931025
19	6	0	-4.616880	1.589589	0.557913
20	6	0	-5.936938	1.183570	0.586931
21	6	0	-6.369307	0.042367	-0.133515
22	6	0	-5.496492	-0.708318	-0.886957
23	8	0	-6.924797	1.811667	1.282411
24	6	0	-6.556525	2.947684	2.040129

25	1	0	-4.271949	2.455012	1.105143
26	1	0	-7.417020	-0.217816	-0.067535
27	1	0	-5.840734	-1.576365	-1.435109
28	1	0	-6.157228	3.736546	1.396623
29	1	0	-7.466019	3.296773	2.521357
30	1	0	-5.815088	2.688315	2.800613
31	6	0	2.181932	1.226752	1.043311
32	6	0	3.041716	2.201798	0.350153
33	6	0	1.699975	0.112659	0.183150
34	6	0	1.666219	0.289999	-1.317714
35	6	0	3.202080	2.141070	-1.037217
36	8	0	2.555016	1.245379	-1.839869
37	8	0	1.895953	1.306413	2.223656
38	6	0	0.733940	-0.736779	0.710252
39	6	0	0.024088	-1.647382	-0.104402
40	1	0	1.885859	-0.636592	-1.836247
41	1	0	0.414738	-0.569130	1.736613
42	6	0	-1.185424	-2.243058	0.496594
43	8	0	-1.736641	-1.823233	1.486708
44	1	0	0.568821	-2.260174	-0.811375
45	8	0	-1.654010	-3.274483	-0.235029
46	6	0	-2.866339	-3.847261	0.278440
47	1	0	-2.697228	-4.241631	1.278106
48	1	0	-3.647707	-3.089189	0.322476
49	1	0	-3.127014	-4.645634	-0.409995
50	6	0	3.724102	3.180537	1.081980
51	6	0	4.562013	4.076405	0.443854
52	6	0	4.719004	3.997231	-0.944126
53	6	0	4.044917	3.040577	-1.687487
54	1	0	3.576342	3.194441	2.153869
55	1	0	5.096205	4.826442	1.010779
56	1	0	5.375908	4.691839	-1.452081
57	1	0	4.152373	2.968749	-2.761098
58	30	0	2.949773	-1.672271	0.715496
59	17	0	3.265877	-2.754597	-1.160432
60	17	0	3.700694	-1.807129	2.722937

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cis-endo-IM2-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.722061 a.u.

Enthalpy H = -4189.688125 a.u.

Entropy S = 215.427 cal/mol/K

Gibbs free energy G = -4189.790481 a.u.

Total free energy in solution E_{sol} = -4190.90114 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.368145	-1.379482	0.535241	
2	7	0	-0.176410	-0.355395	2.061734
3	6	0	0.064218	-1.583808	1.262834
4	6	0	0.182788	-2.784508	2.213862
5	6	0	2.412211	-0.740087	1.151270
6	6	0	0.866325	-0.119032	3.069191
7	6	0	2.322854	-0.118777	2.513956
8	1	0	0.245058	-3.704101	1.631745
9	1	0	-0.690150	-2.837573	2.867695
10	1	0	1.089419	-2.721453	2.811768
11	6	0	3.491682	-0.723016	0.210910
12	6	0	3.028292	-1.377282	-0.951144
13	7	0	1.729376	-1.778001	-0.726552
14	1	0	1.112492	-2.224729	-1.388117
15	1	0	0.754915	-0.873865	3.844552
16	1	0	0.645647	0.842423	3.533739
17	1	0	2.963610	-0.647305	3.226767
18	1	0	2.694046	0.907165	2.457077

19	6	0	4.800545	-0.205753	0.253585
20	6	0	5.599518	-0.360550	-0.865470
21	6	0	5.121402	-1.017828	-2.021672
22	6	0	3.842636	-1.529550	-2.078193
23	8	0	6.887580	0.088207	-0.962638
24	6	0	7.421692	0.745556	0.165920
25	1	0	5.156608	0.289547	1.145889
26	1	0	5.797547	-1.106656	-2.861142
27	1	0	3.485770	-2.031651	-2.968537
28	1	0	7.437217	0.085473	1.037987
29	1	0	8.439316	1.022900	-0.097326
30	1	0	6.848891	1.645911	0.407095
31	6	0	-1.591876	1.829598	-0.676793
32	6	0	-0.639430	2.902074	-0.585150
33	6	0	-1.267523	0.611865	0.089527
34	6	0	-0.519826	0.836235	1.364388
35	6	0	0.489937	2.719395	0.238869
36	8	0	0.674296	1.628813	1.000406
37	8	0	-2.635031	1.860803	-1.361436
38	6	0	-1.509994	-0.597386	-0.424180
39	6	0	-1.208526	-1.805916	0.401346
40	1	0	-1.089788	1.487701	2.034266
41	1	0	-1.917649	-0.719002	-1.421827
42	6	0	-1.180482	-3.045674	-0.470113
43	8	0	-0.663828	-3.101583	-1.566314
44	1	0	-2.021869	-1.937799	1.121828
45	8	0	-1.818395	-4.064018	0.092612
46	6	0	-1.878390	-5.262147	-0.704172
47	1	0	-2.397392	-5.052704	-1.636444
48	1	0	-0.872007	-5.617205	-0.915491
49	1	0	-2.428899	-5.977971	-0.103670
50	6	0	-0.788610	4.082778	-1.335870
51	6	0	0.186217	5.053583	-1.294224
52	6	0	1.324315	4.848666	-0.495592
53	6	0	1.481467	3.705265	0.265840
54	1	0	-1.675455	4.189071	-1.946588
55	1	0	0.083466	5.962502	-1.870282
56	1	0	2.096417	5.607318	-0.466590
57	1	0	2.350720	3.547283	0.889036
58	30	0	-3.921948	0.619266	-0.387076
59	17	0	-4.704598	-1.105580	-1.450149
60	17	0	-4.200974	1.506604	1.585829

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cis-exo-TS1-V

Imaginary frequency: -166.2868 cm^{-1}

Standard orientation:

Electronic energy E = -4189.676411 a.u.

Enthalpy H = -4189.641476 a.u.

Entropy S = 219.250 cal/mol/K

Gibbs free energy G = -4189.745649 a.u.

Total free energy in solution E_{sol}= -4190.86100 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.817703	-1.716081	-0.553572
2	7	0	0.308583	-1.871621	0.480297
3	6	0	-0.374922	-1.797009	-0.618214
4	6	0	0.279780	-1.796336	-1.965166
5	6	0	-2.485240	-1.383141	0.605747
6	6	0	-0.436219	-2.111302	1.725652
7	6	0	-1.718594	-1.284211	1.886213
8	1	0	-0.027509	-0.926552	-2.549766
9	1	0	-0.048522	-2.698322	-2.492537
10	1	0	1.361757	-1.833418	-1.888164
11	6	0	-3.827434	-1.083557	0.238444
12	6	0	-3.914782	-1.279152	-1.160776

13	7	0	-2.682914	-1.666331	-1.623580
14	1	0	-2.426491	-1.751200	-2.591651
15	1	0	0.249144	-1.950734	2.558305
16	1	0	-0.706970	-3.170938	1.721762
17	1	0	-1.505157	-0.236052	2.125088
18	1	0	-2.282136	-1.689871	2.729042
19	6	0	-4.956263	-0.650909	0.966881
20	6	0	-6.129175	-0.431840	0.272955
21	6	0	-6.203446	-0.646171	-1.128547
22	6	0	-5.116872	-1.072221	-1.854483
23	1	0	-4.883671	-0.496416	2.033654
24	1	0	-5.188266	-1.229583	-2.922936
25	1	0	-7.155793	-0.461300	-1.606862
26	8	0	-7.293461	-0.006955	0.832878
27	6	0	-7.289231	0.227110	2.228732
28	1	0	-7.057034	-0.688790	2.778605
29	1	0	-6.567079	1.004124	2.493547
30	1	0	-8.292098	0.559692	2.481268
31	6	0	3.179957	-0.286274	-1.125162
32	6	0	4.056006	-1.315259	-0.517805
33	6	0	2.078495	0.159433	-0.262623
34	6	0	1.770277	-0.620099	0.891155
35	6	0	3.776147	-1.825854	0.746278
36	8	0	2.693639	-1.389163	1.480214
37	8	0	3.351692	0.121946	-2.261984
38	6	0	0.996949	0.881180	-0.922320
39	6	0	-0.180327	1.241832	-0.367392
40	1	0	1.112977	-0.200506	1.638828
41	1	0	1.162423	1.079758	-1.977249
42	6	0	-1.298868	1.645546	-1.240572
43	8	0	-1.321794	1.517076	-2.447093
44	1	0	-0.395070	1.164499	0.690086
45	8	0	-2.331653	2.099634	-0.519581
46	6	0	-3.505202	2.423360	-1.276354
47	1	0	-3.283582	3.216493	-1.987935
48	1	0	-3.859026	1.542668	-1.809159
49	1	0	-4.240528	2.748331	-0.547077
50	6	0	5.173468	-1.795282	-1.205845
51	6	0	5.989499	-2.754129	-0.629366
52	6	0	5.691663	-3.245251	0.645883
53	6	0	4.583630	-2.786052	1.342916
54	1	0	5.371764	-1.383141	-2.186518
55	1	0	6.858497	-3.119406	-1.159885
56	1	0	6.330276	-3.992420	1.098992
57	1	0	4.332074	-3.149444	2.329698
58	30	0	2.363259	2.185542	0.564149
59	17	0	1.536740	2.231983	2.599056
60	17	0	3.530650	3.528702	-0.651529

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cis-exo-IM1-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.681769 a.u.

Enthalpy H = -4189.646957 a.u.

Entropy S = 217.478 cal/mol/K

Gibbs free energy G = -4189.750288 a.u.

Total free energy in solution E_{sol}= -4190.87551 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.896221	1.640813	0.017982
2	7	0	0.167414	1.079350	-0.941148
3	6	0	-0.472163	1.572310	0.096737
4	6	0	0.212982	2.044638	1.338268
5	6	0	-2.627669	0.919882	-0.916266

6	6	0	-0.573393	0.968376	-2.215694
7	6	0	-1.927557	0.274326	-2.064105
8	1	0	0.251375	1.260693	2.097074
9	1	0	-0.346026	2.891006	1.740301
10	1	0	1.222346	2.384925	1.125922
11	6	0	-3.966755	0.883810	-0.462054
12	6	0	-4.002007	1.622485	0.745834
13	7	0	-2.743640	2.080526	1.017671
14	1	0	-2.472381	2.548167	1.864260
15	1	0	0.073866	0.461013	-2.926638
16	1	0	-0.740895	1.988450	-2.567764
17	1	0	-1.838951	-0.801970	-1.890676
18	1	0	-2.478409	0.408944	-2.997160
19	6	0	-5.136672	0.268197	-0.963715
20	6	0	-6.298132	0.413710	-0.237740
21	6	0	-6.319338	1.169376	0.969536
22	6	0	-5.196642	1.777665	1.470384
23	1	0	-5.097058	-0.300650	-1.881137
24	1	0	-5.232711	2.342462	2.392417
25	1	0	-7.267791	1.243365	1.484365
26	8	0	-7.498055	-0.121905	-0.573093
27	6	0	-7.546235	-0.912133	-1.748171
28	1	0	-7.281734	-0.320240	-2.627962
29	1	0	-6.873392	-1.770025	-1.667987
30	1	0	-8.571827	-1.258290	-1.835807
31	6	0	2.757927	0.523369	1.252267
32	6	0	3.536779	1.540270	0.496695
33	6	0	1.850228	-0.289104	0.437654
34	6	0	1.460916	0.254015	-0.904675
35	6	0	3.343350	1.716908	-0.873232
36	8	0	2.463793	0.942956	-1.594653
37	8	0	2.876980	0.401396	2.463538
38	6	0	0.797544	-0.980121	1.167879
39	6	0	-0.319342	-1.508679	0.630602
40	1	0	1.184983	-0.568643	-1.561603
41	1	0	0.908576	-0.988796	2.249394
42	6	0	-1.452142	-1.888115	1.480782
43	8	0	-1.501037	-1.837510	2.690153
44	1	0	-0.459768	-1.611643	-0.436003
45	8	0	-2.516726	-2.232539	0.717843
46	6	0	-3.714170	-2.494160	1.453557
47	1	0	-3.555121	-3.303236	2.163762
48	1	0	-4.026799	-1.600349	1.993617
49	1	0	-4.460147	-2.769574	0.713272
50	6	0	4.476245	2.334592	1.157910
51	6	0	5.213066	3.278652	0.461386
52	6	0	5.011117	3.433655	-0.912246
53	6	0	4.078340	2.657292	-1.586511
54	1	0	4.610906	2.165946	2.218224
55	1	0	5.948100	3.884190	0.974168
56	1	0	5.588650	4.164212	-1.464210
57	1	0	3.912292	2.755928	-2.650642
58	30	0	3.121982	-1.858826	-0.205337
59	17	0	2.088150	-2.915967	-1.850314
60	17	0	5.149266	-2.031773	0.540113

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cis-exo-TS2-V Imaginary frequency: -267.3131 cm^{-1}

Standard orientation: Electronic energy E = -4189.673593 a.u.

Enthalpy H = -4189.639651 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 212.239cal/mol/K

Gibbs free energy G = -4189.740493 a.u.

Total free energy in solution E_{sol}= -4190.85785 a.u.

1	6	0	1.792060	1.069761	-0.617819
2	7	0	-0.317065	1.464041	0.427821
3	6	0	0.342693	1.051912	-0.701726
4	6	0	-0.272740	1.356136	-2.047049
5	6	0	2.498098	1.016532	0.560964
6	6	0	0.491081	1.932444	1.576736
7	6	0	1.751103	1.108459	1.853508
8	1	0	0.010792	0.614500	-2.794394
9	1	0	0.093869	2.342783	-2.345962
10	1	0	-1.355806	1.418251	-1.991184
11	6	0	3.868251	0.838025	0.215295
12	6	0	3.924296	0.792123	-1.197930
13	7	0	2.648308	0.942076	-1.688105
14	1	0	2.371733	0.829472	-2.648462
15	1	0	-0.174209	1.963409	2.437213
16	1	0	0.789665	2.957454	1.348662
17	1	0	1.501506	0.113976	2.241718
18	1	0	2.335814	1.615065	2.624295
19	6	0	5.049505	0.711930	0.975418
20	6	0	6.240571	0.538273	0.298264
21	6	0	6.279366	0.496209	-1.118936
22	6	0	5.138987	0.626024	-1.876967
23	1	0	5.003888	0.744900	2.054324
24	1	0	5.183920	0.597860	-2.958329
25	1	0	7.246394	0.360419	-1.583990
26	8	0	7.455727	0.395558	0.893454
27	6	0	7.487323	0.420055	2.307729
28	1	0	7.123576	1.376770	2.691831
29	1	0	6.888031	-0.392446	2.727305
30	1	0	8.528551	0.287156	2.588093
31	6	0	-3.372044	0.271682	-0.889184
32	6	0	-3.896744	1.597147	-0.502291
33	6	0	-2.161479	-0.160179	-0.143466
34	6	0	-1.562317	0.752189	0.884180
35	6	0	-3.390355	2.258294	0.617650
36	8	0	-2.458182	1.683880	1.436924
37	8	0	-3.834557	-0.377948	-1.808594
38	6	0	-1.273944	-0.965354	-0.866271
39	6	0	0.081217	-1.066842	-0.533469
40	1	0	-1.225816	0.164260	1.738987
41	1	0	-1.625328	-1.352664	-1.820225
42	6	0	1.014885	-1.670171	-1.497753
43	8	0	0.845890	-1.682605	-2.702163
44	1	0	0.397280	-1.063486	0.500739
45	8	0	2.121117	-2.117498	-0.896221
46	6	0	3.124682	-2.639162	-1.776607
47	1	0	2.735426	-3.500147	-2.316570
48	1	0	3.432295	-1.874162	-2.487203
49	1	0	3.954736	-2.919880	-1.136623
50	6	0	-4.899736	2.203651	-1.264815
51	6	0	-5.390842	3.448161	-0.909516
52	6	0	-4.878731	4.093012	0.220602
53	6	0	-3.882830	3.505890	0.988162
54	1	0	-5.273657	1.662603	-2.124202
55	1	0	-6.168550	3.916898	-1.497114
56	1	0	-5.261204	5.064918	0.505382
57	1	0	-3.479551	3.986679	1.868735
58	30	0	-2.553526	-2.138508	0.818483
59	17	0	-1.308437	-2.202965	2.625949
60	17	0	-4.009233	-3.463532	-0.041890

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cis-exo-IM2-V

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.412891	0.192547	-0.497376
2	7	0	0.482719	1.332151	0.329517
3	6	0	0.931131	0.377805	-0.712955
4	6	0	0.655456	0.880587	-2.140543
5	6	0	3.194010	0.850642	0.417224
6	6	0	1.381117	2.444553	0.654938
7	6	0	2.649971	1.916718	1.311178
8	1	0	1.089946	0.202022	-2.872010
9	1	0	1.105424	1.865941	-2.263222
10	1	0	-0.414197	0.967009	-2.331311
11	6	0	4.533335	0.371658	0.242962
12	6	0	4.491237	-0.572410	-0.803055
13	7	0	3.190681	-0.659850	-1.243573
14	1	0	2.829439	-1.281787	-1.948850
15	1	0	0.836436	3.110122	1.326564
16	1	0	1.637070	3.018461	-0.242506
17	1	0	2.418197	1.533328	2.309087
18	1	0	3.369442	2.731627	1.427010
19	6	0	5.754678	0.672869	0.874763
20	6	0	6.891286	0.014593	0.440046
21	6	0	6.832842	-0.932878	-0.607667
22	6	0	5.644607	-1.235905	-1.236287
23	1	0	5.785072	1.396365	1.677210
24	1	0	5.611218	-1.961283	-2.039316
25	1	0	7.757798	-1.411873	-0.898835
26	8	0	8.140799	0.205255	0.959331
27	6	0	8.257588	1.126759	2.022408
28	1	0	7.955391	2.130662	1.710231
29	1	0	7.652613	0.818829	2.879955
30	1	0	9.307832	1.135061	2.302755
31	6	0	-3.213367	0.844824	0.025908
32	6	0	-3.538969	2.223958	-0.275938
33	6	0	-1.779920	0.527820	0.048288
34	6	0	-0.874904	1.673478	0.366819
35	6	0	-2.501681	3.120812	-0.608690
36	8	0	-1.200269	2.776002	-0.567902
37	8	0	-4.091851	-0.023172	0.195006
38	6	0	-1.314138	-0.674632	-0.288902
39	6	0	0.163393	-0.935764	-0.386410
40	1	0	-1.118519	2.079158	1.355028
41	1	0	-1.987322	-1.478780	-0.571384
42	6	0	0.373169	-2.123243	-1.318688
43	8	0	1.079243	-2.172113	-2.301601
44	1	0	0.503413	-1.266894	0.603347
45	8	0	-0.364880	-3.142372	-0.894632
46	6	0	-0.348145	-4.331328	-1.706762
47	1	0	-0.622651	-4.080409	-2.728518
48	1	0	0.646360	-4.771921	-1.688291
49	1	0	-1.084070	-4.988306	-1.257152
50	6	0	-4.879153	2.647001	-0.337866
51	6	0	-5.185901	3.930698	-0.732401
52	6	0	-4.146920	4.808029	-1.080904
53	6	0	-2.821121	4.417572	-1.020799
54	1	0	-5.649753	1.933349	-0.078676
55	1	0	-6.214561	4.259935	-0.779591

Imaginary frequency: none
Electronic energy E = -4189.734831 a.u.
Enthalpy H = -4189.700876 a.u.
Entropy S = 213.344 cal/mol/K
Gibbs free energy G = -4189.802243 a.u.
Total free energy in solution E_{sol}= -4190.91577 a.u.

56	1	0	-4.384084	5.815933	-1.397366
57	1	0	-2.014658	5.090116	-1.277755
58	30	0	-3.709895	-1.776590	1.049811
59	17	0	-3.935667	-3.423131	-0.347443
60	17	0	-3.082690	-1.448896	3.092753

cis-COM-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.474572 a.u.

Enthalpy H = -3501.453639 a.u.

Entropy S = 154.359 cal/mol/K

Gibbs free energy G = -3501.526980 a.u.

Total free energy in solution E_{sol}= -3502.21159 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.404820	-1.335359	0.053400
2	6	0	3.685001	-0.605688	0.102016
3	6	0	1.264697	-0.517896	-0.399660
4	6	0	1.443613	0.798729	-0.679910
5	6	0	3.739016	0.743487	-0.238698
6	8	0	2.612254	1.433977	-0.617261
7	8	0	2.295313	-2.511197	0.356057
8	6	0	-0.034248	-1.161995	-0.471131
9	6	0	-1.129470	-0.689092	-1.100223
10	1	0	0.642714	1.476042	-0.951089
11	1	0	-0.098263	-2.116188	0.043416
12	6	0	-2.395644	-1.443994	-1.026002
13	8	0	-2.577068	-2.621509	-0.945898
14	1	0	-1.122476	0.203400	-1.716207
15	8	0	-3.437274	-0.524238	-0.985025
16	6	0	-4.752751	-1.094587	-0.762677
17	1	0	-4.951805	-1.824097	-1.541722
18	1	0	-4.775035	-1.561460	0.218886
19	1	0	-5.441024	-0.258084	-0.819963
20	6	0	4.865212	-1.249730	0.489692
21	6	0	6.057937	-0.551459	0.528387
22	6	0	6.085693	0.805566	0.180118
23	6	0	4.929430	1.463429	-0.205115
24	1	0	4.802095	-2.297539	0.751963
25	1	0	6.970195	-1.049480	0.827735
26	1	0	7.019886	1.350740	0.212311
27	1	0	4.922642	2.510534	-0.475103
28	30	0	-2.486600	0.791871	0.391396
29	17	0	-2.949518	-0.159679	2.268477
30	17	0	-1.844396	2.667048	-0.478846

cis-endo-TS1-VI

Imaginary frequency: -155.0924 cm^{-1}

Standard orientation:

Electronic energy E = -4189.684792 a.u.

Enthalpy H = -4189.649355 a.u.

Entropy S = 224.532 cal/mol/K

Gibbs free energy G = -4189.756037 a.u.

Total free energy in solution E_{sol}= -4190.85703 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.278436	1.194667	1.100438
2	7	0	0.052574	1.494013	0.370116
3	6	0	0.856810	1.321801	1.360480
4	6	0	0.347294	1.198269	2.767237
5	6	0	2.770295	0.932307	-0.158107
6	6	0	0.596805	1.708474	-0.969657

7	6	0	1.815011	0.844408	-1.306348
8	1	0	0.375579	0.154385	3.087343
9	1	0	-0.672034	1.566963	2.846030
10	1	0	0.974904	1.785777	3.441147
11	6	0	4.167920	0.697672	-0.018402
12	6	0	4.465100	0.846051	1.356602
13	7	0	3.299862	1.134829	2.022862
14	1	0	3.217590	1.292120	3.011235
15	1	0	0.880628	2.764911	-1.027024
16	1	0	-0.209527	1.537659	-1.683265
17	1	0	2.256057	1.211464	-2.234767
18	1	0	1.519681	-0.196657	-1.478748
19	6	0	5.192039	0.385045	-0.937305
20	6	0	6.475171	0.238145	-0.450734
21	6	0	6.757782	0.396720	0.930659
22	6	0	5.773591	0.700690	1.840576
23	8	0	7.563815	-0.059274	-1.211644
24	6	0	7.351113	-0.225068	-2.600114
25	1	0	4.959763	0.270509	-1.986112
26	1	0	7.785345	0.268287	1.242908
27	1	0	6.005523	0.817089	2.891311
28	1	0	6.959528	0.691693	-3.049170
29	1	0	8.322612	-0.454778	-3.028980
30	1	0	6.660020	-1.049502	-2.795519
31	30	0	-2.070067	-2.918733	0.759299
32	17	0	-1.240417	-2.111545	2.624487
33	17	0	-3.794758	-4.092234	0.170648
34	6	0	-3.059308	1.799229	-1.588778
35	6	0	-3.250832	3.099875	-0.902930
36	6	0	-2.385513	0.792760	-0.776983
37	6	0	-1.974556	1.100919	0.531010
38	6	0	-2.909856	3.246867	0.438549
39	8	0	-2.399735	2.198390	1.172441
40	8	0	-3.422046	1.616769	-2.742574
41	6	0	-2.071798	-0.458597	-1.349595
42	6	0	-1.239186	-1.412908	-0.816519
43	1	0	-1.753516	0.305186	1.230360
44	1	0	-2.536139	-0.663991	-2.310274
45	6	0	-0.975462	-2.649504	-1.555418
46	8	0	-1.119428	-2.902241	-2.717778
47	1	0	-0.580248	-1.192492	0.017424
48	8	0	-0.578692	-3.617251	-0.630984
49	6	0	-0.458103	-4.958478	-1.154813
50	1	0	-1.435664	-5.303303	-1.483038
51	1	0	0.243724	-4.952830	-1.983800
52	1	0	-0.087721	-5.557651	-0.329540
53	6	0	-3.793223	4.193870	-1.581725
54	6	0	-3.982650	5.399944	-0.927794
55	6	0	-3.635534	5.521337	0.421563
56	6	0	-3.099419	4.446187	1.115029
57	1	0	-4.058020	4.054015	-2.621537
58	1	0	-4.402137	6.245781	-1.455865
59	1	0	-3.786785	6.461711	0.935496
60	1	0	-2.829118	4.512754	2.160061

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cis-endo-IM1-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.695584 a.u.

Enthalpy H = -4189.660454 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 222.065 cal/mol/K

Gibbs free energy G = -4189.765964 a.u.

Total free energy in solution E_{sol}= -4190.88363 a.u.

1	6	0	-2.415276	0.350511	-1.091746
2	7	0	-0.325707	1.079832	-0.319196
3	6	0	-1.052701	0.695161	-1.343936
4	6	0	-0.467261	0.570251	-2.711204
5	6	0	-2.899466	0.089649	0.180416
6	6	0	-0.974344	1.352876	0.981086
7	6	0	-1.989951	0.278269	1.349744
8	1	0	0.188504	-0.308660	-2.746051
9	1	0	0.122515	1.450049	-2.959417
10	1	0	-1.247662	0.431705	-3.454989
11	6	0	-4.213067	-0.417129	0.033211
12	6	0	-4.484972	-0.425883	-1.357082
13	7	0	-3.378332	0.019430	-2.024257
14	1	0	-3.321326	0.161390	-3.017061
15	1	0	-1.470562	2.323673	0.891220
16	1	0	-0.184947	1.421181	1.722025
17	1	0	-2.531647	0.605726	2.238144
18	1	0	-1.486235	-0.662054	1.598384
19	6	0	-5.188699	-0.856641	0.958036
20	6	0	-6.401813	-1.275517	0.458754
21	6	0	-6.663660	-1.264212	-0.941207
22	6	0	-5.730584	-0.846695	-1.854722
23	8	0	-7.438554	-1.725619	1.207935
24	6	0	-7.244376	-1.786091	2.610127
25	1	0	-4.971426	-0.854886	2.016092
26	1	0	-7.639266	-1.605979	-1.259578
27	1	0	-5.946623	-0.850917	-2.914840
28	1	0	-7.049674	-0.791811	3.020287
29	1	0	-8.168761	-2.177223	3.024632
30	1	0	-6.416949	-2.455031	2.860016
31	30	0	3.109455	-2.143227	-0.674331
32	17	0	1.828840	-2.138379	-2.495555
33	17	0	5.231714	-2.594070	-0.455720
34	6	0	2.184232	2.672886	1.434869
35	6	0	1.654247	3.878966	0.740539
36	6	0	1.914113	1.413069	0.759092
37	6	0	1.148798	1.408566	-0.518706
38	6	0	1.184082	3.788647	-0.568473
39	8	0	1.215259	2.602146	-1.263961
40	8	0	2.757854	2.769224	2.512420
41	6	0	2.300041	0.227880	1.333570
42	6	0	1.989004	-1.069831	0.882083
43	1	0	1.519857	0.624628	-1.178338
44	1	0	2.905655	0.309944	2.232220
45	6	0	2.349986	-2.205520	1.722943
46	8	0	2.777874	-2.237723	2.845969
47	1	0	1.127626	-1.229234	0.238770
48	8	0	2.233176	-3.363329	0.948956
49	6	0	2.774877	-4.554761	1.549582
50	1	0	3.846129	-4.431387	1.693168
51	1	0	2.284332	-4.733501	2.502785
52	1	0	2.567393	-5.353850	0.845079
53	6	0	1.647798	5.119999	1.378111
54	6	0	1.176595	6.246982	0.721337
55	6	0	0.716159	6.137017	-0.592479
56	6	0	0.717320	4.910189	-1.244784
57	1	0	2.032884	5.162131	2.388649
58	1	0	1.173849	7.207517	1.218941
59	1	0	0.354382	7.014124	-1.113860
60	1	0	0.375805	4.806678	-2.266042

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cis-endo-TS2-VI

Imaginary frequency: -175.9002 cm^{-1}

Standard orientation:

Electronic energy E = -4189.673113a.u.

Enthalpy H = -4189.639047 a.u.

Entropy S = 213.773 cal/mol/K

Gibbs free energy G = -4189.740618 a.u.

Total free energy in solution E_{sol}= -4190.85827 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.024130	-0.924854	-1.274027	
2	7	0	-1.348089	-0.994719	-1.338427
3	6	0	-0.231981	-0.261769	-1.557917
4	6	0	-0.229097	0.789188	-2.641393
5	6	0	1.152776	-1.991825	-0.422508
6	6	0	-1.223700	-2.376243	-0.816445
7	6	0	-0.075817	-2.600007	0.174027
8	1	0	0.545728	1.533750	-2.462339
9	1	0	-1.173545	1.318586	-2.737091
10	1	0	-0.033698	0.282039	-3.590771
11	6	0	2.551438	-2.239479	-0.272032
12	6	0	3.219815	-1.273295	-1.066654
13	7	0	2.269211	-0.462487	-1.649805
14	1	0	2.449984	0.235401	-2.349158
15	1	0	-1.058057	-3.014159	-1.687519
16	1	0	-2.181891	-2.649757	-0.380672
17	1	0	0.041844	-3.676220	0.318289
18	1	0	-0.288319	-2.158181	1.151197
19	6	0	3.294894	-3.179698	0.449512
20	6	0	4.677026	-3.148195	0.360816
21	6	0	5.330198	-2.188608	-0.443070
22	6	0	4.609544	-1.247976	-1.161910
23	8	0	5.341057	-4.092195	1.087689
24	6	0	6.754485	-4.086610	1.047944
25	1	0	2.825713	-3.925364	1.077180
26	1	0	6.408199	-2.175387	-0.507916
27	1	0	5.122182	-0.518520	-1.776381
28	1	0	7.158722	-3.142756	1.423136
29	1	0	7.074039	-4.898195	1.696097
30	1	0	7.124584	-4.265572	0.034694
31	6	0	-3.293025	-0.847664	1.493044
32	6	0	-4.399868	-1.585035	0.846595
33	6	0	-2.427828	-0.092756	0.574879
34	6	0	-2.562086	-0.239150	-0.909410
35	6	0	-4.553541	-1.561336	-0.541098
36	8	0	-3.709723	-0.895682	-1.386793
37	8	0	-3.117249	-0.866265	2.700964
38	6	0	-1.295147	0.494579	1.047693
39	6	0	-0.374497	1.174923	0.198452
40	1	0	-2.529879	0.716729	-1.425701
41	1	0	-1.037982	0.336815	2.090711
42	6	0	0.989246	1.272877	0.653715
43	8	0	1.558898	0.580371	1.453438
44	1	0	-0.734035	1.858467	-0.559485
45	8	0	1.680705	2.299256	-0.030837
46	6	0	3.065201	2.446098	0.367386
47	1	0	3.113433	2.730473	1.415663
48	1	0	3.574789	1.499224	0.208616
49	1	0	3.468798	3.227148	-0.270525
50	6	0	-5.314508	-2.301863	1.624508
51	6	0	-6.366610	-2.978484	1.033128
52	6	0	-6.509595	-2.939221	-0.357342
53	6	0	-5.611112	-2.237540	-1.147020
54	1	0	-5.164670	-2.297287	2.696252
55	1	0	-7.073516	-3.529622	1.638270
56	1	0	-7.331089	-3.462077	-0.830517

57	1	0	-5.705725	-2.197074	-2.223614
58	30	0	0.337940	3.854593	0.191141
59	17	0	-0.537884	4.342786	-1.726266
60	17	0	0.631225	4.555683	2.201210

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cis-endo-IM2-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.694959 a.u.

Enthalpy H = -4189.661008 a.u.

Entropy S = 212.419 cal/mol/K

Gibbs free energy G = -4189.761935 a.u.

Total free energy in solution E_{sol} = -4190.87866 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.894620	-0.608011	-0.727715
2	7	0	-1.465076	-0.844675	-1.052595
3	6	0	-0.404300	0.143390	-0.839100
4	6	0	-0.350755	1.110311	-2.027489
5	6	0	1.019082	-1.747394	0.012491
6	6	0	-1.351727	-2.179743	-0.402442
7	6	0	-0.212589	-2.338838	0.614351
8	1	0	0.493824	1.800202	-1.925553
9	1	0	-1.248024	1.723406	-2.103255
10	1	0	-0.222055	0.545741	-2.950036
11	6	0	2.401044	-2.131717	-0.038750
12	6	0	3.052376	-1.160354	-0.840260
13	7	0	2.107515	-0.247346	-1.263689
14	1	0	2.323980	0.593307	-1.774962
15	1	0	-1.203474	-2.910738	-1.198022
16	1	0	-2.302067	-2.410015	0.078682
17	1	0	-0.084382	-3.402871	0.822002
18	1	0	-0.463718	-1.851392	1.561119
19	6	0	3.145120	-3.178393	0.516258
20	6	0	4.509196	-3.232623	0.271973
21	6	0	5.146413	-2.253335	-0.519052
22	6	0	4.423252	-1.212091	-1.080967
23	8	0	5.172715	-4.279026	0.848394
24	6	0	6.564516	-4.379728	0.626661
25	1	0	2.692666	-3.942884	1.133997
26	1	0	6.210193	-2.303038	-0.698767
27	1	0	4.915415	-0.461522	-1.686524
28	1	0	7.094803	-3.507846	1.019930
29	1	0	6.888950	-5.269027	1.160838
30	1	0	6.791360	-4.493255	-0.436975
31	6	0	-4.296084	-0.025497	1.236373
32	6	0	-5.319316	-0.686646	0.407823
33	6	0	-2.982669	0.145641	0.562447
34	6	0	-2.779860	-0.262255	-0.875799
35	6	0	-4.981373	-1.232080	-0.836455
36	8	0	-3.724536	-1.210615	-1.359151
37	8	0	-4.499854	0.355415	2.374367
38	6	0	-1.957355	0.710557	1.199295
39	6	0	-0.657708	1.009682	0.509192
40	1	0	-2.861735	0.615926	-1.521527
41	1	0	-2.075044	1.011385	2.233982
42	6	0	0.472935	0.876066	1.492866
43	8	0	0.477748	0.285549	2.529816
44	1	0	-0.694207	2.064981	0.211495
45	8	0	1.613989	1.544584	1.054505
46	6	0	2.843949	1.162419	1.743208
47	1	0	2.817205	1.555426	2.755234
48	1	0	2.905893	0.078060	1.745496
49	1	0	3.649620	1.594147	1.156674

50	6	0	-6.633203	-0.799856	0.877444
51	6	0	-7.598504	-1.441097	0.123950
52	6	0	-7.246390	-1.985627	-1.116115
53	6	0	-5.951025	-1.886108	-1.598170
54	1	0	-6.854042	-0.370419	1.846092
55	1	0	-8.613606	-1.523874	0.487684
56	1	0	-7.994100	-2.491368	-1.713976
57	1	0	-5.662867	-2.301609	-2.554108
58	30	0	1.629941	3.217923	-0.109608
59	17	0	3.241491	2.949686	-1.528579
60	17	0	0.128023	4.620694	0.500177

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cis-exo-TS1-VI

Imaginary frequency: -211.7019 cm^{-1}

Standard orientation:

Electronic energy E = -4189.679927 a.u.

Enthalpy H = -4189.645850 a.u.

Entropy S = 208.397 cal/mol/K

Gibbs free energy G = -4189.744866 a.u.

Total free energy in solution E_{sol}= -4190.86385 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.201008	-1.122360	1.562605
2	7	0	-2.143700	-1.335739	0.248595
3	6	0	-1.572269	-0.775069	1.281359
4	6	0	-2.294831	0.208574	2.148637
5	6	0	0.598719	-1.696630	0.588671
6	6	0	-1.505600	-2.534746	-0.315220
7	6	0	-0.016134	-2.349730	-0.605307
8	1	0	-1.877652	1.211517	2.051392
9	1	0	-2.176591	-0.125293	3.184691
10	1	0	-3.355573	0.231452	1.921215
11	6	0	1.940352	-1.397590	0.936481
12	6	0	1.900358	-0.712693	2.173372
13	7	0	0.590178	-0.549513	2.534824
14	1	0	0.264288	-0.028659	3.330299
15	1	0	-2.065781	-2.806812	-1.208191
16	1	0	-1.637007	-3.328143	0.423344
17	1	0	0.168831	-1.757613	-1.504284
18	1	0	0.424660	-3.333237	-0.785349
19	6	0	3.181462	-1.612593	0.271941
20	6	0	4.343165	-1.234995	0.938928
21	6	0	4.278238	-0.577364	2.201934
22	6	0	3.082432	-0.317200	2.823593
23	1	0	3.210337	-2.187431	-0.643591
24	1	0	3.056781	0.194750	3.777040
25	1	0	5.218369	-0.283293	2.647479
26	8	0	5.583115	-1.437983	0.482997
27	6	0	5.730005	-1.995319	-0.820524
28	1	0	5.327556	-3.010419	-0.850054
29	1	0	5.238539	-1.360854	-1.559690
30	1	0	6.798015	-2.014313	-1.011081
31	30	0	2.863287	0.477208	-0.936884
32	17	0	1.867355	-0.370737	-2.714154
33	17	0	4.852915	1.431308	-1.035264
34	6	0	-4.303630	1.495629	-0.195650
35	6	0	-5.405508	0.493003	-0.163803
36	6	0	-3.030497	0.972296	-0.635931
37	6	0	-2.912627	-0.432393	-0.959408
38	6	0	-5.223510	-0.781465	-0.696079
39	8	0	-4.037708	-1.148653	-1.288042
40	8	0	-4.495803	2.648937	0.181201
41	6	0	-1.883391	1.767377	-0.477999
42	6	0	-0.558927	1.398433	-0.539551
43	1	0	-2.159699	-0.640126	-1.718132

44	1	0	-2.090689	2.781820	-0.148370
45	6	0	0.397746	2.340052	-0.024735
46	8	0	0.216333	3.470879	0.350126
47	1	0	-0.209268	0.437597	-0.883442
48	8	0	1.709020	1.789380	0.163387
49	6	0	2.549296	2.668477	0.965510
50	1	0	2.814521	3.547400	0.386411
51	1	0	1.995711	2.958165	1.853477
52	1	0	3.435741	2.097357	1.212937
53	6	0	-6.646294	0.820133	0.386834
54	6	0	-7.676768	-0.106852	0.402142
55	6	0	-7.473482	-1.376617	-0.144803
56	6	0	-6.247857	-1.721466	-0.698253
57	1	0	-6.763915	1.819661	0.784516
58	1	0	-8.636701	0.151713	0.829057
59	1	0	-8.276565	-2.102610	-0.139915
60	1	0	-6.068719	-2.695642	-1.132890

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cis-exo-IM1-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.679158 a.u.

Enthalpy H = -4189.644770 a.u.

Entropy S = 209.321 cal/mol/K

Gibbs free energy G = -4189.744226 a.u.

Total free energy in solution E_{sol}= -4190.86545 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-0.239432	-1.174158	1.486690	
2	7	0	-2.129243	-1.297947	0.099615
3	6	0	-1.589485	-0.787370	1.181648
4	6	0	-2.322931	0.162202	2.077245
5	6	0	0.582885	-1.715913	0.509165
6	6	0	-1.501054	-2.499284	-0.474546
7	6	0	-0.004603	-2.321930	-0.721625
8	1	0	-1.943399	1.179652	1.976705
9	1	0	-2.164678	-0.177410	3.105556
10	1	0	-3.389765	0.152771	1.878740
11	6	0	1.915471	-1.434351	0.895923
12	6	0	1.849536	-0.792741	2.154874
13	7	0	0.534098	-0.641661	2.497063
14	1	0	0.195263	-0.135270	3.296458
15	1	0	-2.045452	-2.740025	-1.385185
16	1	0	-1.660545	-3.304988	0.244385
17	1	0	0.209902	-1.700706	-1.594250
18	1	0	0.430632	-3.303869	-0.922496
19	6	0	3.169306	-1.629567	0.249156
20	6	0	4.315954	-1.273248	0.950147
21	6	0	4.225081	-0.656412	2.233673
22	6	0	3.018860	-0.416847	2.841097
23	1	0	3.216025	-2.168123	-0.687325
24	1	0	2.974172	0.064460	3.809625
25	1	0	5.156537	-0.375977	2.705499
26	8	0	5.565225	-1.460404	0.514557
27	6	0	5.739617	-1.971653	-0.804505
28	1	0	5.341243	-2.986192	-0.876908
29	1	0	5.260532	-1.313312	-1.530734
30	1	0	6.811188	-1.981154	-0.974461
31	30	0	2.880356	0.524849	-0.913256
32	17	0	1.944812	-0.303683	-2.729929
33	17	0	4.881103	1.457647	-0.912413
34	6	0	-4.297915	1.505866	-0.201052
35	6	0	-5.394368	0.496272	-0.141206
36	6	0	-3.027813	0.988311	-0.650416
37	6	0	-2.903892	-0.432705	-0.988729

38	6	0	-5.221649	-0.776468	-0.681771
39	8	0	-4.056043	-1.134353	-1.316749
40	8	0	-4.494414	2.659791	0.174054
41	6	0	-1.887183	1.780840	-0.494699
42	6	0	-0.555507	1.414939	-0.553589
43	1	0	-2.211108	-0.581193	-1.819149
44	1	0	-2.095441	2.792383	-0.156267
45	6	0	0.389639	2.342805	-0.008129
46	8	0	0.213954	3.469515	0.383025
47	1	0	-0.200954	0.460946	-0.911194
48	8	0	1.700210	1.776667	0.204625
49	6	0	2.516352	2.629769	1.056789
50	1	0	2.803591	3.523860	0.512331
51	1	0	1.935277	2.897182	1.934129
52	1	0	3.392800	2.048679	1.316917
53	6	0	-6.618433	0.816251	0.448789
54	6	0	-7.644760	-0.115083	0.494401
55	6	0	-7.452600	-1.382085	-0.061404
56	6	0	-6.242332	-1.720140	-0.653016
57	1	0	-6.727806	1.814847	0.851257
58	1	0	-8.592058	0.138714	0.951301
59	1	0	-8.251824	-2.111925	-0.033815
60	1	0	-6.073268	-2.692453	-1.095940

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cis-exo-TS2-VI

Imaginary frequency: -162.6235 cm^{-1}

Standard orientation:

Electronic energy E = -4189.676742 a.u.

Enthalpy H = -4189.643754 a.u.

Entropy S = 201.810 cal/mol/K

Gibbs free energy G = -4189.739641 a.u.

Total free energy in solution E_{sol}= -4190.86193 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.074827	-0.646416	1.566199
2	7	0	-2.068272	-1.135080	0.402690
3	6	0	-1.441244	-0.321514	1.238767
4	6	0	-2.145021	0.766637	1.989077
5	6	0	0.689000	-1.466101	0.757423
6	6	0	-1.448633	-2.448593	0.141065
7	6	0	0.027828	-2.360336	-0.239478
8	1	0	-1.623527	1.722683	1.908424
9	1	0	-2.155093	0.450656	3.039106
10	1	0	-3.175489	0.880242	1.671958
11	6	0	2.048137	-1.167622	1.048300
12	6	0	2.043851	-0.235963	2.116420
13	7	0	0.741315	0.075390	2.409856
14	1	0	0.440654	0.804697	3.034112
15	1	0	-2.044918	-2.930821	-0.630568
16	1	0	-1.553764	-3.024522	1.062362
17	1	0	0.179035	-1.986665	-1.254165
18	1	0	0.454532	-3.365958	-0.207186
19	6	0	3.276896	-1.590401	0.468593
20	6	0	4.454227	-1.137017	1.051820
21	6	0	4.423520	-0.244180	2.158647
22	6	0	3.243027	0.208660	2.695596
23	1	0	3.274361	-2.314520	-0.334512
24	1	0	3.244307	0.905668	3.523736
25	1	0	5.377333	0.086672	2.545095
26	8	0	5.684271	-1.462290	0.633053
27	6	0	5.792960	-2.210780	-0.573446
28	1	0	5.360689	-3.206410	-0.449360
29	1	0	5.306378	-1.678646	-1.392767
30	1	0	6.856757	-2.294574	-0.771533

31	6	0	-4.409090	1.374678	-0.596655
32	6	0	-5.440040	0.349536	-0.279434
33	6	0	-3.086653	0.840366	-0.867435
34	6	0	-2.869614	-0.613873	-0.852030
35	6	0	-5.172379	-1.005387	-0.467116
36	8	0	-3.982417	-1.435079	-1.002517
37	8	0	-4.672325	2.571415	-0.549899
38	6	0	-1.994396	1.685453	-0.760954
39	6	0	-0.650825	1.313309	-0.724929
40	1	0	-2.171225	-0.915651	-1.634791
41	1	0	-2.233381	2.718048	-0.523809
42	6	0	0.242212	2.216374	-0.072509
43	8	0	-0.056069	3.193719	0.583525
44	1	0	-0.265718	0.410508	-1.175568
45	8	0	1.620622	1.859544	-0.113053
46	6	0	2.436315	2.801835	0.639565
47	1	0	2.340880	3.786922	0.193787
48	1	0	2.084286	2.830172	1.667056
49	1	0	3.455800	2.443470	0.572165
50	6	0	-6.690176	0.729928	0.212155
51	6	0	-7.649783	-0.224918	0.510420
52	6	0	-7.363413	-1.577464	0.309026
53	6	0	-6.126746	-1.975399	-0.181557
54	1	0	-6.872925	1.788973	0.339937
55	1	0	-8.617336	0.074058	0.891049
56	1	0	-8.110343	-2.327846	0.535313
57	1	0	-5.886774	-3.016131	-0.352574
58	30	0	2.761935	0.348057	-0.996481
59	17	0	1.773733	-0.705300	-2.662725
60	17	0	4.774658	1.231874	-1.230493

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cis-exo-IM2-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.730332 a.u.

Enthalpy H = -4189.696597 a.u.

Entropy S = 207.289 cal/mol/K

Gibbs free energy G = -4189.795086 a.u.

Total free energy in solution E_{sol}= -4190.90813 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.755987	0.220636	-0.600547
2	7	0	-1.357354	0.690460	0.459363
3	6	0	-0.722504	-0.096962	-0.603351
4	6	0	-1.270530	0.199624	-2.011578
5	6	0	1.405091	1.027028	0.330047
6	6	0	-0.776573	1.969150	0.848768
7	6	0	0.631214	1.740029	1.404590
8	1	0	-0.866270	-0.500870	-2.745492
9	1	0	-0.998658	1.215414	-2.300360
10	1	0	-2.352426	0.113739	-2.031931
11	6	0	2.686595	1.364546	-0.235540
12	6	0	2.760239	0.735341	-1.489011
13	7	0	1.572761	0.063451	-1.696783
14	1	0	1.382505	-0.533165	-2.484108
15	1	0	-1.428154	2.395931	1.612105
16	1	0	-0.739789	2.675551	0.010566
17	1	0	0.572066	1.161608	2.327571
18	1	0	1.114296	2.694805	1.621136
19	6	0	3.764108	2.127641	0.246885
20	6	0	4.886504	2.226156	-0.553074
21	6	0	4.947214	1.581140	-1.814030
22	6	0	3.902301	0.829061	-2.293433
23	1	0	3.705941	2.594633	1.219178
24	1	0	3.968923	0.327070	-3.249529

25	1	0	5.859567	1.695441	-2.383315
26	8	0	6.005858	2.922983	-0.227797
27	6	0	6.040830	3.524145	1.053206
28	1	0	5.259176	4.282298	1.152063
29	1	0	5.925041	2.773587	1.838884
30	1	0	7.016113	3.995181	1.137615
31	6	0	-4.767368	-0.920325	0.199795
32	6	0	-5.492984	0.366467	0.099566
33	6	0	-3.284924	-0.784596	0.212490
34	6	0	-2.760044	0.577078	0.579803
35	6	0	-4.791544	1.553982	-0.155278
36	8	0	-3.432369	1.585914	-0.241035
37	8	0	-5.325990	-2.000531	0.222288
38	6	0	-2.484798	-1.792336	-0.130448
39	6	0	-1.003479	-1.568376	-0.149552
40	1	0	-3.046831	0.812685	1.611440
41	1	0	-2.902968	-2.757504	-0.390727
42	6	0	-0.245431	-2.570813	-0.967925
43	8	0	-0.627186	-3.147215	-1.949880
44	1	0	-0.637420	-1.635559	0.879562
45	8	0	1.012016	-2.742317	-0.460909
46	6	0	1.818930	-3.735999	-1.149120
47	1	0	1.261510	-4.667112	-1.184924
48	1	0	2.033443	-3.387814	-2.156729
49	1	0	2.728438	-3.819200	-0.568281
50	6	0	-6.890449	0.388353	0.156616
51	6	0	-7.582501	1.571442	-0.031711
52	6	0	-6.871622	2.747301	-0.295546
53	6	0	-5.486224	2.746548	-0.356829
54	1	0	-7.399602	-0.548800	0.340761
55	1	0	-8.662923	1.587964	0.016603
56	1	0	-7.406759	3.675692	-0.450578
57	1	0	-4.923484	3.648655	-0.554874
58	30	0	1.952352	-1.229239	0.920972
59	17	0	0.934040	-1.543985	2.852383
60	17	0	4.030255	-1.709468	0.397974

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cis-COM-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.484007 a.u.

Enthalpy H = -3501.463968 a.u.

Entropy S = 150.143 cal/mol/K

Gibbs free energy G = -3501.535306 a.u.

Total free energy in solution E_{sol} = -3502.22559 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	2.922016	-0.768036	0.011083	
2	6	0	4.392833	-0.661307	0.013994
3	6	0	2.219735	0.530762	0.015824
4	6	0	2.940698	1.676225	0.050063
5	6	0	5.008418	0.587432	0.035321
6	8	0	4.272851	1.748781	0.060704
7	8	0	2.333700	-1.835161	0.004520
8	6	0	0.765486	0.500768	0.006031
9	6	0	-0.071710	1.543402	-0.119069
10	1	0	2.500323	2.663169	0.081353
11	1	0	0.343734	-0.493933	0.101843
12	6	0	-1.510466	1.312899	-0.100368
13	8	0	-2.026228	0.198124	0.037974
14	1	0	0.240033	2.570529	-0.248697
15	8	0	-2.212751	2.418852	-0.245798
16	6	0	-3.648469	2.299839	-0.241519
17	1	0	-3.971935	1.696405	-1.090269
18	1	0	-3.983356	1.876250	0.705927

19	1	0	-4.018331	3.313586	-0.345741
20	30	0	-3.798680	-0.678576	0.059309
21	17	0	-4.431431	-1.088056	-1.965035
22	17	0	-4.577275	-0.705637	2.073030
23	6	0	5.195505	-1.807721	-0.005349
24	6	0	6.573202	-1.691596	-0.004410
25	6	0	7.167967	-0.423171	0.016383
26	6	0	6.393298	0.724682	0.037117
27	1	0	4.698023	-2.768425	-0.021227
28	1	0	7.193591	-2.577467	-0.019914
29	1	0	8.246488	-0.334351	0.016959
30	1	0	6.828157	1.714459	0.054778

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cis-endo-TS1-VII

Imaginary frequency: -304.3765 cm^{-1}

Standard orientation:

Electronic energy E = -4189.698130 a.u.

Enthalpy H = -4189.663860 a.u.

Entropy S = 208.437 cal/mol/K

Gibbs free energy G = -4189.762895 a.u.

Total free energy in solution E_{sol}= -4190.87627 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.096503	1.671916	-1.353806
2	7	0	-2.240697	1.394073	-1.060528
3	6	0	-1.208659	2.182373	-0.994568
4	6	0	-1.338370	3.637537	-0.641820
5	6	0	0.369301	0.325112	-1.446297
6	6	0	-2.056193	0.079855	-1.713186
7	6	0	-0.752162	-0.663854	-1.387133
8	1	0	-0.599378	3.930845	0.105168
9	1	0	-2.337352	3.890874	-0.296164
10	1	0	-1.159549	4.219851	-1.551430
11	6	0	1.788690	0.202504	-1.518111
12	6	0	2.314253	1.516601	-1.509364
13	7	0	1.268643	2.396670	-1.386156
14	1	0	1.349481	3.397709	-1.362146
15	1	0	-2.080873	0.292016	-2.785570
16	1	0	-2.922510	-0.531838	-1.474945
17	1	0	-0.617257	-1.448236	-2.135544
18	1	0	-0.782660	-1.168862	-0.419340
19	6	0	2.670456	-0.911171	-1.593457
20	6	0	4.030406	-0.655144	-1.718360
21	6	0	4.527454	0.674687	-1.744621
22	6	0	3.690410	1.758085	-1.645469
23	8	0	4.975072	-1.606662	-1.799841
24	6	0	4.568998	-2.951959	-1.571806
25	1	0	2.269817	-1.912345	-1.653274
26	1	0	5.598773	0.798085	-1.816919
27	1	0	4.086909	2.765461	-1.652878
28	1	0	3.908583	-3.299210	-2.369871
29	1	0	5.482323	-3.538555	-1.569883
30	1	0	4.066003	-3.042692	-0.607009
31	6	0	-3.486170	-1.036968	1.087339
32	6	0	-4.781716	-1.061742	0.359782
33	6	0	-2.844819	0.267023	1.144256
34	6	0	-3.371209	1.353771	0.377253
35	6	0	-5.288923	0.099832	-0.216463
36	8	0	-4.629850	1.307377	-0.127674
37	8	0	-3.018716	-2.048289	1.593775
38	6	0	-1.533538	0.360988	1.652645
39	6	0	-0.801473	1.515257	1.765183
40	1	0	-3.163577	2.361180	0.705174
41	1	0	-1.047715	-0.585900	1.879292
42	6	0	0.626749	1.455356	1.859221

43	8	0	1.301783	0.422161	1.730626
44	1	0	-1.247695	2.499023	1.769363
45	8	0	1.213384	2.638591	2.044269
46	6	0	2.652377	2.618621	2.115095
47	1	0	2.984947	1.920647	2.879146
48	1	0	3.073211	2.311771	1.158688
49	1	0	2.938709	3.636700	2.360064
50	6	0	-5.510095	-2.247049	0.239810
51	6	0	-6.720374	-2.261813	-0.435167
52	6	0	-7.212738	-1.082142	-1.000223
53	6	0	-6.501383	0.105548	-0.896013
54	1	0	-5.091679	-3.135333	0.694693
55	1	0	-7.283180	-3.181371	-0.524011
56	1	0	-8.158449	-1.088706	-1.526690
57	1	0	-6.861553	1.030554	-1.325268
58	30	0	2.461924	-0.928662	0.851202
59	17	0	4.499455	-0.508349	1.588802
60	17	0	1.279444	-2.798815	0.781348

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cis-endo-IM-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.722451 a.u.

Enthalpy H = -4189.688792 a.u.

Entropy S = 206.252 cal/mol/K

Gibbs free energy G = -4189.786789 a.u.

Total free energy in solution E_{sol}= -4190.89940 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.346643	1.276050	-1.282028
2	7	0	-2.060850	1.167806	-1.354778
3	6	0	-0.925211	1.944077	-0.861477
4	6	0	-1.009709	3.383425	-1.374136
5	6	0	0.534730	-0.075458	-1.273013
6	6	0	-1.823373	-0.215283	-1.834002
7	6	0	-0.651701	-0.981813	-1.200072
8	1	0	-0.250629	4.012318	-0.900920
9	1	0	-1.984871	3.812969	-1.143203
10	1	0	-0.882688	3.393021	-2.456624
11	6	0	1.954122	-0.289712	-1.367779
12	6	0	2.555093	0.987776	-1.488817
13	7	0	1.554177	1.928052	-1.400717
14	1	0	1.675638	2.919749	-1.511168
15	1	0	-1.638476	-0.151500	-2.907920
16	1	0	-2.754107	-0.765578	-1.702345
17	1	0	-0.476731	-1.891146	-1.780374
18	1	0	-0.859278	-1.298475	-0.177433
19	6	0	2.769761	-1.452971	-1.367791
20	6	0	4.135818	-1.290175	-1.545217
21	6	0	4.700596	-0.005446	-1.738318
22	6	0	3.930491	1.132634	-1.711923
23	8	0	5.025677	-2.304874	-1.525276
24	6	0	4.541763	-3.578086	-1.117648
25	1	0	2.313324	-2.425400	-1.256943
26	1	0	5.773403	0.049660	-1.858602
27	1	0	4.383523	2.108736	-1.828542
28	1	0	3.849419	-3.987418	-1.857369
29	1	0	5.416138	-4.217943	-1.044241
30	1	0	4.046241	-3.508185	-0.146176
31	6	0	-3.738417	-0.488162	1.414479

32	6	0	-4.909081	-0.822300	0.586552
33	6	0	-2.872469	0.572584	0.845146
34	6	0	-3.195508	1.281530	-0.444919
35	6	0	-5.152183	-0.145201	-0.613784
36	8	0	-4.363063	0.844378	-1.117140
37	8	0	-3.487923	-1.031813	2.473351
38	6	0	-1.698583	0.890750	1.395040
39	6	0	-0.898608	1.994934	0.770980
40	1	0	-3.343647	2.348811	-0.252452
41	1	0	-1.334048	0.363443	2.269098
42	6	0	0.521902	1.978107	1.268040
43	8	0	1.127850	0.952416	1.543035
44	1	0	-1.337341	2.960296	1.043387
45	8	0	1.064773	3.175470	1.373136
46	6	0	2.454875	3.188591	1.788670
47	1	0	2.553531	2.699738	2.754090
48	1	0	3.060163	2.650782	1.062213
49	1	0	2.721942	4.238299	1.843235
50	6	0	-5.789971	-1.828576	1.001670
51	6	0	-6.895127	-2.158561	0.240930
52	6	0	-7.127854	-1.471921	-0.956250
53	6	0	-6.268995	-0.473443	-1.385410
54	1	0	-5.566143	-2.329509	1.934518
55	1	0	-7.572181	-2.937162	0.564670
56	1	0	-7.990912	-1.720567	-1.560878
57	1	0	-6.435504	0.065474	-2.307970
58	30	0	2.322938	-0.659657	0.986881
59	17	0	4.275486	0.039780	1.741031
60	17	0	1.172705	-2.479569	1.460944

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cis-exo-TS1-VII

Imaginary frequency: -251.3803 cm^{-1}

Standard orientation:

Electronic energy E = -4189.695484 a.u.

Enthalpy H = -4189.661216 a.u.

Entropy S = 213.925 cal/mol/K

Gibbs free energy G = -4189.762859 a.u.

Total free energy in solution E_{sol}= -4190.87712 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.053932	1.207316	-0.588390
2	6	0	-5.202533	0.407308	-0.091130
3	6	0	-2.972338	0.416504	-1.151456
4	6	0	-3.073808	-1.004689	-1.169260
5	8	0	-4.264703	-1.623468	-1.006653
6	8	0	-4.028974	2.427131	-0.479959
7	6	0	-1.731541	1.034956	-1.381327
8	6	0	-0.552746	0.399577	-1.686438
9	1	0	-2.500764	-1.534670	-1.921673
10	1	0	-1.705472	2.102351	-1.182959
11	6	0	0.695660	1.048161	-1.489466
12	8	0	0.838039	2.240824	-1.123924
13	1	0	-0.494381	-0.647835	-1.940224
14	8	0	1.745609	0.251256	-1.675177
15	6	0	3.042031	0.767697	-1.357317
16	1	0	3.246229	1.681711	-1.914024
17	1	0	3.124079	0.925836	-0.278387
18	1	0	3.740627	-0.014751	-1.635998
19	6	0	-5.252780	-0.967855	-0.305602
20	6	0	-6.253609	1.019052	0.596428
21	6	0	-7.323284	0.267629	1.054970
22	6	0	-7.353695	-1.110737	0.822295
23	6	0	-6.320956	-1.737483	0.139353
24	1	0	-6.323287	-2.801236	-0.055345
25	1	0	-8.189323	-1.700232	1.177035

26	1	0	-8.134854	0.744198	1.588416
27	1	0	-6.194098	2.088995	0.747270
28	30	0	2.046686	3.135308	0.087271
29	17	0	1.747450	2.364673	2.133943
30	17	0	3.440830	4.553234	-0.750276
31	6	0	0.209501	-1.486464	0.986853
32	7	0	-1.989369	-1.768029	0.159986
33	6	0	-1.158964	-1.048847	0.856948
34	6	0	-1.601080	0.195103	1.564230
35	6	0	0.753447	-2.487024	0.205411
36	6	0	-1.572883	-3.121782	-0.232230
37	6	0	-0.127174	-3.253511	-0.728820
38	1	0	-1.077460	1.081811	1.201481
39	1	0	-1.345873	0.074674	2.621610
40	1	0	-2.674306	0.334796	1.486349
41	6	0	2.160128	-2.444444	0.401629
42	6	0	2.401522	-1.398836	1.325799
43	7	0	1.203435	-0.838472	1.680541
44	1	0	1.118566	0.046632	2.163897
45	1	0	-2.287436	-3.484366	-0.971928
46	1	0	-1.686531	-3.741280	0.661642
47	1	0	-0.006645	-2.878361	-1.751900
48	1	0	0.127705	-4.315297	-0.753007
49	6	0	3.239451	-3.179589	-0.137111
50	6	0	4.515456	-2.838268	0.262796
51	6	0	4.740096	-1.783306	1.188505
52	6	0	3.703780	-1.062102	1.730638
53	8	0	5.652476	-3.448900	-0.169379
54	6	0	5.502852	-4.506765	-1.095761
55	1	0	6.506967	-4.855928	-1.319901
56	1	0	5.022170	-4.158947	-2.014409
57	1	0	4.917643	-5.324593	-0.666424
58	1	0	3.053182	-3.979378	-0.839313
59	1	0	5.766887	-1.570945	1.454753
60	1	0	3.881394	-0.255668	2.430318

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cis-exo-IM1-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.698841 a.u.

Enthalpy H = -4189.664712 a.u.

Entropy S = 213.407 cal/mol/K

Gibbs free energy G = -4189.766109 a.u.

Total free energy in solution E_{sol} = -4190.88566 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.017921	1.204116	-0.656772
2	6	0	-5.102224	0.383619	-0.048572
3	6	0	-2.913115	0.442328	-1.204431
4	6	0	-2.946363	-1.043616	-1.178263
5	8	0	-4.190400	-1.653604	-0.983246
6	8	0	-4.057826	2.429013	-0.617333
7	6	0	-1.728630	1.086956	-1.500522
8	6	0	-0.521897	0.468297	-1.831870
9	1	0	-2.583698	-1.442330	-2.127545
10	1	0	-1.729584	2.162260	-1.346618
11	6	0	0.707547	1.105181	-1.629347
12	8	0	0.866469	2.301972	-1.246394
13	1	0	-0.464624	-0.573393	-2.110014
14	8	0	1.774913	0.311741	-1.832447
15	6	0	3.055396	0.819023	-1.462195
16	1	0	3.259684	1.776655	-1.938956
17	1	0	3.130644	0.897465	-0.371882
18	1	0	3.772184	0.073573	-1.793435
19	6	0	-5.123086	-1.000911	-0.212701

20	6	0	-6.112846	0.990783	0.699506
21	6	0	-7.123523	0.230541	1.267653
22	6	0	-7.130590	-1.153985	1.084068
23	6	0	-6.133750	-1.776769	0.343967
24	1	0	-6.124213	-2.846381	0.183414
25	1	0	-7.919109	-1.753507	1.521017
26	1	0	-7.904695	0.705651	1.845920
27	1	0	-6.073687	2.067137	0.805585
28	30	0	1.985451	3.077439	0.096312
29	17	0	1.469034	2.274232	2.102251
30	17	0	3.552007	4.454020	-0.469220
31	6	0	0.111792	-1.512941	0.906658
32	7	0	-1.944488	-1.676383	-0.206201
33	6	0	-1.201294	-1.014920	0.661564
34	6	0	-1.674443	0.185098	1.418714
35	6	0	0.728794	-2.466564	0.106644
36	6	0	-1.543403	-3.052812	-0.556718
37	6	0	-0.066658	-3.184573	-0.933117
38	1	0	-1.216280	1.102095	1.042949
39	1	0	-1.350833	0.055165	2.454619
40	1	0	-2.754908	0.277674	1.401307
41	6	0	2.109431	-2.429836	0.409943
42	6	0	2.268998	-1.436143	1.408799
43	7	0	1.047641	-0.913452	1.722261
44	1	0	0.942598	-0.009257	2.170505
45	1	0	-2.205692	-3.389486	-1.351091
46	1	0	-1.734712	-3.665528	0.326722
47	1	0	0.150160	-2.765228	-1.921439
48	1	0	0.178005	-4.247995	-0.974055
49	6	0	3.233923	-3.123524	-0.096612
50	6	0	4.472286	-2.783776	0.401601
51	6	0	4.616732	-1.771395	1.394852
52	6	0	3.539485	-1.096224	1.908897
53	8	0	5.646197	-3.347697	0.017060
54	6	0	5.583339	-4.355522	-0.974397
55	1	0	6.607874	-4.672367	-1.147096
56	1	0	5.158452	-3.964585	-1.902710
57	1	0	4.988903	-5.206004	-0.630112
58	1	0	3.106686	-3.884649	-0.852461
59	1	0	5.621821	-1.555101	1.731390
60	1	0	3.659010	-0.322455	2.655464

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cis-exo-TS2-VII

Imaginary frequency: -197.2077 cm^{-1}

Standard orientation:

Electronic energy E = -4189.694765 a.u.

Enthalpy H = -4189.661019 a.u.

Entropy S = 209.945 cal/mol/K

Gibbs free energy G = -4189.760771 a.u.

Total free energy in solution E_{sol}= -4190.87752 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.325281	0.790717	-0.858006
2	6	0	-5.440699	0.003501	-0.276338
3	6	0	-3.014283	0.124250	-0.879784
4	6	0	-2.956393	-1.316488	-0.429882
5	8	0	-3.888222	-1.613431	0.613402
6	8	0	-4.504829	1.915761	-1.300840
7	6	0	-1.925645	0.846424	-1.261658
8	6	0	-0.604638	0.333559	-1.404198
9	1	0	-3.181114	-1.980237	-1.271538
10	1	0	-2.089028	1.911962	-1.396461
11	6	0	0.526432	1.155978	-1.288187
12	8	0	0.510657	2.340011	-0.845900
13	1	0	-0.423528	-0.648389	-1.807984

14	8	0	1.678226	0.556143	-1.618452
15	6	0	2.893873	1.267279	-1.389296
16	1	0	2.888112	2.231347	-1.898874
17	1	0	3.068829	1.382634	-0.315278
18	1	0	3.680105	0.636871	-1.792699
19	6	0	-5.172596	-1.169341	0.428822
20	6	0	-6.759104	0.448007	-0.388130
21	6	0	-7.792591	-0.271710	0.190686
22	6	0	-7.505605	-1.442479	0.897209
23	6	0	-6.199283	-1.898230	1.020438
24	1	0	-5.957267	-2.799497	1.567089
25	1	0	-8.308281	-2.006378	1.355449
26	1	0	-8.814312	0.072118	0.101613
27	1	0	-6.933865	1.367763	-0.930830
28	30	0	1.723921	3.380814	0.217524
29	17	0	1.914674	2.463455	2.227754
30	17	0	2.686042	5.098228	-0.666094
31	6	0	0.577569	-1.357968	0.710473
32	7	0	-1.657140	-1.756001	0.070729
33	6	0	-0.781255	-0.906888	0.635150
34	6	0	-1.230838	0.188802	1.555639
35	6	0	1.079983	-2.425082	-0.010977
36	6	0	-1.245146	-3.147950	-0.194591
37	6	0	0.144961	-3.263779	-0.821787
38	1	0	-0.604426	1.074893	1.457539
39	1	0	-1.117484	-0.206735	2.570427
40	1	0	-2.271176	0.454434	1.413000
41	6	0	2.488280	-2.411198	0.160015
42	6	0	2.774332	-1.310992	1.006557
43	7	0	1.601372	-0.688744	1.335291
44	1	0	1.538413	0.190381	1.837455
45	1	0	-2.006340	-3.599554	-0.826614
46	1	0	-1.242756	-3.671638	0.764561
47	1	0	0.138715	-2.935842	-1.867353
48	1	0	0.435956	-4.316261	-0.816179
49	6	0	3.536364	-3.222408	-0.329899
50	6	0	4.825672	-2.898821	0.036895
51	6	0	5.095466	-1.788569	0.883591
52	6	0	4.091240	-0.992879	1.378022
53	8	0	5.936609	-3.577668	-0.357534
54	6	0	5.740230	-4.701102	-1.193501
55	1	0	6.728386	-5.107518	-1.390218
56	1	0	5.268929	-4.410751	-2.136532
57	1	0	5.125139	-5.456284	-0.696436
58	1	0	3.317219	-4.060748	-0.975250
59	1	0	6.131460	-1.595555	1.127777
60	1	0	4.303078	-0.149153	2.022264

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cis-exo-IM2-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.726393 a.u.

Enthalpy H = -4189.692670 a.u.

Entropy S = 211.313 cal/mol/K

Gibbs free energy G = -4189.793072 a.u.

Total free energy in solution E_{sol}= -4190.91038 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.454185	-0.004971	1.143847
2	6	0	5.278373	-0.828829	0.232909
3	6	0	2.996494	-0.306726	1.077485
4	6	0	2.641457	-1.659200	0.527907
5	8	0	3.316994	-1.844759	-0.756340
6	8	0	4.907609	0.874438	1.851502
7	6	0	2.079026	0.589117	1.432722

8	6	0	0.618048	0.264301	1.261469
9	1	0	3.059030	-2.436615	1.179852
10	1	0	2.396017	1.547800	1.827970
11	6	0	-0.233345	1.491435	1.165926
12	8	0	-0.027069	2.386602	0.340342
13	1	0	0.255846	-0.308293	2.117170
14	8	0	-1.209917	1.523408	2.035098
15	6	0	-2.157328	2.605336	1.945024
16	1	0	-1.646287	3.564428	2.023652
17	1	0	-2.714098	2.511833	1.010894
18	1	0	-2.828966	2.465694	2.784106
19	6	0	4.665917	-1.676261	-0.703457
20	6	0	6.670580	-0.685610	0.229228
21	6	0	7.444987	-1.374200	-0.686544
22	6	0	6.821371	-2.206304	-1.623254
23	6	0	5.444026	-2.362652	-1.636350
24	1	0	4.949205	-3.006397	-2.350777
25	1	0	7.420396	-2.742673	-2.348423
26	1	0	8.521004	-1.264823	-0.686756
27	1	0	7.107401	-0.012274	0.955386
28	30	0	-1.046021	3.809494	-0.585171
29	17	0	-2.297866	2.728992	-2.002101
30	17	0	-0.745546	5.782100	0.202472
31	6	0	-0.981758	-1.136286	-0.063144
32	7	0	1.250592	-1.856482	0.417912
33	6	0	0.447936	-0.690696	0.021907
34	6	0	0.882297	-0.064009	-1.313683
35	6	0	-1.460152	-2.381459	0.225642
36	6	0	0.826820	-3.169594	-0.065795
37	6	0	-0.537971	-3.521433	0.525981
38	1	0	0.195433	0.721726	-1.629250
39	1	0	0.874820	-0.846214	-2.073551
40	1	0	1.884635	0.354970	-1.261051
41	6	0	-2.888611	-2.323614	0.067383
42	6	0	-3.195312	-1.008761	-0.332434
43	7	0	-2.018620	-0.279113	-0.378483
44	1	0	-1.932289	0.562537	-0.934319
45	1	0	1.588385	-3.885786	0.247193
46	1	0	0.775169	-3.197130	-1.160281
47	1	0	-0.438875	-3.696977	1.601217
48	1	0	-0.909632	-4.443824	0.072155
49	6	0	-3.915724	-3.272763	0.216560
50	6	0	-5.213715	-2.872985	-0.055185
51	6	0	-5.501728	-1.554498	-0.473357
52	6	0	-4.505035	-0.612412	-0.615765
53	8	0	-6.307944	-3.682743	0.049032
54	6	0	-6.084153	-5.016952	0.454009
55	1	0	-7.060156	-5.494922	0.474447
56	1	0	-5.636955	-5.057173	1.451462
57	1	0	-5.435439	-5.541055	-0.253790
58	1	0	-3.682361	-4.279102	0.534071
59	1	0	-6.535547	-1.310888	-0.677802
60	1	0	-4.729388	0.395531	-0.942011

5.2.2 trans-2a as diene

trans-endo-TS-I Imaginary frequency: -344.2917 cm^{-1}

Standard orientation: Electronic energy E = -4189.680077 a.u.

Enthalpy H = -4189.645642 a.u.

Center Atomic Atomic Coordinates (Angstroms) Entropy S = 213.921 cal/mol/K

Number	Number	Type	X	Y	Z
1	6	0	0.635509	0.643973	-0.965506
2	7	0	-1.649291	0.088898	-1.313511
3	6	0	-0.630832	0.837172	-1.657272
4	6	0	-0.644748	1.659804	-2.914604
5	6	0	0.804558	-0.227615	0.105590
6	6	0	-1.430492	-1.057771	-0.407392
7	6	0	-0.410321	-0.862007	0.718360
8	1	0	-0.147038	2.620723	-2.779307
9	1	0	-1.658556	1.818767	-3.277539
10	1	0	-0.110152	1.085865	-3.679039
11	6	0	2.166619	-0.047852	0.551262
12	6	0	2.743974	0.923132	-0.304818
13	7	0	1.782712	1.335636	-1.190526
14	1	0	1.914020	2.030968	-1.907911
15	1	0	-1.083485	-1.871969	-1.053976
16	1	0	-2.396339	-1.356357	-0.009076
17	1	0	-0.185167	-1.838597	1.148475
18	1	0	-0.805205	-0.222608	1.512758
19	6	0	2.943060	-0.663345	1.562011
20	6	0	4.266548	-0.281060	1.675147
21	6	0	4.825638	0.700791	0.812350
22	6	0	4.087648	1.304432	-0.176456
23	8	0	5.133901	-0.788754	2.580075
24	6	0	4.663321	-1.846655	3.402614
25	1	0	2.498741	-1.419237	2.192205
26	1	0	5.870141	0.942453	0.953579
27	1	0	4.530709	2.034088	-0.840946
28	1	0	4.322428	-2.687389	2.793664
29	1	0	5.509943	-2.149835	4.011197
30	1	0	3.850382	-1.504823	4.047789
31	30	0	2.009779	-1.796184	-1.023848
32	17	0	1.644455	-3.668991	0.022632
33	17	0	2.686698	-1.242721	-3.012828
34	6	0	-3.566975	0.604106	1.476333
35	6	0	-4.590314	-0.380335	1.052037
36	6	0	-2.969253	1.370661	0.393473
37	6	0	-3.179280	0.966798	-0.963462
38	6	0	-4.858018	-0.573827	-0.301665
39	8	0	-4.198369	0.123777	-1.286744
40	8	0	-3.264841	0.750544	2.656350
41	6	0	-1.933545	2.278905	0.696923
42	6	0	-1.245102	2.995075	-0.241328
43	1	0	-3.081167	1.705309	-1.746159
44	1	0	-1.611842	2.300187	1.732777
45	6	0	0.041579	3.642467	-0.010924
46	8	0	0.726948	4.106953	-0.909165
47	1	0	-1.633122	3.154073	-1.235261
48	8	0	0.448140	3.610236	1.267745
49	6	0	1.747241	4.161702	1.505396
50	1	0	2.506867	3.562188	1.004426
51	1	0	1.796099	5.185524	1.140309
52	1	0	1.885531	4.126741	2.581507
53	6	0	-5.296972	-1.130720	1.995124
54	6	0	-6.254994	-2.044813	1.589256
55	6	0	-6.511616	-2.218099	0.225643
56	6	0	-5.815779	-1.487813	-0.727260
57	1	0	-5.065377	-0.963924	3.038908
58	1	0	-6.802560	-2.622876	2.321423
59	1	0	-7.258971	-2.931590	-0.096906
60	1	0	-5.993726	-1.609485	-1.786941

Gibbs free energy G = -4189.747282 a.u.

Total free energy in solution E_{sol} = -4190.86113 a.u.

trans-endo-IM-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-0.771201	0.840929	0.592082	
2	7	0	1.481567	0.071763	1.009635
3	6	0	0.580263	1.224853	1.116219
4	6	0	0.458082	1.644711	2.586075
5	6	0	-0.991806	-0.071581	-0.417460
6	6	0	1.211697	-1.008737	0.024099
7	6	0	0.193663	-0.697181	-1.079529
8	1	0	-0.092217	2.585587	2.669699
9	1	0	1.444264	1.802735	3.022417
10	1	0	-0.049707	0.861106	3.148841
11	6	0	-2.413733	-0.020282	-0.710647
12	6	0	-2.963799	0.936746	0.169621
13	7	0	-1.934316	1.475611	0.913328
14	1	0	-2.071788	1.996256	1.764534
15	1	0	0.854899	-1.883200	0.574514
16	1	0	2.159644	-1.298178	-0.428936
17	1	0	-0.068214	-1.630794	-1.578306
18	1	0	0.601050	-0.006414	-1.822019
19	6	0	-3.245652	-0.743643	-1.592971
20	6	0	-4.604255	-0.485443	-1.549791
21	6	0	-5.139715	0.478802	-0.657448
22	6	0	-4.340604	1.190536	0.205950
23	8	0	-5.525202	-1.111987	-2.319724
24	6	0	-5.064258	-2.178603	-3.135364
25	1	0	-2.816268	-1.488657	-2.245862
26	1	0	-6.211704	0.620287	-0.668634
27	1	0	-4.764859	1.904811	0.899119
28	1	0	-4.576375	-2.945783	-2.529001
29	1	0	-5.947799	-2.591502	-3.613202
30	1	0	-4.371296	-1.815233	-3.898147
31	30	0	-1.935882	-1.604061	0.978774
32	17	0	-1.634949	-3.533139	0.009969
33	17	0	-2.512620	-0.965476	2.980220
34	6	0	4.192832	0.817933	-1.308668
35	6	0	5.036444	-0.281249	-0.811968
36	6	0	3.090312	1.199632	-0.394626
37	6	0	2.865132	0.525066	0.935498
38	6	0	4.751120	-0.905779	0.408302
39	8	0	3.707404	-0.579701	1.217896
40	8	0	4.369907	1.369660	-2.380084
41	6	0	2.182098	2.118602	-0.730586
42	6	0	1.123228	2.491345	0.262237
43	1	0	3.020182	1.242656	1.746025
44	1	0	2.217754	2.605517	-1.697573
45	6	0	-0.010980	3.223801	-0.414495
46	8	0	-0.351893	3.046935	-1.557300
47	1	0	1.561333	3.166707	1.004751
48	8	0	-0.620510	4.078637	0.422993
49	6	0	-1.771851	4.729813	-0.139252
50	1	0	-1.480998	5.313098	-1.009915
51	1	0	-2.507623	3.983461	-0.436407
52	1	0	-2.156787	5.372601	0.646222
53	6	0	6.130822	-0.716855	-1.570318
54	6	0	6.931070	-1.751757	-1.126684
55	6	0	6.633854	-2.367690	0.094943

Imaginary frequency: none cm^{-1}
Electronic energy E = -4189.713118 a.u.
Enthalpy H = -4189.679399 a.u.
Entropy S = 209.646 cal/mol/K
Gibbs free energy G = -4189.779008 a.u.
Total free energy in solution E_{sol}= -4190.89299 a.u. 1

56	6	0	5.556517	-1.953827	0.860001
57	1	0	6.316957	-0.211062	-2.508805
58	1	0	7.775490	-2.084495	-1.714756
59	1	0	7.252544	-3.181003	0.452566
60	1	0	5.312586	-2.421057	1.804155

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trans-exo-TS-I

Imaginary frequency: -351.8176 cm^{-1}

Standard orientation:

Electronic energy E = -4189.669954 a.u.

Enthalpy H = -4189.635464 a.u.

Entropy S = 215.570 cal/mol/K

Gibbs free energy G = -4189.737888 a.u.

Total free energy in solution E_{sol}= -4190.85409 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.541594	0.368394	0.350589	
2	7	0	-1.477986	-0.647998	-0.405420
3	6	0	-0.904029	0.224471	0.401313
4	6	0	-1.633189	0.744381	1.601971
5	6	0	1.334321	-0.186322	-0.643240
6	6	0	-0.619999	-1.512788	-1.239187
7	6	0	0.655935	-0.866441	-1.795150
8	1	0	-1.381481	1.784259	1.811339
9	1	0	-1.329768	0.112757	2.445111
10	1	0	-2.708321	0.644705	1.488743
11	6	0	2.680986	0.270886	-0.384343
12	6	0	2.612392	1.067942	0.784687
13	7	0	1.298815	1.139584	1.179979
14	1	0	0.998709	1.469257	2.082990
15	1	0	-1.243795	-1.920421	-2.033424
16	1	0	-0.328995	-2.355038	-0.602647
17	1	0	0.441966	-0.135224	-2.581004
18	1	0	1.277527	-1.650278	-2.229075
19	6	0	3.928170	0.005015	-0.997490
20	6	0	5.057983	0.546916	-0.412848
21	6	0	4.967923	1.349345	0.756172
22	6	0	3.765043	1.614388	1.364125
23	1	0	3.971462	-0.621950	-1.875292
24	1	0	3.714085	2.210595	2.265135
25	1	0	5.893669	1.732913	1.162634
26	8	0	6.316793	0.363786	-0.871005
27	6	0	6.481803	-0.519999	-1.970098
28	1	0	6.086004	-1.510375	-1.731994
29	1	0	5.986543	-0.128046	-2.861707
30	1	0	7.551827	-0.581445	-2.144652
31	30	0	2.316226	-1.768312	0.703289
32	17	0	2.823496	-3.403078	-0.642528
33	17	0	1.932417	-1.586421	2.835921
34	6	0	-4.681883	1.113995	-0.160161
35	6	0	-5.308147	-0.223713	-0.023479
36	6	0	-3.404543	1.112525	-0.856967
37	6	0	-2.854308	-0.121365	-1.345734
38	6	0	-4.756101	-1.332738	-0.661952
39	8	0	-3.652066	-1.224893	-1.472721
40	8	0	-5.191408	2.116945	0.326104
41	6	0	-2.559997	2.222367	-0.734739
42	6	0	-1.236168	2.222183	-1.111487
43	1	0	-2.269645	-0.027327	-2.257112
44	1	0	-2.953337	3.057191	-0.164435
45	6	0	-0.262454	3.238566	-0.728486
46	8	0	0.871426	3.292252	-1.160290
47	1	0	-0.846871	1.528846	-1.842558
48	8	0	-0.714739	4.076362	0.234180
49	6	0	0.226253	5.077275	0.632279

50	1	0	1.128158	4.611883	1.028762
51	1	0	0.499231	5.699995	-0.217632
52	1	0	-0.274941	5.665236	1.395331
53	6	0	-6.461544	-0.392954	0.746737
54	6	0	-7.045352	-1.642330	0.872053
55	6	0	-6.477304	-2.740289	0.218402
56	6	0	-5.333422	-2.593358	-0.552651
57	1	0	-6.871992	0.485155	1.227790
58	1	0	-7.937987	-1.770324	1.469768
59	1	0	-6.930649	-3.718744	0.312516
60	1	0	-4.878357	-3.427612	-1.068886

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trans-exo-IM-I

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.735147 a.u.

Enthalpy H = -4189.701689 a.u.

Entropy S = 207.741 cal/mol/K

Gibbs free energy G = -4189.800393 a.u.

Total free energy in solution E_{sol}= -4190.91514 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.935846	0.541768	0.223937	
2	7	0	-0.342589	-0.363536	0.164379
3	6	0	0.475494	0.902862	0.323351
4	6	0	0.130760	1.513435	1.688709
5	6	0	2.479554	-0.714168	0.163790
6	6	0	0.295591	-1.529169	0.864881
7	6	0	1.636524	-1.940128	0.273305
8	1	0	0.843584	2.298496	1.939343
9	1	0	0.193576	0.756410	2.471460
10	1	0	-0.874955	1.940661	1.680085
11	6	0	3.898185	-0.547969	0.034619
12	6	0	4.140277	0.840285	0.022728
13	7	0	2.929298	1.487022	0.140907
14	1	0	2.765490	2.484546	0.107499
15	1	0	-0.421932	-2.343428	0.849688
16	1	0	0.418908	-1.239096	1.906428
17	1	0	1.498818	-2.441913	-0.689593
18	1	0	2.090482	-2.671900	0.946838
19	6	0	4.968787	-1.455946	-0.064092
20	6	0	6.248097	-0.940456	-0.175540
21	6	0	6.475747	0.455132	-0.189865
22	6	0	5.436924	1.354684	-0.090516
23	1	0	4.780181	-2.520039	-0.052676
24	1	0	5.623000	2.420944	-0.098961
25	1	0	7.499641	0.791761	-0.279835
26	8	0	7.378883	-1.697402	-0.280873
27	6	0	7.215959	-3.100055	-0.250559
28	1	0	6.758171	-3.423079	0.688732
29	1	0	6.603489	-3.444716	-1.088643
30	1	0	8.213754	-3.522803	-0.332626
31	30	0	-2.246099	-0.192122	1.036770
32	17	0	-2.488257	-1.634038	2.674993
33	17	0	-3.463545	1.630185	0.851431
34	6	0	-2.875737	0.069832	-2.143554
35	6	0	-3.325698	-1.158129	-1.441441
36	6	0	-1.466076	0.402717	-1.815811
37	6	0	-0.548149	-0.664439	-1.291008
38	6	0	-2.379868	-2.132016	-1.100654
39	8	0	-1.052717	-1.968541	-1.431898
40	8	0	-3.608770	0.785549	-2.788090
41	6	0	-1.144098	1.667500	-1.549582
42	6	0	0.156364	1.936764	-0.859286

43	1	0	0.419282	-0.668643	-1.797626
44	1	0	-1.841326	2.466531	-1.759461
45	6	0	0.290491	3.360741	-0.340622
46	8	0	1.355457	3.873556	-0.061212
47	1	0	0.966313	1.817891	-1.585143
48	8	0	-0.872985	3.971131	-0.197205
49	6	0	-0.821487	5.293181	0.370077
50	1	0	-0.355020	5.249739	1.351827
51	1	0	-0.248779	5.950822	-0.279836
52	1	0	-1.855705	5.610017	0.442718
53	6	0	-4.673879	-1.367908	-1.130432
54	6	0	-5.061633	-2.536771	-0.497338
55	6	0	-4.107408	-3.511722	-0.191113
56	6	0	-2.766207	-3.322023	-0.494687
57	1	0	-5.380035	-0.589599	-1.387803
58	1	0	-6.098590	-2.694383	-0.234900
59	1	0	-4.411086	-4.422790	0.306969
60	1	0	-2.015725	-4.063025	-0.255346

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trans-endo-TS-II

Imaginary frequency: -471.1310 cm^{-1}

Standard orientation:

Electronic energy E = -4189.686841 a.u.

Enthalpy H = -4189.653495 a.u.

Entropy S = 204.992 cal/mol/K

Gibbs free energy G = -4189.750893 a.u.

Total free energy in solution E_{sol}= -4190.86255 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.521355	-0.982350	-0.465032	
2	7	0	0.861723	-0.670453	-0.359488
3	6	0	-0.213965	-1.477834	-0.110214
4	6	0	0.005538	-2.963449	-0.035577
5	6	0	-1.821430	0.337492	-0.715511
6	6	0	0.575342	0.632159	-1.044477
7	6	0	-0.728286	1.353528	-0.690389
8	1	0	-0.764997	-3.447083	0.563765
9	1	0	0.983180	-3.210913	0.372782
10	1	0	-0.025821	-3.363442	-1.054863
11	6	0	-3.228534	0.415327	-0.907899
12	6	0	-3.727404	-0.901322	-0.762213
13	7	0	-2.671484	-1.741942	-0.505495
14	1	0	-2.754767	-2.678054	-0.144508
15	1	0	0.547832	0.386420	-2.107149
16	1	0	1.441402	1.274811	-0.899854
17	1	0	-0.883147	2.123316	-1.450429
18	1	0	-0.682008	1.864213	0.274412
19	6	0	-4.109670	1.481284	-1.187296
20	6	0	-5.455545	1.195161	-1.302566
21	6	0	-5.939962	-0.129895	-1.153142
22	6	0	-5.094862	-1.183115	-0.891190
23	8	0	-6.423630	2.115573	-1.562866
24	6	0	-6.008553	3.458040	-1.726284
25	1	0	-3.725206	2.484731	-1.299452
26	1	0	-7.005387	-0.282623	-1.260593
27	1	0	-5.476072	-2.191165	-0.789366
28	1	0	-5.320893	3.555891	-2.570607
29	1	0	-6.910910	4.030311	-1.923031
30	1	0	-5.527062	3.833398	-0.819198
31	6	0	1.511106	1.920899	1.977039
32	6	0	2.768284	2.285790	1.283229
33	6	0	1.172269	0.498849	1.935717
34	6	0	1.897942	-0.392593	1.099370
35	6	0	3.493052	1.332836	0.573523
36	8	0	3.088090	0.003224	0.524041

37	8	0	0.808588	2.754098	2.530570
38	6	0	-0.060789	0.053604	2.406064
39	6	0	-0.480152	-1.255928	2.251322
40	1	0	1.994031	-1.433840	1.383476
41	1	0	-0.753112	0.808461	2.761270
42	6	0	-1.876572	-1.664112	2.449770
43	8	0	-2.271848	-2.809065	2.315959
44	1	0	0.219342	-2.078489	2.241887
45	8	0	-2.690938	-0.635871	2.714268
46	6	0	-4.076976	-0.972322	2.858654
47	1	0	-4.475374	-1.319786	1.907132
48	1	0	-4.197919	-1.746798	3.613021
49	1	0	-4.567654	-0.052689	3.160523
50	6	0	3.238608	3.601582	1.302733
51	6	0	4.403211	3.938806	0.633178
52	6	0	5.105599	2.960215	-0.075780
53	6	0	4.656157	1.647010	-0.113288
54	1	0	2.660804	4.330695	1.855155
55	1	0	4.766572	4.957321	0.652948
56	1	0	6.010473	3.221770	-0.607980
57	1	0	5.175430	0.877494	-0.668309
58	30	0	2.709159	-1.333171	-1.233527
59	17	0	3.189156	-0.209681	-3.034183
60	17	0	3.498161	-3.179949	-0.368440

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trans-endo-IM-II

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.724164 a.u.

Enthalpy H = -4189.690556 a.u.

Entropy S = 208.612 cal/mol/K

Gibbs free energy G = -4189.789674 a.u.

Total free energy in solution E_{sol}= -4190.90151 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.611355	-0.758376	-0.269176	
2	7	0	0.845021	-0.570156	-0.295878
3	6	0	-0.330815	-1.416277	0.153861
4	6	0	-0.173373	-2.812687	-0.443493
5	6	0	-1.833865	0.584934	-0.363566
6	6	0	0.512387	0.768259	-0.905084
7	6	0	-0.680564	1.530918	-0.327277
8	1	0	-0.955385	-3.481586	-0.086604
9	1	0	0.787020	-3.245429	-0.164178
10	1	0	-0.222107	-2.750787	-1.533337
11	6	0	-3.233556	0.763141	-0.616529
12	6	0	-3.802319	-0.526102	-0.654174
13	7	0	-2.794717	-1.442210	-0.430379
14	1	0	-2.893810	-2.440975	-0.461094
15	1	0	0.298601	0.572177	-1.954045
16	1	0	1.423957	1.361978	-0.883007
17	1	0	-0.860255	2.382996	-0.988161
18	1	0	-0.486206	1.932344	0.668401
19	6	0	-4.040648	1.896578	-0.822621
20	6	0	-5.389816	1.700048	-1.059425
21	6	0	-5.944243	0.399733	-1.098106
22	6	0	-5.165669	-0.719521	-0.900476
23	8	0	-6.289407	2.702280	-1.271949
24	6	0	-5.794086	4.025774	-1.246196
25	1	0	-3.604931	2.884665	-0.787608
26	1	0	-7.005209	0.315983	-1.290163
27	1	0	-5.600841	-1.710471	-0.937523
28	1	0	-5.042040	4.179904	-2.024886
29	1	0	-6.648120	4.671454	-1.432884
30	1	0	-5.360706	4.264692	-0.271036

31	6	0	1.836986	1.556378	2.437599
32	6	0	2.961944	2.058162	1.617726
33	6	0	1.261821	0.275955	1.968462
34	6	0	1.834300	-0.463875	0.812217
35	6	0	3.470588	1.320794	0.545048
36	8	0	3.016485	0.056382	0.228662
37	8	0	1.382405	2.162154	3.388511
38	6	0	0.120708	-0.251792	2.416342
39	6	0	-0.364235	-1.510003	1.755886
40	1	0	2.089617	-1.488923	1.090692
41	1	0	-0.462554	0.212971	3.200565
42	6	0	-1.758729	-1.845196	2.263972
43	8	0	-2.458896	-1.087073	2.881980
44	1	0	0.291201	-2.346473	2.030274
45	8	0	-2.114851	-3.104397	1.963606
46	6	0	-3.445649	-3.453807	2.385299
47	1	0	-3.528542	-3.362260	3.465740
48	1	0	-4.167152	-2.788006	1.912934
49	1	0	-3.589852	-4.482538	2.070678
50	6	0	3.512010	3.316095	1.888569
51	6	0	4.536306	3.821193	1.107294
52	6	0	5.018430	3.068077	0.032896
53	6	0	4.491804	1.817054	-0.256056
54	1	0	3.102246	3.869400	2.723444
55	1	0	4.957329	4.794080	1.321220
56	1	0	5.812343	3.460063	-0.589266
57	1	0	4.845111	1.223928	-1.089258
58	30	0	2.447274	-1.235264	-1.568296
59	17	0	2.699900	-0.052059	-3.375164
60	17	0	3.349151	-3.100426	-0.855580

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trans-exo-TS-II

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.672189 a.u.

Enthalpy H = -4189.638153 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	1.659493	0.054303	0.490312	
2	7	0	-0.560183	-0.446443	-0.340250
3	6	0	0.254842	0.409415	0.379537
4	6	0	-0.359292	1.171025	1.518881
5	6	0	2.336715	-0.708348	-0.427143
6	6	0	0.147270	-1.578409	-1.025835
7	6	0	1.555968	-1.295292	-1.556949
8	1	0	0.238136	2.050740	1.756899
9	1	0	-0.423750	0.514122	2.390995
10	1	0	-1.376796	1.482446	1.294190
11	6	0	3.708257	-0.714223	-0.037976
12	6	0	3.792623	0.071134	1.134851
13	7	0	2.536531	0.556057	1.425181
14	1	0	2.277871	1.026986	2.274157
15	1	0	-0.521515	-1.943510	-1.804650
16	1	0	0.227923	-2.378037	-0.289936
17	1	0	1.556634	-0.636807	-2.432787
18	1	0	1.975540	-2.248008	-1.886992
19	6	0	4.863513	-1.323088	-0.567145
20	6	0	6.058234	-1.135966	0.100968
21	6	0	6.123106	-0.357277	1.282849
22	6	0	5.005488	0.247749	1.810508
23	1	0	4.798469	-1.915356	-1.468408
24	1	0	5.069936	0.840405	2.714174

Entropy S = 208.601 cal/mol/K

Gibbs free energy G = -4189.737266 a.u.

Total free energy in solution E_{sol}= -4190.85265 a.u. 1

25	1	0	7.089995	-0.254451	1.756377
26	8	0	7.252968	-1.661130	-0.288201
27	6	0	7.256930	-2.450924	-1.461057
28	1	0	6.614026	-3.328065	-1.346031
29	1	0	6.927834	-1.869919	-2.326826
30	1	0	8.285346	-2.770208	-1.606413
31	30	0	-2.201822	-1.381518	0.636340
32	17	0	-2.133830	-3.554526	0.233568
33	17	0	-3.043927	-0.550075	2.483986
34	6	0	-3.127948	2.126458	-0.873556
35	6	0	-4.036067	0.969960	-0.696599
36	6	0	-1.788257	1.751113	-1.338646
37	6	0	-1.521526	0.411309	-1.740805
38	6	0	-3.671710	-0.289200	-1.183214
39	8	0	-2.541978	-0.455314	-1.964606
40	8	0	-3.440677	3.265149	-0.570798
41	6	0	-0.704654	2.551650	-1.008520
42	6	0	0.589825	2.049033	-1.066720
43	1	0	-0.742916	0.235619	-2.470350
44	1	0	-0.908994	3.493258	-0.511655
45	6	0	1.772113	2.806700	-0.614046
46	8	0	2.889652	2.614941	-1.030906
47	1	0	0.860759	1.314486	-1.810619
48	8	0	1.482232	3.704818	0.349033
49	6	0	2.617780	4.445231	0.818166
50	1	0	3.362841	3.763132	1.225196
51	1	0	3.062358	5.006935	-0.000858
52	1	0	2.235980	5.112998	1.583943
53	6	0	-5.212432	1.089414	0.039771
54	6	0	-6.006814	-0.024230	0.274431
55	6	0	-5.633185	-1.268469	-0.230882
56	6	0	-4.467571	-1.412325	-0.978338
57	1	0	-5.463881	2.066370	0.430415
58	1	0	-6.908558	0.068994	0.864008
59	1	0	-6.244842	-2.139804	-0.039842
60	1	0	-4.164094	-2.364058	-1.391344

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trans-exo-IM-II

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.729775 a.u.

Enthalpy H = -4189.696505 a.u.

Entropy S = 204.768 cal/mol/K

Gibbs free energy G = -4189.793796 a.u.

Total free energy in solution E_{sol}= -4190.90962 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.935846	0.541768	0.223937
2	7	0	-0.342589	-0.363536	0.164379
3	6	0	0.475494	0.902862	0.323351
4	6	0	0.130760	1.513435	1.688709
5	6	0	2.479554	-0.714168	0.163790
6	6	0	0.295591	-1.529169	0.864881
7	6	0	1.636524	-1.940128	0.273305
8	1	0	0.843584	2.298496	1.939343
9	1	0	0.193576	0.756410	2.471460
10	1	0	-0.874955	1.940661	1.680085
11	6	0	3.898185	-0.547969	0.034619
12	6	0	4.140277	0.840285	0.022728
13	7	0	2.929298	1.487022	0.140907
14	1	0	2.765490	2.484546	0.107499
15	1	0	-0.421932	-2.343428	0.849688
16	1	0	0.418908	-1.239096	1.906428
17	1	0	1.498818	-2.441913	-0.689593

18	1	0	2.090482	-2.671900	0.946838
19	6	0	4.968787	-1.455946	-0.064092
20	6	0	6.248097	-0.940456	-0.175540
21	6	0	6.475747	0.455132	-0.189865
22	6	0	5.436924	1.354684	-0.090516
23	1	0	4.780181	-2.520039	-0.052676
24	1	0	5.623000	2.420944	-0.098961
25	1	0	7.499641	0.791761	-0.279835
26	8	0	7.378883	-1.697402	-0.280873
27	6	0	7.215959	-3.100055	-0.250559
28	1	0	6.758171	-3.423079	0.688732
29	1	0	6.603489	-3.444716	-1.088643
30	1	0	8.213754	-3.522803	-0.332626
31	30	0	-2.246099	-0.192122	1.036770
32	17	0	-2.488257	-1.634038	2.674993
33	17	0	-3.463545	1.630185	0.851431
34	6	0	-2.875737	0.069832	-2.143554
35	6	0	-3.325698	-1.158129	-1.441441
36	6	0	-1.466076	0.402717	-1.815811
37	6	0	-0.548149	-0.664439	-1.291008
38	6	0	-2.379868	-2.132016	-1.100654
39	8	0	-1.052717	-1.968541	-1.431898
40	8	0	-3.608770	0.785549	-2.788090
41	6	0	-1.144098	1.667500	-1.549582
42	6	0	0.156364	1.936764	-0.859286
43	1	0	0.419282	-0.668643	-1.797626
44	1	0	-1.841326	2.466531	-1.759461
45	6	0	0.290491	3.360741	-0.340622
46	8	0	1.355457	3.873556	-0.061212
47	1	0	0.966313	1.817891	-1.585143
48	8	0	-0.872985	3.971131	-0.197205
49	6	0	-0.821487	5.293181	0.370077
50	1	0	-0.355020	5.249739	1.351827
51	1	0	-0.248779	5.950822	-0.279836
52	1	0	-1.855705	5.610017	0.442718
53	6	0	-4.673879	-1.367908	-1.130432
54	6	0	-5.061633	-2.536771	-0.497338
55	6	0	-4.107408	-3.511722	-0.191113
56	6	0	-2.766207	-3.322023	-0.494687
57	1	0	-5.380035	-0.589599	-1.387803
58	1	0	-6.098590	-2.694383	-0.234900
59	1	0	-4.411086	-4.422790	0.306969
60	1	0	-2.015725	-4.063025	-0.255346

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trans-COM-III

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.457489 a.u.

Enthalpy H = -3501.436232 a.u.

Entropy S = 208.601 cal/mol/K

Gibbs free energy G = -3501.511236 a.u.

Total free energy in solution E_{sol} = -3502.20223 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.771307	2.219618	-0.003796
2	6	0	0.689418	2.413261	-0.096013
3	6	0	-1.216338	0.813056	-0.091304
4	6	0	-0.314987	-0.166534	-0.254043
5	6	0	1.549491	1.330026	-0.235483
6	8	0	1.044846	0.031872	-0.286128
7	8	0	-1.552339	3.144848	0.113451
8	6	0	-2.658106	0.549368	-0.044638
9	6	0	-3.210386	-0.591850	0.375966
10	1	0	-0.556840	-1.208028	-0.412297
11	1	0	-3.288496	1.373399	-0.353968

12	6	0	-4.673005	-0.828106	0.384936
13	8	0	-5.175758	-1.850378	0.788039
14	1	0	-2.632585	-1.422101	0.763038
15	8	0	-5.378127	0.207076	-0.096793
16	6	0	-6.798290	0.012903	-0.085270
17	1	0	-7.062558	-0.849688	-0.693762
18	1	0	-7.145250	-0.148599	0.933554
19	1	0	-7.220097	0.923465	-0.498543
20	6	0	1.236803	3.700089	-0.063388
21	6	0	2.603427	3.881026	-0.172176
22	6	0	3.442525	2.771854	-0.320562
23	6	0	2.923474	1.486821	-0.356328
24	1	0	0.552367	4.530687	0.046121
25	1	0	3.024577	4.876692	-0.145211
26	1	0	4.512130	2.908242	-0.407909
27	1	0	3.571702	0.627198	-0.452674
28	30	0	2.183748	-1.742130	-0.007689
29	17	0	1.161356	-3.111194	-1.290401
30	17	0	3.686133	-1.427859	1.471363

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trans-endo-TS-III

Imaginary frequency: -289.4825 cm^{-1}

Standard orientation:

Electronic energy E = -4189.661738 a.u.

Enthalpy H = -4189.627028 a.u.

Entropy S = 216.281 cal/mol/K

Gibbs free energy G = -4189.729790 a.u.

Total free energy in solution E_{sol}= -4190.84757 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.919194	-0.717674	-1.380907
2	7	0	0.307477	0.037212	-1.039194
3	6	0	-0.504871	-0.958904	-1.236776
4	6	0	-0.006757	-2.372850	-1.303781
5	6	0	-2.509473	0.474397	-1.021097
6	6	0	-0.240097	1.398776	-1.181564
7	6	0	-1.649158	1.623159	-0.612515
8	1	0	-0.378603	-2.965353	-0.463969
9	1	0	1.077814	-2.427326	-1.325431
10	1	0	-0.381223	-2.827918	-2.224860
11	6	0	-3.913124	0.249066	-0.993047
12	6	0	-4.114306	-1.099247	-1.373114
13	7	0	-2.890119	-1.670111	-1.608840
14	1	0	-2.733022	-2.637563	-1.826874
15	1	0	-0.264032	1.586668	-2.258592
16	1	0	0.467996	2.091194	-0.734428
17	1	0	-2.021433	2.567817	-1.015055
18	1	0	-1.645819	1.711924	0.477089
19	6	0	-5.013696	1.067732	-0.659711
20	6	0	-6.275366	0.511705	-0.723698
21	6	0	-6.461048	-0.839160	-1.120057
22	6	0	-5.401811	-1.651109	-1.448966
23	8	0	-7.428598	1.169306	-0.429296
24	6	0	-7.308657	2.514071	-0.003136
25	1	0	-4.850642	2.091284	-0.355599
26	1	0	-7.477073	-1.208979	-1.151434
27	1	0	-5.561535	-2.679939	-1.744907
28	1	0	-6.856116	3.132623	-0.782847
29	1	0	-8.319946	2.858582	0.194004
30	1	0	-6.711737	2.583184	0.909891
31	6	0	1.763987	1.973653	1.506016
32	6	0	2.801679	2.306443	0.485231
33	6	0	1.171939	0.662518	1.362062
34	6	0	1.568765	-0.186576	0.312218
35	6	0	3.245861	1.357212	-0.425712

36	8	0	2.804648	0.025298	-0.311928
37	8	0	1.428357	2.799542	2.347258
38	6	0	-0.064483	0.381587	2.036421
39	6	0	-0.832015	-0.719343	1.883113
40	1	0	1.424598	-1.251229	0.415556
41	1	0	-0.462253	1.198050	2.632043
42	6	0	-2.231210	-0.691459	2.319420
43	8	0	-2.787508	0.223927	2.888090
44	1	0	-0.507572	-1.609449	1.362682
45	8	0	-2.881163	-1.812265	1.929971
46	6	0	-4.284934	-1.804291	2.209094
47	1	0	-4.456907	-1.708248	3.279743
48	1	0	-4.766609	-0.975278	1.691692
49	1	0	-4.663331	-2.753846	1.841296
50	6	0	3.296045	3.606363	0.373113
51	6	0	4.204354	3.927850	-0.625078
52	6	0	4.620909	2.951942	-1.531590
53	6	0	4.139706	1.650963	-1.441319
54	1	0	2.940943	4.335819	1.089050
55	1	0	4.588908	4.935906	-0.704253
56	1	0	5.326386	3.200263	-2.313215
57	1	0	4.461953	0.880279	-2.127570
58	30	0	4.236224	-1.445676	-0.027480
59	17	0	3.124701	-3.256096	0.342822
60	17	0	6.238644	-0.760099	-0.303048

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trans-endo-IM-III

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.724159 a.u.

Enthalpy H = -4189.690553 a.u.

Entropy S = 208.589 cal/mol/K

Gibbs free energy G = -4189.789660 a.u.

Total free energy in solution E_{sol}= -4190.90152 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.538706	-0.915546	-0.285332
2	7	0	0.914317	-0.651426	-0.272266
3	6	0	-0.246554	-1.500688	0.209173
4	6	0	-0.034688	-2.934383	-0.269300
5	6	0	-1.791825	0.405119	-0.527128
6	6	0	0.555867	0.576051	-1.066704
7	6	0	-0.663102	1.377163	-0.610593
8	1	0	-0.797116	-3.598346	0.136474
9	1	0	0.936751	-3.304015	0.059264
10	1	0	-0.071812	-2.963404	-1.360951
11	6	0	-3.198020	0.524330	-0.778489
12	6	0	-3.737084	-0.774118	-0.666699
13	7	0	-2.704227	-1.640936	-0.375984
14	1	0	-2.803647	-2.617500	-0.157432
15	1	0	0.362497	0.226769	-2.079674
16	1	0	1.451921	1.190766	-1.120914
17	1	0	-0.854654	2.128676	-1.381122
18	1	0	-0.489473	1.913728	0.323994
19	6	0	-4.036624	1.610811	-1.090087
20	6	0	-5.386467	1.361101	-1.266629
21	6	0	-5.911676	0.053168	-1.146711
22	6	0	-5.101735	-1.021922	-0.853502
23	8	0	-6.315729	2.313762	-1.563017
24	6	0	-5.854083	3.641912	-1.707296
25	1	0	-3.623711	2.605598	-1.177373
26	1	0	-6.974786	-0.072801	-1.300458
27	1	0	-5.511796	-2.021174	-0.775955
28	1	0	-5.127159	3.719898	-2.520454
29	1	0	-6.729144	4.241482	-1.943306

30	1	0	-5.401633	4.004946	-0.780211
31	6	0	1.589594	1.814554	2.266288
32	6	0	2.718235	2.313766	1.451239
33	6	0	1.137233	0.450669	1.911368
34	6	0	1.825412	-0.354952	0.868390
35	6	0	3.342774	1.508176	0.494483
36	8	0	3.001906	0.186296	0.296687
37	8	0	1.037707	2.478504	3.122715
38	6	0	0.021664	-0.122411	2.369228
39	6	0	-0.324006	-1.474788	1.812865
40	1	0	2.133158	-1.323948	1.267566
41	1	0	-0.616543	0.375849	3.085506
42	6	0	-1.686219	-1.992398	2.244745
43	8	0	-2.021726	-3.150957	2.143948
44	1	0	0.399117	-2.218407	2.168772
45	8	0	-2.477071	-1.030987	2.712047
46	6	0	-3.811491	-1.445588	3.051865
47	1	0	-4.321253	-1.795537	2.156543
48	1	0	-3.776505	-2.240120	3.793738
49	1	0	-4.296176	-0.558920	3.445545
50	6	0	3.157934	3.633231	1.608442
51	6	0	4.187747	4.131295	0.830335
52	6	0	4.787969	3.307784	-0.126871
53	6	0	4.372268	1.995413	-0.301940
54	1	0	2.660068	4.238457	2.354641
55	1	0	4.523115	5.151566	0.956544
56	1	0	5.587766	3.692395	-0.746105
57	1	0	4.817685	1.345561	-1.043718
58	30	0	2.617542	-1.367310	-1.367980
59	17	0	3.566913	-3.070633	-0.373826
60	17	0	2.931867	-0.366727	-3.273799

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trans-exo-TS1-III

Imaginary frequency: -217.3364 cm^{-1}

Standard orientation:

Electronic energy E = -4189.659210 a.u.

Enthalpy H = -4189.624524 a.u.

Entropy S = 220.769 cal/mol/K

Gibbs free energy G = -4189.729418 a.u.

Total free energy in solution E_{sol}= -4190.84841 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.909432	-0.672498	-1.200314
2	7	0	-0.393361	-0.154223	-0.966068
3	6	0	0.530865	-1.074995	-1.075677
4	6	0	0.177358	-2.524840	-1.203478
5	6	0	2.349311	0.601820	-0.909229
6	6	0	0.012380	1.243165	-1.202632
7	6	0	1.346221	1.659464	-0.575110
8	1	0	0.776361	-3.143596	-0.533241
9	1	0	0.387518	-2.814253	-2.239302
10	1	0	-0.878622	-2.697520	-1.024192
11	6	0	3.770082	0.558399	-0.902224
12	6	0	4.134679	-0.771905	-1.221109
13	7	0	2.988563	-1.505505	-1.398125
14	1	0	2.946657	-2.498467	-1.547498
15	1	0	-0.793382	1.886943	-0.855210
16	1	0	0.085634	1.351656	-2.288108
17	1	0	1.259809	1.788714	0.509462
18	1	0	1.626168	2.632636	-0.983709

19	6	0	4.764815	1.525379	-0.642701
20	6	0	6.085112	1.130307	-0.715149
21	6	0	6.434123	-0.204499	-1.050007
22	6	0	5.479768	-1.159409	-1.308843
23	1	0	4.480930	2.537155	-0.391861
24	1	0	5.761941	-2.173621	-1.560897
25	1	0	7.488353	-0.442580	-1.095152
26	8	0	7.151873	1.942906	-0.485373
27	6	0	6.873999	3.282488	-0.124041
28	1	0	6.332327	3.799337	-0.920635
29	1	0	6.291395	3.326020	0.799962
30	1	0	7.837906	3.759441	0.029461
31	6	0	-2.668979	-2.398482	0.779627
32	6	0	-3.632275	-1.901043	-0.245446
33	6	0	-1.596855	-1.479181	1.090266
34	6	0	-1.544887	-0.218724	0.459873
35	6	0	-3.601000	-0.585661	-0.690383
36	8	0	-2.719254	0.323456	-0.078108
37	8	0	-2.765260	-3.533359	1.231474
38	6	0	-0.391187	-1.987835	1.660818
39	6	0	0.774893	-1.304979	1.771948
40	1	0	-1.012259	0.578046	0.963098
41	1	0	-0.387327	-3.051978	1.876387
42	6	0	2.035742	-2.021395	1.960716
43	8	0	2.185329	-3.227653	1.923284
44	1	0	0.851782	-0.232627	1.655836
45	8	0	3.066708	-1.160736	2.090486
46	6	0	4.356817	-1.770764	2.159949
47	1	0	4.455385	-2.342045	3.082032
48	1	0	4.505747	-2.436239	1.311238
49	1	0	5.070653	-0.952495	2.129431
50	6	0	-4.550972	-2.771968	-0.832416
51	6	0	-5.400469	-2.325532	-1.833861
52	6	0	-5.332518	-1.000587	-2.267080
53	6	0	-4.425149	-0.114303	-1.698231
54	1	0	-4.566358	-3.792682	-0.473736
55	1	0	-6.113777	-3.003929	-2.282720
56	1	0	-5.989214	-0.650294	-3.052130
57	1	0	-4.369114	0.916354	-2.018094
58	30	0	-3.321390	2.164442	0.629035
59	17	0	-1.585768	3.025574	1.584543
60	17	0	-5.312833	2.698508	0.063821

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trans-exo-IM1-III

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.664942 a.u.

Enthalpy H = -4189.630607 a.u.

Entropy S = 217.434 cal/mol/K

Gibbs free energy G = -4189.733917 a.u.

Total free energy in solution E_{sol} = -4190.86620 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.367896	-0.151287	0.941117
2	7	0	0.206320	-0.165734	0.053463
3	6	0	0.978220	0.186674	1.057276
4	6	0	0.524022	0.932694	2.274018
5	6	0	2.982432	-0.441511	-0.265541
6	6	0	0.760887	-1.007329	-1.038700
7	6	0	2.138221	-0.544936	-1.490073
8	1	0	0.027937	1.858478	1.985165
9	1	0	1.387576	1.181570	2.885517
10	1	0	-0.182983	0.348169	2.862572
11	6	0	4.377144	-0.500259	-0.027428
12	6	0	4.555796	-0.260559	1.356032

13	7	0	3.333556	-0.018483	1.921791
14	1	0	3.165024	0.056419	2.909595
15	1	0	0.046662	-0.986421	-1.858392
16	1	0	0.820704	-2.026887	-0.648216
17	1	0	2.082576	0.418710	-2.007463
18	1	0	2.533324	-1.275035	-2.197869
19	6	0	5.489962	-0.744557	-0.864085
20	6	0	6.738522	-0.756043	-0.281998
21	6	0	6.899430	-0.532001	1.114646
22	6	0	5.832789	-0.287480	1.941661
23	1	0	5.346295	-0.915110	-1.921009
24	1	0	5.976533	-0.112722	2.999667
25	1	0	7.908932	-0.558194	1.502167
26	8	0	7.902378	-0.972648	-0.943656
27	6	0	7.820352	-1.182385	-2.342512
28	1	0	7.230946	-2.074469	-2.569340
29	1	0	7.380535	-0.314840	-2.840892
30	1	0	8.841238	-1.322779	-2.685293
31	6	0	-2.508825	0.638374	1.920817
32	6	0	-2.510504	-0.858337	2.052167
33	6	0	-1.921778	1.129045	0.720807
34	6	0	-1.250940	0.197568	-0.182553
35	6	0	-2.199253	-1.678805	0.976453
36	8	0	-1.901526	-1.094752	-0.267478
37	8	0	-2.936804	1.325293	2.852835
38	6	0	-1.779112	2.528774	0.501381
39	6	0	-0.964411	3.132834	-0.402256
40	1	0	-1.243378	0.574140	-1.204932
41	1	0	-2.358550	3.152753	1.173295
42	6	0	-0.863591	4.580006	-0.563645
43	8	0	-0.108050	5.133174	-1.337954
44	1	0	-0.316332	2.584076	-1.075970
45	8	0	-1.691875	5.273705	0.253320
46	6	0	-1.598089	6.691215	0.119232
47	1	0	-0.589931	7.031233	0.352613
48	1	0	-1.843857	6.994569	-0.897246
49	1	0	-2.314426	7.100988	0.825693
50	6	0	-2.836247	-1.466575	3.263113
51	6	0	-2.847411	-2.851510	3.376341
52	6	0	-2.536470	-3.646238	2.273394
53	6	0	-2.206029	-3.060272	1.054952
54	1	0	-3.095354	-0.815841	4.088297
55	1	0	-3.109470	-3.316259	4.317680
56	1	0	-2.554385	-4.724911	2.356649
57	1	0	-1.975490	-3.655223	0.180158
58	30	0	-3.279357	-1.247397	-1.764680
59	17	0	-2.128097	-0.590417	-3.477507
60	17	0	-5.067997	-2.238509	-1.156792

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trans-exo-TS2-III

Imaginary frequency: -39.9693 cm^{-1}

Standard orientation:

Electronic energy E = -4189.65906 a.u.

Enthalpy H = -4189.62463 a.u.

Entropy S = 216.278 cal/mol/K

Gibbs free energy G = -4189.72739 a.u.

Total free energy in solution E_{sol}= -4190.85315 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.006023	0.427784	1.057665
2	7	0	-0.272686	-0.084086	0.697920
3	6	0	0.652917	0.858413	0.925704
4	6	0	0.287563	2.246631	1.354747
5	6	0	2.465677	-0.811920	0.643926
6	6	0	0.145055	-1.499464	0.834721

7	6	0	1.478272	-1.825654	0.164471
8	1	0	0.938689	2.985886	0.889129
9	1	0	0.419183	2.276265	2.442386
10	1	0	-0.745948	2.492096	1.143631
11	6	0	3.877733	-0.788045	0.744200
12	6	0	4.225053	0.493616	1.237761
13	7	0	3.077010	1.214673	1.426947
14	1	0	3.033847	2.178752	1.705308
15	1	0	-0.656978	-2.115434	0.437746
16	1	0	0.232002	-1.686150	1.907099
17	1	0	1.396178	-1.810314	-0.927690
18	1	0	1.765914	-2.839994	0.447756
19	6	0	4.881074	-1.742173	0.463858
20	6	0	6.192127	-1.379881	0.683919
21	6	0	6.523500	-0.091150	1.184106
22	6	0	5.563034	0.848260	1.466892
23	1	0	4.608952	-2.714840	0.080996
24	1	0	5.834509	1.825570	1.843655
25	1	0	7.573226	0.123524	1.332381
26	8	0	7.267856	-2.179567	0.459008
27	6	0	7.010833	-3.468106	-0.066960
28	1	0	6.400817	-4.057955	0.622493
29	1	0	6.507255	-3.401171	-1.034761
30	1	0	7.980517	-3.941633	-0.191473
31	6	0	-2.650073	2.284693	-0.430812
32	6	0	-3.469734	1.692850	0.673298
33	6	0	-1.564483	1.454736	-0.882773
34	6	0	-1.374907	0.102734	-0.336586
35	6	0	-3.360508	0.350084	1.009054
36	8	0	-2.570690	-0.489836	0.203490
37	8	0	-2.856852	3.437272	-0.803230
38	6	0	-0.454437	2.054187	-1.493045
39	6	0	0.763869	1.441152	-1.669852
40	1	0	-1.069063	-0.593600	-1.117961
41	1	0	-0.544159	3.118107	-1.686173
42	6	0	2.003054	2.145380	-1.956315
43	8	0	3.080824	1.606516	-2.117610
44	1	0	0.883151	0.367279	-1.648889
45	8	0	1.867134	3.497239	-1.948107
46	6	0	3.070730	4.208527	-2.239935
47	1	0	3.837840	3.980650	-1.500547
48	1	0	3.445147	3.935040	-3.225044
49	1	0	2.805391	5.261506	-2.209447
50	6	0	-4.315647	2.494598	1.438327
51	6	0	-5.022084	1.952758	2.504045
52	6	0	-4.886141	0.600593	2.817568
53	6	0	-4.046809	-0.217303	2.067453
54	1	0	-4.395887	3.537867	1.162484
55	1	0	-5.681680	2.578083	3.091059
56	1	0	-5.438613	0.175229	3.644884
57	1	0	-3.944127	-1.272729	2.281171
58	30	0	-3.460918	-1.995762	-0.844597
59	17	0	-1.839885	-2.971309	-1.896653
60	17	0	-5.531009	-2.229637	-0.370841

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trans-exo-IM2-III

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.704039 a.u.

Enthalpy H = -4189.670446 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 210.230 cal/mol/K

Gibbs free energy G = -4189.770333 a.u.

Total free energy in solution E_{sol}= -4190.88746 a.u.

1	6	0	-1.744516	1.166996	-0.548269
2	7	0	0.625270	0.712579	-0.971045
3	6	0	-0.386940	1.791064	-0.781469
4	6	0	-0.360326	2.658836	-2.047853
5	6	0	-2.046564	-0.168855	-0.628733
6	6	0	0.099061	-0.429078	-1.739082
7	6	0	-1.028408	-1.179793	-1.028359
8	1	0	-1.167764	3.392525	-2.035015
9	1	0	-0.497324	2.035243	-2.929657
10	1	0	0.603114	3.164618	-2.122386
11	6	0	-3.435013	-0.307588	-0.301503
12	6	0	-3.914376	0.990821	-0.038184
13	7	0	-2.869416	1.875136	-0.203735
14	1	0	-2.873793	2.860340	0.020395
15	1	0	0.929868	-1.084020	-1.994880
16	1	0	-0.293164	-0.036239	-2.676130
17	1	0	-0.672161	-1.718282	-0.133690
18	1	0	-1.434205	-1.949500	-1.688678
19	6	0	-4.298797	-1.414608	-0.214777
20	6	0	-5.616340	-1.183034	0.139164
21	6	0	-6.083407	0.125015	0.403262
22	6	0	-5.248167	1.217799	0.317928
23	1	0	-3.926880	-2.409432	-0.414993
24	1	0	-5.616757	2.215085	0.521524
25	1	0	-7.123972	0.236745	0.676211
26	8	0	-6.564139	-2.157194	0.264089
27	6	0	-6.147857	-3.488460	0.038369
28	1	0	-5.786515	-3.621009	-0.985371
29	1	0	-5.361271	-3.779801	0.739946
30	1	0	-7.025239	-4.110359	0.196540
31	6	0	3.505999	1.407357	1.033343
32	6	0	4.183605	0.306827	0.316975
33	6	0	2.040931	1.466338	0.809933
34	6	0	1.254740	0.305804	0.278068
35	6	0	3.442541	-0.728783	-0.246002
36	8	0	2.081324	-0.856896	0.028675
37	8	0	4.108350	2.266011	1.646681
38	6	0	1.408776	2.635342	0.869206
39	6	0	-0.037379	2.688890	0.491243
40	1	0	0.540728	-0.057953	1.028661
41	1	0	1.939550	3.523678	1.183568
42	6	0	-0.545573	4.106334	0.286637
43	8	0	-1.713674	4.427941	0.345578
44	1	0	-0.626430	2.286657	1.322236
45	8	0	0.424466	4.972076	0.006925
46	6	0	-0.012104	6.321249	-0.238227
47	1	0	-0.673005	6.341074	-1.102289
48	1	0	-0.540011	6.703306	0.632311
49	1	0	0.894327	6.886221	-0.426532
50	6	0	5.564312	0.338277	0.115808
51	6	0	6.184944	-0.647447	-0.636162
52	6	0	5.418217	-1.665839	-1.201994
53	6	0	4.039907	-1.715836	-1.015431
54	1	0	6.117107	1.155250	0.560762
55	1	0	7.255190	-0.623529	-0.789796
56	1	0	5.892551	-2.433195	-1.799657
57	1	0	3.442272	-2.503720	-1.454753
58	30	0	1.192902	-2.672343	0.469233
59	17	0	0.574772	-2.478530	2.522913
60	17	0	1.296495	-4.063748	-1.177077

trans-COM-IV

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -3501.484084 a.u.

Enthalpy H = -3501.462982 a.u.

Entropy S = 158.706 cal/mol/K

Gibbs free energy G = -3501.538388 a.u.

Total free energy in solution E_{sol}= -4190.85265 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.402644	-1.941182	0.205145
2	17	0	-1.304249	-1.600542	2.338815
3	17	0	-2.558392	-3.056065	-1.238307
4	6	0	-0.192990	0.611328	-0.425465
5	6	0	-1.420935	1.385363	-0.367353
6	6	0	1.040837	1.343887	-0.256183
7	6	0	0.971963	2.678467	-0.014607
8	6	0	-1.355130	2.748824	-0.071489
9	8	0	-0.156878	3.376051	0.101876
10	8	0	-0.182639	-0.624385	-0.622286
11	6	0	2.318274	0.627972	-0.340733
12	6	0	3.430152	0.994089	0.302418
13	1	0	1.842899	3.307399	0.103097
14	1	0	2.324343	-0.260771	-0.958687
15	6	0	4.719636	0.276441	0.166932
16	8	0	5.730440	0.624389	0.730166
17	1	0	3.468692	1.832322	0.986872
18	8	0	4.645671	-0.791122	-0.640906
19	6	0	5.873709	-1.518942	-0.778316
20	1	0	6.644318	-0.875527	-1.198400
21	1	0	6.201287	-1.884140	0.192872
22	1	0	5.649458	-2.343660	-1.447060
23	6	0	-2.682937	0.805280	-0.587359
24	6	0	-3.823788	1.570926	-0.480779
25	6	0	-3.729157	2.933705	-0.154267
26	6	0	-2.500702	3.533624	0.045081
27	1	0	-2.751378	-0.234530	-0.883846
28	1	0	-4.791736	1.121606	-0.653855
29	1	0	-4.629799	3.526800	-0.066344
30	1	0	-2.400226	4.583025	0.284291

trans-endo-TS1-IV

Imaginary frequency: -232.2591 cm^{-1}

Standard orientation:

Electronic energy E = -4189.697289 a.u.

Enthalpy H = -4189.662800 a.u.

Entropy S = 213.613 cal/mol/K

Gibbs free energy G = -4189.764294 a.u.

Total free energy in solution E_{sol}= -4190.87613 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.920310	2.395856	-1.041138
2	7	0	-1.452879	2.380420	-0.930894
3	6	0	-0.333066	2.978412	-0.633117
4	6	0	-0.329835	4.288283	0.103117
5	6	0	1.008556	1.092912	-1.486318
6	6	0	-1.390791	1.296542	-1.927493
7	6	0	-0.224738	0.311909	-1.790391
8	1	0	0.402797	4.298405	0.911228
9	1	0	-1.318661	4.532532	0.487176
10	1	0	-0.060167	5.069173	-0.614741
11	6	0	2.380356	0.727594	-1.435883
12	6	0	3.083813	1.868251	-0.984715
13	7	0	2.184605	2.888193	-0.774526
14	1	0	2.372403	3.667071	-0.165072
15	1	0	-1.303545	1.800775	-2.894274
16	1	0	-2.346479	0.777012	-1.919464

17	1	0	-0.128324	-0.245395	-2.724788
18	1	0	-0.398459	-0.441562	-1.019527
19	6	0	3.052671	-0.484660	-1.693099
20	6	0	4.416518	-0.516224	-1.483021
21	6	0	5.117701	0.642797	-1.054879
22	6	0	4.475078	1.834634	-0.806658
23	8	0	5.194664	-1.615543	-1.653296
24	6	0	4.526034	-2.819256	-2.001199
25	1	0	2.491448	-1.353851	-2.005054
26	1	0	6.187328	0.550212	-0.920375
27	1	0	5.024175	2.704362	-0.469711
28	1	0	4.048006	-2.730215	-2.979979
29	1	0	5.293701	-3.587182	-2.037877
30	1	0	3.771462	-3.079679	-1.255153
31	6	0	-2.587782	-0.543063	0.535293
32	6	0	-3.895342	-0.477058	-0.119256
33	6	0	-2.034785	0.673849	0.983561
34	6	0	-2.622128	1.895665	0.549720
35	6	0	-4.486587	0.766736	-0.338987
36	8	0	-3.867668	1.929958	0.044083
37	8	0	-2.033174	-1.677341	0.664614
38	6	0	-0.736767	0.694252	1.611746
39	6	0	-0.102714	1.784500	2.075838
40	1	0	-2.416683	2.810101	1.081819
41	1	0	-0.197829	-0.244060	1.643610
42	6	0	1.344802	1.794289	2.348799
43	8	0	2.001432	2.821050	2.368154
44	1	0	-0.574460	2.752561	2.155455
45	8	0	1.856311	0.575381	2.493191
46	6	0	3.280317	0.491742	2.632939
47	1	0	3.762852	0.849800	1.724944
48	1	0	3.606112	1.086161	3.484270
49	1	0	3.485014	-0.562138	2.789643
50	6	0	-4.568278	-1.628266	-0.545472
51	6	0	-5.804156	-1.524451	-1.158668
52	6	0	-6.381105	-0.265123	-1.359048
53	6	0	-5.726429	0.888506	-0.954471
54	1	0	-4.093533	-2.585360	-0.379530
55	1	0	-6.323813	-2.415104	-1.484700
56	1	0	-7.347693	-0.185001	-1.839056
57	1	0	-6.147014	1.873290	-1.104101
58	30	0	-0.309032	-2.538152	0.777743
59	17	0	0.583956	-2.741950	2.745106
60	17	0	0.407679	-3.220253	-1.177827

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trans-endo-IM1-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.703272 a.u.

Enthalpy H = -4189.668848 a.u.

Entropy S = 211.812 cal/mol/K

Gibbs free energy G = -4189.769486 a.u.

Total free energy in solution E_{sol} = -4190.88710 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.982916	-2.505748	-0.720552
2	7	0	1.358564	-2.355235	-0.510083
3	6	0	0.233787	-2.959998	-0.143088
4	6	0	0.215562	-4.144417	0.778623
5	6	0	-1.072515	-1.292143	-1.390102
6	6	0	1.326741	-1.550169	-1.749845
7	6	0	0.152958	-0.576118	-1.841407
8	1	0	-0.551235	-4.036825	1.546268
9	1	0	1.179591	-4.334774	1.242422
10	1	0	-0.027844	-5.014071	0.160188

11	6	0	-2.438147	-0.926592	-1.405710
12	6	0	-3.142217	-1.972537	-0.762162
13	7	0	-2.254058	-2.949973	-0.383344
14	1	0	-2.436382	-3.549862	0.406608
15	1	0	1.250836	-2.275067	-2.562990
16	1	0	2.279981	-1.038987	-1.840462
17	1	0	0.061085	-0.251975	-2.880894
18	1	0	0.301313	0.332316	-1.255788
19	6	0	-3.102908	0.233467	-1.858002
20	6	0	-4.460793	0.312846	-1.638096
21	6	0	-5.164709	-0.757084	-1.015141
22	6	0	-4.532163	-1.896135	-0.576179
23	8	0	-5.233985	1.375123	-1.967541
24	6	0	-4.560463	2.517731	-2.480136
25	1	0	-2.535231	1.037539	-2.303101
26	1	0	-6.231461	-0.630538	-0.884691
27	1	0	-5.083392	-2.689985	-0.089793
28	1	0	-4.098288	2.294606	-3.444948
29	1	0	-5.323231	3.280158	-2.608158
30	1	0	-3.795461	2.865423	-1.782179
31	6	0	2.618567	0.557376	0.405718
32	6	0	3.885545	0.315799	-0.301712
33	6	0	1.977509	-0.548285	0.961276
34	6	0	2.380142	-1.927436	0.544228
35	6	0	4.359282	-0.990489	-0.441457
36	8	0	3.668927	-2.078239	0.028161
37	8	0	2.204198	1.766392	0.480732
38	6	0	0.737871	-0.409460	1.651852
39	6	0	0.054780	-1.414127	2.248693
40	1	0	2.290926	-2.653884	1.344562
41	1	0	0.257923	0.561762	1.636774
42	6	0	-1.379547	-1.346423	2.529345
43	8	0	-2.072822	-2.345240	2.662916
44	1	0	0.493912	-2.380695	2.434354
45	8	0	-1.865898	-0.105231	2.535454
46	6	0	-3.286706	0.016699	2.668820
47	1	0	-3.779879	-0.414368	1.798192
48	1	0	-3.622608	-0.492301	3.569951
49	1	0	-3.474970	1.083564	2.729301
50	6	0	4.642370	1.368909	-0.822975
51	6	0	5.849468	1.121407	-1.458007
52	6	0	6.309669	-0.191152	-1.578622
53	6	0	5.567817	-1.252254	-1.075331
54	1	0	4.257367	2.372511	-0.706832
55	1	0	6.432112	1.941146	-1.855858
56	1	0	7.252297	-0.391011	-2.071619
57	1	0	5.901738	-2.277169	-1.161999
58	30	0	0.522008	2.666611	0.647197
59	17	0	-0.161773	3.306381	2.606762
60	17	0	-0.492824	2.940452	-1.293772

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trans-endo-TS2-IV Imaginary frequency: -280.7259 cm^{-1}

Standard orientation: Electronic energy E = -4189.696145 a.u.

Enthalpy H = -4189.662511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 209.451 cal/mol/K

Gibbs free energy G = -4189.762028 a.u.

Total free energy in solution E_{sol}= -4190.87591 a.u.

1	6	0	1.093476	2.164783	-0.673129
2	7	0	-1.286020	2.277549	-0.765212
3	6	0	-0.136616	2.750563	-0.176000
4	6	0	-0.124065	4.191166	0.280896
5	6	0	1.156625	0.956265	-1.327952
6	6	0	-1.167386	1.356942	-1.918905
7	6	0	-0.087444	0.280961	-1.803896
8	1	0	0.618461	4.353826	1.061423
9	1	0	-1.101526	4.499653	0.649797
10	1	0	0.113473	4.811221	-0.587492
11	6	0	2.529772	0.588100	-1.390324
12	6	0	3.256422	1.634299	-0.777998
13	7	0	2.366873	2.602579	-0.365135
14	1	0	2.572976	3.291986	0.340561
15	1	0	-0.931882	1.989999	-2.776623
16	1	0	-2.149254	0.924482	-2.094693
17	1	0	0.060901	-0.164972	-2.790546
18	1	0	-0.374896	-0.539143	-1.144346
19	6	0	3.189664	-0.556562	-1.877967
20	6	0	4.561197	-0.619602	-1.729606
21	6	0	5.283571	0.448655	-1.138563
22	6	0	4.652537	1.577187	-0.664518
23	8	0	5.328498	-1.674837	-2.113118
24	6	0	4.643697	-2.814249	-2.605668
25	1	0	2.615124	-1.365166	-2.305994
26	1	0	6.357083	0.337881	-1.063204
27	1	0	5.217370	2.381261	-0.209884
28	1	0	4.123421	-2.585026	-3.539450
29	1	0	5.406309	-3.565954	-2.789996
30	1	0	3.924537	-3.186130	-1.871598
31	6	0	-2.683580	-0.507081	0.425371
32	6	0	-3.887557	-0.383052	-0.389775
33	6	0	-2.068461	0.711497	0.844861
34	6	0	-2.416782	2.003822	0.174044
35	6	0	-4.314551	0.886628	-0.800209
36	8	0	-3.643229	2.035473	-0.514315
37	8	0	-2.252476	-1.653543	0.721858
38	6	0	-0.898578	0.710104	1.572684
39	6	0	-0.209230	1.899747	1.839745
40	1	0	-2.449295	2.840343	0.867681
41	1	0	-0.423252	-0.227121	1.832397
42	6	0	1.185386	1.870097	2.302916
43	8	0	1.817456	2.863906	2.619865
44	1	0	-0.749515	2.788690	2.129388
45	8	0	1.708833	0.644516	2.246576
46	6	0	3.074278	0.514373	2.664685
47	1	0	3.727394	1.006474	1.946086
48	1	0	3.204743	0.956316	3.649920
49	1	0	3.263887	-0.553541	2.686566
50	6	0	-4.627147	-1.513149	-0.766231
51	6	0	-5.777887	-1.378813	-1.519356
52	6	0	-6.197424	-0.102032	-1.909560
53	6	0	-5.473927	1.027528	-1.559279
54	1	0	-4.269594	-2.481369	-0.443696
55	1	0	-6.349193	-2.251264	-1.804803
56	1	0	-7.098285	0.011207	-2.499125
57	1	0	-5.778810	2.019669	-1.861958
58	30	0	-0.534846	-2.498868	1.099398
59	17	0	0.075117	-2.576682	3.179247
60	17	0	0.391978	-3.211633	-0.743627

trans-endo-IM2-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.713892 a.u.

Enthalpy H = -4189.680353 a.u.

Entropy S = 209.369 cal/mol/K

Gibbs free energy G = -4189.779831 a.u.

Total free energy in solution E_{sol}= -4190.89503 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.117119	1.871844	-0.888328
2	7	0	-1.270449	2.255922	-1.241304
3	6	0	-0.069797	2.703075	-0.482133
4	6	0	0.126200	4.199451	-0.730258
5	6	0	1.069416	0.613449	-1.425414
6	6	0	-1.048836	1.313133	-2.350724
7	6	0	-0.196053	0.084497	-2.018561
8	1	0	0.940524	4.610686	-0.134733
9	1	0	-0.792829	4.727115	-0.468411
10	1	0	0.322414	4.360174	-1.790467
11	6	0	2.416318	0.117745	-1.444245
12	6	0	3.233384	1.141554	-0.924107
13	7	0	2.420942	2.211419	-0.602778
14	1	0	2.716936	3.054065	-0.139958
15	1	0	-0.541318	1.872280	-3.138872
16	1	0	-2.029834	1.040141	-2.734402
17	1	0	0.016472	-0.462755	-2.941202
18	1	0	-0.717227	-0.618943	-1.363964
19	6	0	2.981614	-1.104538	-1.845055
20	6	0	4.348746	-1.264991	-1.703577
21	6	0	5.159185	-0.223799	-1.195887
22	6	0	4.618200	0.983047	-0.805227
23	8	0	5.023322	-2.406901	-2.021331
24	6	0	4.242110	-3.511323	-2.437653
25	1	0	2.343461	-1.896533	-2.207919
26	1	0	6.221169	-0.412363	-1.115027
27	1	0	5.248665	1.773538	-0.416917
28	1	0	3.727325	-3.296868	-3.378490
29	1	0	4.937806	-4.333333	-2.585197
30	1	0	3.505577	-3.780657	-1.675796
31	6	0	-2.642879	-0.473880	0.629552
32	6	0	-3.850473	-0.577817	-0.158091
33	6	0	-1.972763	0.818249	0.589837
34	6	0	-2.378685	1.911538	-0.363154
35	6	0	-4.223560	0.484346	-1.001167
36	8	0	-3.536882	1.638635	-1.138308
37	8	0	-2.203621	-1.440682	1.286168
38	6	0	-0.894224	1.113157	1.326166
39	6	0	-0.254669	2.444116	1.090621
40	1	0	-2.622577	2.810315	0.209828
41	1	0	-0.481847	0.436743	2.063958
42	6	0	1.078958	2.589077	1.808370
43	8	0	1.658961	3.643512	1.946698
44	1	0	-0.897455	3.246281	1.473945
45	8	0	1.539630	1.420909	2.234750
46	6	0	2.824789	1.430598	2.876800
47	1	0	3.591548	1.665992	2.140605
48	1	0	2.833227	2.168489	3.675561
49	1	0	2.952965	0.425218	3.262375
50	6	0	-4.626007	-1.751696	-0.129452
51	6	0	-5.759462	-1.861138	-0.903704
52	6	0	-6.124441	-0.790943	-1.734938
53	6	0	-5.370161	0.366702	-1.791567
54	1	0	-4.299887	-2.554524	0.517783
55	1	0	-6.358424	-2.760640	-0.877848

56	1	0	-7.011601	-0.869676	-2.350505
57	1	0	-5.637886	1.193652	-2.434448
58	30	0	-0.350398	-2.051185	1.616044
59	17	0	0.419419	-1.614835	3.593000
60	17	0	0.275630	-3.134032	-0.155063

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trans-exo-TS1-IV

Imaginary frequency: -230.4263 cm^{-1}

Standard orientation:

Electronic energy E = -4189.695916 a.u.

Enthalpy H = -4189.660997 a.u.

Entropy S = 208.601 cal/mol/K

Gibbs free energy G = -4189.764464 a.u.

Total free energy in solution E_{sol}= -4190.87618 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.176376	-1.610573	1.185168
2	7	0	-0.563292	-2.639269	-0.051550
3	6	0	-0.211435	-1.879750	0.944594
4	6	0	-1.237473	-1.228242	1.813529
5	6	0	2.170251	-1.980963	0.301536
6	6	0	0.467268	-3.483140	-0.671293
7	6	0	1.859034	-2.851956	-0.867990
8	1	0	-1.258275	-0.145679	1.670761
9	1	0	-0.956193	-1.410569	2.854728
10	1	0	-2.222436	-1.654724	1.645240
11	6	0	3.332606	-1.244966	0.658211
12	6	0	2.977295	-0.451578	1.774358
13	7	0	1.671810	-0.712047	2.111459
14	1	0	1.093157	-0.043484	2.600052
15	1	0	0.075502	-3.853313	-1.620018
16	1	0	0.573774	-4.347814	-0.010852
17	1	0	1.942650	-2.259543	-1.782440
18	1	0	2.575002	-3.672134	-0.961231
19	6	0	4.624838	-1.160507	0.097007
20	6	0	5.516078	-0.277098	0.669367
21	6	0	5.145984	0.514666	1.790588
22	6	0	3.893467	0.441928	2.350881
23	1	0	4.875155	-1.754118	-0.769709
24	1	0	3.621432	1.061283	3.195151
25	1	0	5.893509	1.189986	2.184799
26	8	0	6.788192	-0.069718	0.235641
27	6	0	7.184935	-0.764032	-0.932744
28	1	0	7.168645	-1.845195	-0.770615
29	1	0	6.535274	-0.511729	-1.774992
30	1	0	8.201484	-0.443308	-1.143009
31	6	0	-2.947023	0.070024	-0.424125
32	6	0	-4.085594	-0.769461	-0.041706
33	6	0	-1.895773	-0.556458	-1.100567
34	6	0	-1.895883	-1.981711	-1.238989
35	6	0	-4.067758	-2.129533	-0.348597
36	8	0	-3.020631	-2.694009	-1.031709
37	8	0	-2.989110	1.309932	-0.124652
38	6	0	-0.677270	0.164478	-1.399783
39	6	0	0.323050	-0.227148	-2.203283
40	1	0	-1.339666	-2.418769	-2.057501
41	1	0	-0.497410	1.067439	-0.831060
42	6	0	1.639335	0.440097	-2.188358
43	8	0	2.629644	-0.032213	-2.708873
44	1	0	0.270615	-1.099866	-2.841459
45	8	0	1.636423	1.580653	-1.491408
46	6	0	2.919654	2.188251	-1.288853
47	1	0	3.589159	1.483287	-0.798345
48	1	0	3.342812	2.491659	-2.244658
49	1	0	2.729817	3.048280	-0.654976

50	6	0	-5.192822	-0.248473	0.637910
51	6	0	-6.245741	-1.074232	0.991825
52	6	0	-6.204453	-2.435668	0.671794
53	6	0	-5.116225	-2.972647	0.000883
54	1	0	-5.195860	0.808065	0.867707
55	1	0	-7.101021	-0.667482	1.514198
56	1	0	-7.028009	-3.080585	0.949141
57	1	0	-5.059300	-4.020407	-0.260266
58	30	0	-1.733387	2.723716	0.185916
59	17	0	-2.074039	4.595754	-0.840967
60	17	0	-0.200096	2.234920	1.718751

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trans-exo-IM1-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.705774 a.u.

Enthalpy H = -4189.670623 a.u.

Entropy S = 221.782 cal/mol/K

Gibbs free energy G = -4189.775999 a.u.

Total free energy in solution E_{sol}= -4190.89565 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.031779	-1.507278	-0.286604
2	7	0	-0.283267	-1.522219	1.273597
3	6	0	-0.645799	-1.659011	0.016489
4	6	0	0.312395	-1.934136	-1.088978
5	6	0	-2.959104	-0.985336	0.601480
6	6	0	-1.328360	-1.532920	2.323416
7	6	0	-2.533125	-0.654808	1.992519
8	1	0	0.640159	-0.988699	-1.537957
9	1	0	-0.194621	-2.517575	-1.857927
10	1	0	1.177022	-2.497946	-0.758189
11	6	0	-4.161131	-0.784556	-0.115681
12	6	0	-3.911157	-1.213293	-1.442501
13	7	0	-2.620035	-1.651168	-1.528010
14	1	0	-2.149264	-1.888972	-2.383296
15	1	0	-0.862950	-1.226215	3.256695
16	1	0	-1.657820	-2.570759	2.426402
17	1	0	-2.300879	0.412165	2.071473
18	1	0	-3.317457	-0.873815	2.719286
19	6	0	-5.428875	-0.274841	0.248872
20	6	0	-6.397986	-0.213068	-0.727040
21	6	0	-6.132102	-0.652699	-2.055614
22	6	0	-4.910900	-1.151483	-2.428910
23	1	0	-5.607933	0.056775	1.261111
24	1	0	-4.726573	-1.474758	-3.444702
25	1	0	-6.941359	-0.572761	-2.768904
26	8	0	-7.658493	0.253073	-0.543324
27	6	0	-7.980885	0.748598	0.743930
28	1	0	-7.902421	-0.040069	1.496846
29	1	0	-7.326973	1.581137	1.015216
30	1	0	-9.008674	1.094441	0.683847
31	6	0	2.974462	-0.624712	0.176067
32	6	0	3.485259	-2.003800	0.171614
33	6	0	1.898145	-0.342707	1.000329
34	6	0	1.169314	-1.421295	1.723445
35	6	0	2.848019	-2.977572	0.941214
36	8	0	1.722249	-2.713293	1.679838
37	8	0	3.585810	0.236540	-0.558098
38	6	0	1.481017	1.007301	1.223974
39	6	0	0.440158	1.431547	1.969654
40	1	0	1.061489	-1.159398	2.777728
41	1	0	2.105932	1.791899	0.808195
42	6	0	0.072707	2.845409	2.102164

43	8	0	-0.922686	3.227461	2.685195
44	1	0	-0.226913	0.765847	2.493510
45	8	0	0.934791	3.664078	1.484102
46	6	0	0.604034	5.055172	1.511433
47	1	0	-0.372186	5.215870	1.057551
48	1	0	0.586452	5.415128	2.538994
49	1	0	1.384723	5.543516	0.937277
50	6	0	4.610150	-2.363086	-0.575149
51	6	0	5.091312	-3.663180	-0.543684
52	6	0	4.442006	-4.620930	0.237021
53	6	0	3.316897	-4.285581	0.979652
54	1	0	5.088495	-1.592408	-1.163784
55	1	0	5.966194	-3.932791	-1.119730
56	1	0	4.813337	-5.637228	0.268148
57	1	0	2.796919	-5.011031	1.590424
58	30	0	2.738847	1.775270	-1.332602
59	17	0	3.617396	3.741773	-1.037212
60	17	0	0.964463	1.222343	-2.538412

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trans-exo-TS2-IV

Imaginary frequency: -283.0278 cm^{-1}

Standard orientation:

Electronic energy E = -4189.687524 a.u.

Enthalpy H = -4189.653351 a.u.

Entropy S = 215.898 cal/mol/K

Gibbs free energy G = -4189.755930 a.u.

Total free energy in solution E_{sol}= -4190.86742 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.224705	0.279049	-0.006487
2	7	0	-0.445873	1.718438	-0.654473
3	6	0	-0.792642	0.558941	-0.020786
4	6	0	-0.037907	0.141170	1.214766
5	6	0	-3.177805	1.241573	-0.233217
6	6	0	-1.468537	2.402676	-1.470201
7	6	0	-2.763669	2.595268	-0.697862
8	1	0	1.024473	0.350570	1.167344
9	1	0	-0.182307	-0.915782	1.429216
10	1	0	-0.458238	0.723171	2.039664
11	6	0	-4.443643	0.661925	0.091135
12	6	0	-4.175434	-0.668681	0.491115
13	7	0	-2.808558	-0.872568	0.486359
14	1	0	-2.408988	-1.783797	0.303527
15	1	0	-1.677128	1.816660	-2.375738
16	1	0	-1.031483	3.357147	-1.761249
17	1	0	-3.511742	3.036276	-1.359295
18	1	0	-2.611843	3.283514	0.139364
19	6	0	-5.760015	1.136321	0.059854
20	6	0	-6.784255	0.267373	0.397618
21	6	0	-6.508878	-1.067836	0.767448
22	6	0	-5.209191	-1.544435	0.816668
23	1	0	-6.003867	2.150760	-0.226583
24	1	0	-5.009467	-2.567575	1.106883
25	1	0	-7.316197	-1.738136	1.022853
26	8	0	-8.045782	0.784732	0.344666
27	6	0	-9.125904	-0.072468	0.659138
28	1	0	-9.170943	-0.922815	-0.026527
29	1	0	-9.058093	-0.436275	1.687842
30	1	0	-10.024965	0.528044	0.548229
31	6	0	3.095201	0.947717	-0.485767
32	6	0	3.394747	2.299117	-0.022747
33	6	0	1.832300	0.746808	-1.117385
34	6	0	0.888718	1.876029	-1.326634
35	6	0	2.501388	3.339043	-0.298918
36	8	0	1.384150	3.168473	-1.056473

37	8	0	3.926751	0.022774	-0.271144
38	6	0	1.351970	-0.535171	-1.280242
39	6	0	0.018950	-0.899266	-1.503279
40	1	0	0.619868	1.901167	-2.386435
41	1	0	2.024874	-1.346886	-1.042843
42	6	0	-0.372059	-2.287627	-1.206799
43	8	0	-1.498949	-2.732527	-1.340726
44	1	0	-0.644623	-0.371814	-2.174792
45	8	0	0.630282	-2.997638	-0.671621
46	6	0	0.340623	-4.360625	-0.331568
47	1	0	-0.379077	-4.393803	0.484922
48	1	0	-0.063979	-4.880492	-1.197017
49	1	0	1.292940	-4.783337	-0.029343
50	6	0	4.545992	2.563564	0.730657
51	6	0	4.805264	3.842347	1.187538
52	6	0	3.906276	4.872551	0.892237
53	6	0	2.758206	4.630332	0.153068
54	1	0	5.214467	1.739954	0.940203
55	1	0	5.693645	4.044710	1.769694
56	1	0	4.102762	5.876183	1.247215
57	1	0	2.053439	5.415441	-0.083220
58	30	0	3.669890	-1.783008	0.421914
59	17	0	4.174469	-3.439680	-0.879140
60	17	0	2.853134	-1.635286	2.438065

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trans-exo-IM2-IV

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.724077 a.u.

Enthalpy H = -4189.690179 a.u.

Entropy S = 214.004 cal/mol/K

Gibbs free energy G = -4189.791860 a.u.

Total free energy in solution E_{sol}= -4190.91087 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.897096	-0.004669	0.132657
2	7	0	-0.982231	1.325341	-0.344329
3	6	0	-1.392163	0.042299	0.263899
4	6	0	-0.966791	-0.077189	1.740223
5	6	0	-3.708681	1.026111	-0.257758
6	6	0	-1.793274	2.496779	0.012023
7	6	0	-3.184119	2.382283	-0.595563
8	1	0	0.115965	-0.168952	1.832076
9	1	0	-1.441535	-0.945111	2.202232
10	1	0	-1.290889	0.807225	2.287126
11	6	0	-5.054812	0.528572	-0.236248
12	6	0	-4.978380	-0.819681	0.183799
13	7	0	-3.653558	-1.117075	0.423129
14	1	0	-3.269146	-2.041113	0.557404
15	1	0	-1.270225	3.376181	-0.366598
16	1	0	-1.870084	2.606423	1.099274
17	1	0	-3.130807	2.529311	-1.678446
18	1	0	-3.827781	3.166350	-0.188137
19	6	0	-6.298618	1.095062	-0.529574
20	6	0	-7.435100	0.309333	-0.408676
21	6	0	-7.346875	-1.035628	0.003404
22	6	0	-6.119221	-1.608088	0.303945
23	1	0	-6.404251	2.122699	-0.852086
24	1	0	-6.059601	-2.640688	0.623765
25	1	0	-8.237717	-1.639773	0.092822
26	8	0	-8.618507	0.925148	-0.715457
27	6	0	-9.802648	0.165262	-0.597829
28	1	0	-9.792198	-0.696618	-1.271082
29	1	0	-9.955055	-0.179702	0.428855
30	1	0	-10.615336	0.830691	-0.878423

31	6	0	2.635316	0.619135	-0.911582
32	6	0	3.138531	1.730784	-0.121524
33	6	0	1.191748	0.421750	-0.856242
34	6	0	0.387874	1.604035	-0.435351
35	6	0	2.270181	2.381394	0.780233
36	8	0	0.947575	2.131085	0.825245
37	8	0	3.385628	-0.182456	-1.508659
38	6	0	0.662783	-0.793880	-0.996981
39	6	0	-0.742857	-1.113538	-0.584539
40	1	0	0.534556	2.419174	-1.153228
41	1	0	1.299818	-1.603115	-1.329544
42	6	0	-0.715162	-2.417604	0.219422
43	8	0	-1.677003	-3.119979	0.445261
44	1	0	-1.369329	-1.288820	-1.464147
45	8	0	0.500387	-2.681241	0.677974
46	6	0	0.635941	-3.847515	1.510549
47	1	0	0.020435	-3.730217	2.400408
48	1	0	0.320118	-4.730650	0.960035
49	1	0	1.690429	-3.888025	1.760257
50	6	0	4.510822	2.047818	-0.123318
51	6	0	5.013548	2.974436	0.763837
52	6	0	4.145125	3.589953	1.679023
53	6	0	2.791415	3.307023	1.689800
54	1	0	5.163149	1.572580	-0.847660
55	1	0	6.066101	3.220797	0.756664
56	1	0	4.538040	4.309347	2.386141
57	1	0	2.113485	3.783590	2.384321
58	30	0	4.933567	-1.001082	-0.587310
59	17	0	4.025102	-2.014661	1.108756
60	17	0	6.864652	-0.645506	-1.475523

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trans-COM-V

Standard orientation:

Imaginary frequency: none

Electronic energy E = -3501.466869 a.u.

Enthalpy H = -3501.446589 a.u.

Entropy S = 151.290 cal/mol/K

Gibbs free energy G = -3501.518472 a.u.

Total free energy in solution E_{sol}= -3502.20922 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.523841	-1.298561	-0.189402
2	6	0	-2.927693	-0.851459	-0.139630
3	6	0	-0.604458	-0.328394	-0.821642
4	6	0	-1.100781	0.819392	-1.361310
5	6	0	-3.298704	0.363279	-0.709165
6	8	0	-2.376587	1.175623	-1.333506
7	8	0	-1.148029	-2.371703	0.245085
8	6	0	0.806821	-0.687802	-0.847175
9	6	0	1.847988	0.063126	-1.291575
10	1	0	-0.498266	1.563327	-1.863285
11	1	0	1.016379	-1.661261	-0.412785
12	6	0	3.244078	-0.456933	-1.314744
13	8	0	4.124456	0.070601	-1.948866
14	1	0	1.727268	1.013517	-1.797898
15	8	0	3.398340	-1.544681	-0.556562
16	6	0	4.730648	-2.083302	-0.536270
17	1	0	5.018612	-2.394473	-1.538271
18	1	0	5.426793	-1.329608	-0.175186
19	1	0	4.687581	-2.929559	0.140454
20	6	0	-3.910915	-1.634724	0.474008
21	6	0	-5.222726	-1.197603	0.510778
22	6	0	-5.568904	0.029044	-0.069900
23	6	0	-4.611770	0.819456	-0.685501

24	1	0	-3.603867	-2.575044	0.912241
25	1	0	-5.982755	-1.800619	0.988799
26	1	0	-6.595716	0.368966	-0.038317
27	1	0	-4.851987	1.770646	-1.139795
28	30	0	1.311826	0.859739	0.867644
29	17	0	0.912842	2.925925	0.358003
30	17	0	1.508174	-0.442977	2.555801

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trans-endo-TS1-V

Imaginary frequency: -189.5696 cm^{-1}

Standard orientation:

Electronic energy E = -4189.680096 a.u.

Enthalpy H = -4189.644993 a.u.

Entropy S = 219.622 cal/mol/K

Gibbs free energy G = -4189.749342 a.u.

Total free energy in solution E_{sol}= -4190.87613 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.921799	0.516984	-1.859416
2	7	0	0.376870	1.107243	-1.954840
3	6	0	-0.576321	0.331356	-2.362919
4	6	0	-0.326866	-0.754540	-3.371389
5	6	0	-2.197638	1.300941	-0.762006
6	6	0	0.001732	2.303401	-1.181448
7	6	0	-1.114432	2.123502	-0.142561
8	1	0	-0.756784	-1.704215	-3.048522
9	1	0	0.733671	-0.876926	-3.580706
10	1	0	-0.812913	-0.461277	-4.306992
11	6	0	-3.544692	1.026588	-0.387616
12	6	0	-4.033241	0.075425	-1.313975
13	7	0	-3.040730	-0.202972	-2.222156
14	1	0	-3.023743	-1.033567	-2.790218
15	1	0	-0.330105	3.035897	-1.923714
16	1	0	0.903817	2.699790	-0.718475
17	1	0	-1.474205	3.115748	0.139314
18	1	0	-0.744851	1.653015	0.774066
19	6	0	-4.367585	1.488200	0.661133
20	6	0	-5.645763	0.974274	0.754109
21	6	0	-6.121092	0.018377	-0.180927
22	6	0	-5.336508	-0.433429	-1.216862
23	8	0	-6.550051	1.314428	1.712705
24	6	0	-6.137293	2.263350	2.677412
25	1	0	-3.988188	2.215699	1.364004
26	1	0	-7.132631	-0.341455	-0.049418
27	1	0	-5.712005	-1.163333	-1.922144
28	1	0	-5.885201	3.217203	2.206339
29	1	0	-6.982190	2.399525	3.346866
30	1	0	-5.276105	1.898390	3.243524
31	6	0	2.052207	1.091554	1.094165
32	6	0	3.152139	1.967257	0.632649
33	6	0	1.682978	0.037598	0.142001
34	6	0	2.043313	0.202514	-1.222015
35	6	0	3.603140	1.883567	-0.681733
36	8	0	3.054230	0.994826	-1.584169
37	8	0	1.505815	1.241757	2.176072
38	6	0	0.524199	-0.775836	0.486448
39	6	0	-0.004143	-1.750536	-0.286776
40	1	0	1.925346	-0.603979	-1.924543
41	1	0	0.059212	-0.528798	1.435318
42	6	0	-1.357446	-2.293249	-0.060715
43	8	0	-2.003197	-2.807232	-0.953100
44	1	0	0.453208	-2.079544	-1.209815

45	8	0	-1.816972	-2.097806	1.175244
46	6	0	-3.180171	-2.495872	1.389082
47	1	0	-3.843977	-1.895210	0.769190
48	1	0	-3.301741	-3.549007	1.145099
49	1	0	-3.369290	-2.317241	2.442358
50	6	0	3.741998	2.897377	1.491503
51	6	0	4.769973	3.708415	1.039276
52	6	0	5.210102	3.601036	-0.283736
53	6	0	4.628592	2.691504	-1.155723
54	1	0	3.372200	2.947500	2.507097
55	1	0	5.234299	4.421107	1.707427
56	1	0	6.013919	4.233356	-0.637464
57	1	0	4.949638	2.591397	-2.183259
58	30	0	2.574427	-1.948174	0.691855
59	17	0	3.200917	-2.934496	-1.157194
60	17	0	2.893902	-2.178744	2.809913

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trans-endo-IM1-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.690802 a.u.

Enthalpy H = -4189.656023 a.u.

Entropy S = 216.077 cal/mol/K

Gibbs free energy G = -4189.758688 a.u.

Total free energy in solution E_{sol} = -4190.88710 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.041301	-0.037929	1.711683
2	7	0	-0.254870	0.451152	1.698185
3	6	0	0.695753	-0.404024	2.025115
4	6	0	0.458999	-1.688518	2.763880
5	6	0	2.357117	0.968059	0.812039
6	6	0	0.137602	1.826709	1.320359
7	6	0	1.284085	1.877858	0.312020
8	1	0	0.989119	-2.505691	2.273012
9	1	0	-0.588450	-1.954044	2.870016
10	1	0	0.875244	-1.551257	3.767233
11	6	0	3.727216	0.811446	0.483255
12	6	0	4.192244	-0.303007	1.222776
13	7	0	3.166341	-0.789659	1.988295
14	1	0	3.145351	-1.728567	2.350917
15	1	0	0.455900	2.310311	2.246411
16	1	0	-0.747426	2.337727	0.956080
17	1	0	1.628552	2.912119	0.249483
18	1	0	0.957682	1.585459	-0.691873
19	6	0	4.593684	1.505484	-0.391495
20	6	0	5.889690	1.049811	-0.505351
21	6	0	6.340075	-0.076080	0.239397
22	6	0	5.516839	-0.754825	1.103213
23	8	0	6.839013	1.598755	-1.305004
24	6	0	6.454833	2.713115	-2.090623
25	1	0	4.231483	2.356938	-0.949218
26	1	0	7.369064	-0.378285	0.098028
27	1	0	5.875018	-1.610024	1.660769
28	1	0	6.139729	3.546796	-1.457837
29	1	0	7.335560	2.998514	-2.658337
30	1	0	5.645365	2.447060	-2.775312
31	6	0	-1.901742	1.147841	-0.982187
32	6	0	-2.910099	1.986313	-0.287327
33	6	0	-1.573058	-0.105315	-0.287312
34	6	0	-1.596657	-0.042761	1.228610
35	6	0	-3.228211	1.730129	1.046360
36	8	0	-2.607074	0.752209	1.786779
37	8	0	-1.430389	1.470618	-2.064326
38	6	0	-0.452733	-0.840489	-0.857416

39	6	0	0.112611	-1.938558	-0.311304
40	1	0	-1.722326	-1.025747	1.661761
41	1	0	-0.013659	-0.397967	-1.746592
42	6	0	1.470731	-2.384596	-0.639934
43	8	0	2.143917	-3.059139	0.122015
44	1	0	-0.356061	-2.479678	0.498675
45	8	0	1.941975	-1.910472	-1.800496
46	6	0	3.314877	-2.220147	-2.070006
47	1	0	3.958266	-1.760693	-1.319882
48	1	0	3.465228	-3.297694	-2.064634
49	1	0	3.516789	-1.807070	-3.053271
50	6	0	-3.570518	3.014371	-0.962724
51	6	0	-4.539363	3.766498	-0.318463
52	6	0	-4.849405	3.491291	1.015552
53	6	0	-4.197345	2.478252	1.705914
54	1	0	-3.307226	3.180069	-1.999014
55	1	0	-5.060133	4.553749	-0.846458
56	1	0	-5.609747	4.070677	1.523513
57	1	0	-4.422863	2.250761	2.738827
58	30	0	-3.198351	-1.377984	-0.707004
59	17	0	-3.201253	-2.966702	0.835081
60	17	0	-4.557624	-0.950105	-2.338343

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trans-endo-TS2-V

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.681718 a.u.

Enthalpy H = -4189.647848 a.u.

Entropy S = 210.758 cal/mol/K

Gibbs free energy G = -4189.747986 a.u.

Total free energy in solution E_{sol}= -4190.87591 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.921770	-0.100464	-1.404308
2	7	0	0.310097	0.674885	-1.722847
3	6	0	-0.553946	-0.393356	-1.819929
4	6	0	-0.371722	-1.329999	-2.997368
5	6	0	-2.275223	0.927018	-0.564430
6	6	0	-0.191257	1.980879	-1.237745
7	6	0	-1.237853	1.908542	-0.122578
8	1	0	-0.840511	-2.294045	-2.802840
9	1	0	0.680325	-1.498341	-3.222864
10	1	0	-0.835813	-0.863113	-3.869324
11	6	0	-3.665400	0.773702	-0.283991
12	6	0	-4.092133	-0.376672	-0.986594
13	7	0	-3.018750	-0.885881	-1.680861
14	1	0	-2.975199	-1.813266	-2.070296
15	1	0	-0.645055	2.469491	-2.102169
16	1	0	0.669559	2.575379	-0.941906
17	1	0	-1.661577	2.906494	0.010640
18	1	0	-0.791554	1.618077	0.834422
19	6	0	-4.581032	1.505123	0.499893
20	6	0	-5.884867	1.052240	0.565454
21	6	0	-6.294705	-0.108239	-0.137544
22	6	0	-5.417612	-0.826354	-0.917724
23	8	0	-6.875896	1.648035	1.284620
24	6	0	-6.537684	2.819773	2.000621
25	1	0	-4.253451	2.386100	1.033044
26	1	0	-7.329904	-0.406344	-0.041654
27	1	0	-5.744553	-1.706227	-1.457110
28	1	0	-6.187259	3.604980	1.325132
29	1	0	-7.449086	3.144647	2.494993
30	1	0	-5.767984	2.614499	2.749524
31	6	0	2.045029	1.183510	1.063228
32	6	0	2.930194	2.191708	0.456332

33	6	0	1.651268	0.083682	0.143504
34	6	0	1.696687	0.313267	-1.348635
35	6	0	3.180083	2.174636	-0.919645
36	8	0	2.600982	1.293739	-1.787588
37	8	0	1.671661	1.227242	2.221594
38	6	0	0.702444	-0.830909	0.583415
39	6	0	0.091257	-1.718810	-0.331963
40	1	0	1.952572	-0.590656	-1.891053
41	1	0	0.332707	-0.727215	1.599621
42	6	0	-1.106412	-2.494323	0.040155
43	8	0	-1.601230	-3.345681	-0.673846
44	1	0	0.713348	-2.220135	-1.062563
45	8	0	-1.645314	-2.091423	1.193932
46	6	0	-2.865933	-2.750370	1.564312
47	1	0	-3.644723	-2.517042	0.840524
48	1	0	-2.710433	-3.826115	1.606358
49	1	0	-3.122190	-2.354267	2.541302
50	6	0	3.542131	3.163121	1.257243
51	6	0	4.398535	4.094210	0.699532
52	6	0	4.645835	4.058347	-0.677205
53	6	0	4.042667	3.109883	-1.488660
54	1	0	3.325518	3.144470	2.317332
55	1	0	4.877878	4.838749	1.320180
56	1	0	5.317972	4.780996	-1.122151
57	1	0	4.219516	3.072098	-2.554652
58	30	0	2.937562	-1.681893	0.709612
59	17	0	3.496349	-2.613683	-1.181634
60	17	0	3.440738	-1.899354	2.786410

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trans-endo-IM2-V

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.711481 a.u.

Enthalpy H = -4189.677784 a.u.

Entropy S = 208.601 cal/mol/K

Gibbs free energy G = -4189.779490 a.u.

Total free energy in solution E_{sol}= -4190.89503 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.813667	0.307090	1.544405
2	7	0	-0.276487	1.349621	2.282060
3	6	0	0.595971	0.152975	2.420719
4	6	0	0.953233	0.002659	3.902360
5	6	0	1.967480	1.192320	0.511483
6	6	0	0.329212	2.536415	1.667187
7	6	0	0.986839	2.300033	0.302871
8	1	0	1.558266	-0.881074	4.094501
9	1	0	0.032840	-0.071362	4.484216
10	1	0	1.489985	0.896063	4.223207
11	6	0	3.236724	0.911341	-0.095882
12	6	0	3.802128	-0.159094	0.626831
13	7	0	2.920206	-0.508723	1.627511
14	1	0	3.038256	-1.264631	2.281277
15	1	0	1.102300	2.887448	2.354239
16	1	0	-0.434894	3.309420	1.628947
17	1	0	1.497513	3.213768	-0.014313
18	1	0	0.240460	2.069825	-0.464480
19	6	0	3.937572	1.479677	-1.175514
20	6	0	5.175808	0.951994	-1.498094
21	6	0	5.728116	-0.122038	-0.763903
22	6	0	5.055979	-0.685072	0.299305
23	8	0	5.961682	1.396918	-2.521867
24	6	0	5.448865	2.446588	-3.315563
25	1	0	3.503185	2.297432	-1.732849

26	1	0	6.699541	-0.486781	-1.068740
27	1	0	5.490050	-1.504777	0.858285
28	1	0	5.285454	3.349308	-2.719636
29	1	0	6.199367	2.645490	-4.076162
30	1	0	4.510092	2.155049	-3.795014
31	6	0	-2.370906	0.656866	-0.599503
32	6	0	-2.856431	2.019392	-0.581426
33	6	0	-1.659432	0.228468	0.597472
34	6	0	-1.645024	1.041268	1.865977
35	6	0	-2.832056	2.739299	0.625522
36	8	0	-2.407795	2.234270	1.806791
37	8	0	-2.525921	-0.087114	-1.588714
38	6	0	-0.867674	-0.849765	0.621559
39	6	0	-0.165300	-1.150476	1.905187
40	1	0	-2.102665	0.454377	2.666269
41	1	0	-0.639130	-1.441438	-0.256879
42	6	0	0.775697	-2.342705	1.804248
43	8	0	1.396042	-2.797537	2.740209
44	1	0	-0.902249	-1.413953	2.674199
45	8	0	0.839719	-2.822181	0.570310
46	6	0	1.733136	-3.927151	0.354199
47	1	0	2.759328	-3.590371	0.493329
48	1	0	1.505648	-4.728084	1.053349
49	1	0	1.557060	-4.231355	-0.671722
50	6	0	-3.377689	2.617355	-1.741489
51	6	0	-3.850712	3.911763	-1.707617
52	6	0	-3.820579	4.619202	-0.497086
53	6	0	-3.322583	4.046107	0.660190
54	1	0	-3.387717	2.031282	-2.650657
55	1	0	-4.245258	4.375792	-2.600609
56	1	0	-4.196073	5.633876	-0.460697
57	1	0	-3.305688	4.578372	1.601160
58	30	0	-2.508765	-2.072615	-1.459267
59	17	0	-4.076167	-2.681015	-0.092245
60	17	0	-0.937999	-3.020951	-2.610381

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trans-exo-TS1-V

Imaginary frequency: -134.3246 cm^{-1}

Standard orientation:

Electronic energy E = -4189.676003 a.u.

Enthalpy H = -4189.640552 a.u.

Entropy S = 225.800 cal/mol/K

Gibbs free energy G = -4189.747837 a.u.

Total free energy in solution E_{sol} = -4190.86100 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.257388	-1.662106	-0.107069
2	7	0	-0.210120	-1.322637	1.025712
3	6	0	-0.815489	-1.766285	-0.022143
4	6	0	-0.046011	-2.337501	-1.176675
5	6	0	-2.977840	-0.814885	0.705875
6	6	0	-1.020120	-0.856380	2.158959
7	6	0	-2.264758	-0.049000	1.772437
8	1	0	0.148331	-1.569221	-1.929481
9	1	0	-0.612601	-3.139354	-1.652022
10	1	0	0.902873	-2.749816	-0.842419
11	6	0	-4.317142	-0.812668	0.225403
12	6	0	-4.350841	-1.699251	-0.875864
13	7	0	-3.085183	-2.191572	-1.075539
14	1	0	-2.832231	-2.872127	-1.768855
15	1	0	-0.375991	-0.280341	2.825323
16	1	0	-1.339239	-1.750425	2.704682
17	1	0	-2.017300	0.956307	1.415174
18	1	0	-2.882117	0.071407	2.664881
19	6	0	-5.488567	-0.142658	0.637192

20	6	0	-6.653094	-0.390527	-0.059936
21	6	0	-6.673623	-1.293864	-1.154712
22	6	0	-5.542169	-1.952551	-1.572351
23	1	0	-5.452899	0.541887	1.472050
24	1	0	-5.574905	-2.634745	-2.411965
25	1	0	-7.621520	-1.443001	-1.653962
26	8	0	-7.858010	0.177702	0.215869
27	6	0	-7.901385	1.102626	1.286120
28	1	0	-7.622362	0.624570	2.228972
29	1	0	-7.238333	1.951049	1.097429
30	1	0	-8.929652	1.448620	1.343727
31	6	0	2.723512	-0.829418	-1.196803
32	6	0	3.433740	-2.009286	-0.651079
33	6	0	1.975608	-0.064611	-0.198587
34	6	0	1.712451	-0.647440	1.067615
35	6	0	3.250135	-2.386449	0.676285
36	8	0	2.432581	-1.674877	1.527959
37	8	0	2.757149	-0.544316	-2.384220
38	6	0	1.142527	1.024026	-0.685208
39	6	0	0.321176	1.790083	0.069891
40	1	0	1.383081	-0.028867	1.887318
41	1	0	1.242774	1.229923	-1.746558
42	6	0	-0.562910	2.827417	-0.495219
43	8	0	-1.503187	3.290541	0.112824
44	1	0	0.190871	1.643057	1.134096
45	8	0	-0.235143	3.182873	-1.743404
46	6	0	-1.089163	4.174785	-2.328701
47	1	0	-2.108118	3.797804	-2.396419
48	1	0	-1.079077	5.078271	-1.722816
49	1	0	-0.677943	4.365054	-3.314603
50	6	0	4.278078	-2.775372	-1.459232
51	6	0	4.927846	-3.881480	-0.937760
52	6	0	4.731385	-4.237216	0.400778
53	6	0	3.889715	-3.495720	1.216877
54	1	0	4.403093	-2.463840	-2.487798
55	1	0	5.589284	-4.468040	-1.561065
56	1	0	5.240075	-5.100279	0.810144
57	1	0	3.722352	-3.748587	2.254774
58	30	0	2.993624	1.890384	0.408045
59	17	0	2.787538	2.128740	2.573651
60	17	0	4.241802	2.699945	-1.153178

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trans-exo-IM1-V

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.683933 a.u.

Enthalpy H = -4189.648838 a.u.

Entropy S = 220.557 cal/mol/K

Gibbs free energy G = -4189.753632 a.u.

Total free energy in solution E_{sol}= -4190.87704 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.226377	-1.491320	-0.135605
2	7	0	-0.192251	-0.918802	0.874243
3	6	0	-0.797979	-1.499760	-0.130570
4	6	0	-0.050781	-2.103454	-1.275143
5	6	0	-2.973956	-0.620664	0.641633
6	6	0	-0.989526	-0.452751	2.034410
7	6	0	-2.277873	0.256947	1.626580
8	1	0	0.272052	-1.318497	-1.964251
9	1	0	-0.691838	-2.790639	-1.822820
10	1	0	0.829633	-2.645010	-0.938398
11	6	0	-4.318556	-0.722787	0.210718
12	6	0	-4.337011	-1.690872	-0.822048
13	7	0	-3.058837	-2.126368	-1.039561

14	1	0	-2.806742	-2.876760	-1.657604
15	1	0	-0.352613	0.196260	2.630736
16	1	0	-1.232159	-1.341299	2.624470
17	1	0	-2.089744	1.245443	1.194306
18	1	0	-2.877834	0.402641	2.526691
19	6	0	-5.510885	-0.080614	0.616010
20	6	0	-6.679811	-0.443472	-0.015782
21	6	0	-6.684161	-1.433076	-1.039512
22	6	0	-5.537232	-2.062217	-1.451920
23	1	0	-5.484077	0.668247	1.394077
24	1	0	-5.561034	-2.806401	-2.237072
25	1	0	-7.639567	-1.668605	-1.488889
26	8	0	-7.903020	0.076221	0.253356
27	6	0	-7.969660	1.088181	1.243445
28	1	0	-7.642861	0.705902	2.213842
29	1	0	-7.356982	1.948161	0.962396
30	1	0	-9.013053	1.384238	1.300275
31	6	0	2.676486	-0.755251	-1.195889
32	6	0	3.314568	-1.988187	-0.672602
33	6	0	1.888976	-0.010881	-0.219000
34	6	0	1.312592	-0.731082	0.972946
35	6	0	2.896656	-2.524707	0.542815
36	8	0	1.860733	-1.996640	1.271568
37	8	0	2.839400	-0.398739	-2.356844
38	6	0	1.163831	1.136427	-0.729313
39	6	0	0.317012	1.919509	-0.018353
40	1	0	1.409240	-0.136729	1.877229
41	1	0	1.363917	1.372250	-1.770877
42	6	0	-0.498689	2.988016	-0.601961
43	8	0	-1.459997	3.471602	-0.035300
44	1	0	0.143930	1.773806	1.039005
45	8	0	-0.110740	3.358520	-1.831962
46	6	0	-0.907703	4.388004	-2.426411
47	1	0	-1.937774	4.052295	-2.535913
48	1	0	-0.887638	5.281967	-1.806385
49	1	0	-0.457854	4.580670	-3.395221
50	6	0	4.332976	-2.622426	-1.386276
51	6	0	4.932674	-3.767160	-0.885204
52	6	0	4.504890	-4.287705	0.338543
53	6	0	3.486203	-3.675868	1.056751
54	1	0	4.631408	-2.178978	-2.327188
55	1	0	5.729587	-4.251306	-1.433437
56	1	0	4.971234	-5.178620	0.739374
57	1	0	3.140714	-4.064194	2.005130
58	30	0	3.169268	1.559145	0.521934
59	17	0	2.719668	1.821100	2.673060
60	17	0	4.633781	2.486094	-0.773436

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trans-exo-TS2-V

Imaginary frequency: -281.5936 cm^{-1}

Standard orientation:

Electronic energy E = -4189.665884 a.u.

Enthalpy H = -4189.631704 a.u.

Entropy S = 214.194 cal/mol/K

Gibbs free energy G = -4189.733475 a.u.

Total free energy in solution E_{sol}= -4190.85116 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.862926	0.961152	0.539566
2	7	0	0.273236	1.500825	-0.383147
3	6	0	-0.416333	0.956081	0.673102
4	6	0	0.142585	1.159791	2.062204
5	6	0	-2.520621	1.003071	-0.665213
6	6	0	-0.506385	2.047647	-1.518777

7	6	0	-1.727417	1.214871	-1.914951
8	1	0	-0.188544	0.377772	2.744950
9	1	0	-0.218237	2.132840	2.408602
10	1	0	1.227959	1.199554	2.065011
11	6	0	-3.906866	0.810986	-0.388495
12	6	0	-4.019845	0.655292	1.017288
13	7	0	-2.759361	0.747590	1.563601
14	1	0	-2.536645	0.673802	2.539831
15	1	0	0.189897	2.175200	-2.345190
16	1	0	-0.846646	3.038776	-1.212802
17	1	0	-1.435266	0.262488	-2.372406
18	1	0	-2.299137	1.766098	-2.664321
19	6	0	-5.054639	0.762335	-1.189203
20	6	0	-6.281617	0.559954	-0.581888
21	6	0	-6.381071	0.410426	0.820162
22	6	0	-5.257476	0.460508	1.627357
23	1	0	-5.011108	0.867978	-2.264915
24	1	0	-5.348205	0.343654	2.699760
25	1	0	-7.344318	0.253371	1.282858
26	8	0	-7.359894	0.519993	-1.415846
27	6	0	-8.626117	0.242438	-0.850744
28	1	0	-8.631143	-0.727548	-0.346478
29	1	0	-8.928104	1.022388	-0.146326
30	1	0	-9.325072	0.220325	-1.682528
31	6	0	3.311993	0.269765	0.931862
32	6	0	3.829456	1.628001	0.674101
33	6	0	2.143898	-0.118582	0.100717
34	6	0	1.554138	0.870062	-0.856749
35	6	0	3.345925	2.378612	-0.398794
36	8	0	2.438237	1.875116	-1.287431
37	8	0	3.747672	-0.445194	1.816177
38	6	0	1.260354	-1.025589	0.693778
39	6	0	-0.083206	-1.115283	0.304661
40	1	0	1.267375	0.354262	-1.774545
41	1	0	1.603982	-1.512570	1.602959
42	6	0	-1.065585	-1.916019	1.058230
43	8	0	-2.115917	-2.303740	0.606693
44	1	0	-0.356654	-0.992039	-0.734490
45	8	0	-0.698386	-2.101456	2.346293
46	6	0	-1.628197	-2.878756	3.113628
47	1	0	-2.593648	-2.375557	3.150532
48	1	0	-1.758097	-3.859314	2.661115
49	1	0	-1.191903	-2.963992	4.103808
50	6	0	4.808906	2.173946	1.510194
51	6	0	5.299846	3.445988	1.273753
52	6	0	4.811240	4.181125	0.189005
53	6	0	3.838692	3.656037	-0.649622
54	1	0	5.165970	1.563599	2.329389
55	1	0	6.059794	3.867031	1.917910
56	1	0	5.194281	5.175246	-0.003494
57	1	0	3.453701	4.207143	-1.496661
58	30	0	2.631817	-1.999841	-1.022471
59	17	0	1.528433	-1.890526	-2.910886
60	17	0	4.009924	-3.399775	-0.149686

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trans-exo-IM2-V

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.701992 a.u.

Enthalpy H = -4189.668253 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 210.074 cal/mol/K

Gibbs free energy G = -4189.768066 a.u.

Total free energy in solution E_{sol}= -4190.88169 a.u.

1	6	0	-1.897643	0.324100	0.946899
2	7	0	0.224338	1.547605	0.848333
3	6	0	-0.448183	0.319972	1.368409
4	6	0	-0.276854	0.295432	2.890398
5	6	0	-2.512852	1.286467	0.191083
6	6	0	-0.654908	2.722284	0.783455
7	6	0	-1.819640	2.553634	-0.194130
8	1	0	-0.808616	-0.542184	3.339248
9	1	0	-0.667434	1.220942	3.312715
10	1	0	0.784704	0.228886	3.135493
11	6	0	-3.875540	0.869023	0.015476
12	6	0	-4.015207	-0.360854	0.701059
13	7	0	-2.794068	-0.673386	1.260553
14	1	0	-2.575586	-1.491928	1.803260
15	1	0	-0.040661	3.585826	0.541376
16	1	0	-1.053672	2.873058	1.788216
17	1	0	-1.455063	2.537354	-1.226594
18	1	0	-2.498981	3.406412	-0.110864
19	6	0	-4.977491	1.424572	-0.640922
20	6	0	-6.187881	0.748236	-0.605884
21	6	0	-6.314665	-0.477349	0.078699
22	6	0	-5.230134	-1.039321	0.736535
23	1	0	-4.916065	2.361001	-1.179868
24	1	0	-5.336367	-1.980353	1.261265
25	1	0	-7.260971	-0.997176	0.100105
26	8	0	-7.221822	1.346827	-1.272060
27	6	0	-8.473404	0.693019	-1.265633
28	1	0	-8.411382	-0.291735	-1.737454
29	1	0	-8.861271	0.583698	-0.248928
30	1	0	-9.145007	1.325450	-1.840775
31	6	0	3.550725	0.896523	0.208936
32	6	0	3.708187	2.344933	0.057014
33	6	0	2.139769	0.422412	0.087487
34	6	0	1.031743	1.333535	-0.368973
35	6	0	2.647780	3.113630	-0.435266
36	8	0	1.477486	2.571748	-0.876137
37	8	0	4.448395	0.123349	0.478885
38	6	0	1.740793	-0.715749	0.670500
39	6	0	0.248000	-0.914735	0.701151
40	1	0	0.472994	0.888429	-1.201745
41	1	0	2.434395	-1.299546	1.272860
42	6	0	-0.069786	-2.296725	1.212259
43	8	0	-0.866247	-2.662460	2.033865
44	1	0	-0.116416	-0.935161	-0.335830
45	8	0	0.725798	-3.174210	0.539019
46	6	0	0.584656	-4.580540	0.872910
47	1	0	0.685057	-4.697512	1.947657
48	1	0	-0.390388	-4.922668	0.538053
49	1	0	1.393848	-5.073941	0.346459
50	6	0	4.913191	2.966003	0.406664
51	6	0	5.059051	4.333548	0.269571
52	6	0	3.992183	5.090084	-0.228790
53	6	0	2.792909	4.491515	-0.583656
54	1	0	5.712344	2.339253	0.780527
55	1	0	5.988204	4.815571	0.540678
56	1	0	4.100623	6.161279	-0.342688
57	1	0	1.965640	5.062049	-0.983689
58	30	0	2.141601	-2.364203	-0.942659
59	17	0	0.973469	-1.718390	-2.659924
60	17	0	3.809029	-3.637748	-0.426077

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trans-COM-VI

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.008240	-1.227604	-0.145232
2	6	0	-3.343329	-0.609463	-0.068513
3	6	0	-0.953447	-0.311820	-0.607033
4	6	0	-1.241539	0.984193	-0.873273
5	6	0	-3.516501	0.731815	-0.404438
6	8	0	-2.461419	1.519626	-0.796602
7	8	0	-1.785408	-2.393567	0.134066
8	6	0	0.409315	-0.828315	-0.683000
9	6	0	1.337963	-0.389599	-1.558386
10	1	0	-0.497275	1.723900	-1.144380
11	1	0	0.631072	-1.643889	0.000868
12	6	0	2.734156	-0.891529	-1.539100
13	8	0	3.430228	-1.163847	-2.470346
14	1	0	1.104728	0.308253	-2.351812
15	8	0	3.166516	-0.966109	-0.233843
16	6	0	4.521222	-1.435327	-0.028501
17	1	0	4.623251	-2.417126	-0.480920
18	1	0	5.213344	-0.732489	-0.484834
19	1	0	4.645432	-1.480548	1.048159
20	6	0	-4.458352	-1.353544	0.334265
21	6	0	-5.705547	-0.760439	0.392511
22	6	0	-5.854075	0.589853	0.048358
23	6	0	-4.764887	1.345265	-0.351569
24	1	0	-4.301703	-2.392635	0.591927
25	1	0	-6.567391	-1.335018	0.704031
26	1	0	-6.831007	1.052925	0.096023
27	1	0	-4.852912	2.389527	-0.617726
28	30	0	2.005800	0.538184	0.713389
29	17	0	2.364285	2.471273	-0.218943
30	17	0	1.454462	-0.274105	2.635076

Imaginary frequency: none
Electronic energy E = -3501.475951 a.u.
Enthalpy H = -3501.454852 a.u.
Entropy S = 155.351 cal/mol/K
Gibbs free energy G = -3501.528665 a.u.
Total free energy in solution E_{sol}= -3502.21394 a.u.

trans-endo-TS1-VI

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.278436	1.194667	1.100438
2	7	0	0.052574	1.494013	0.370116
3	6	0	0.856810	1.321801	1.360480
4	6	0	0.347294	1.198269	2.767237
5	6	0	2.770295	0.932307	-0.158107
6	6	0	0.596805	1.708474	-0.969657
7	6	0	1.815011	0.844408	-1.306348
8	1	0	0.375579	0.154385	3.087343
9	1	0	-0.672034	1.566963	2.846030
10	1	0	0.974904	1.785777	3.441147
11	6	0	4.167920	0.697672	-0.018402
12	6	0	4.465100	0.846051	1.356602
13	7	0	3.299862	1.134829	2.022862
14	1	0	3.217590	1.292120	3.011235
15	1	0	0.880628	2.764911	-1.027024
16	1	0	-0.209527	1.537659	-1.683265
17	1	0	2.256057	1.211464	-2.234767

Imaginary frequency: -266.7123 cm^{-1}
Electronic energy E = -4189.673802 a.u.
Enthalpy H = -4189.639110 a.u.
Entropy S = 217.179 cal/mol/K
Gibbs free energy G = -4189.742298 a.u.
Total free energy in solution E_{sol}= -4190.39687 a.u.

18	1	0	1.519681	-0.196657	-1.478748
19	6	0	5.192039	0.385045	-0.937305
20	6	0	6.475171	0.238145	-0.450734
21	6	0	6.757782	0.396720	0.930659
22	6	0	5.773591	0.700690	1.840576
23	8	0	7.563815	-0.059274	-1.211644
24	6	0	7.351113	-0.225068	-2.600114
25	1	0	4.959763	0.270509	-1.986112
26	1	0	7.785345	0.268287	1.242908
27	1	0	6.005523	0.817089	2.891311
28	1	0	6.959528	0.691693	-3.049170
29	1	0	8.322612	-0.454778	-3.028980
30	1	0	6.660020	-1.049502	-2.795519
31	30	0	-2.070067	-2.918733	0.759299
32	17	0	-1.240417	-2.111545	2.624487
33	17	0	-3.794758	-4.092234	0.170648
34	6	0	-3.059308	1.799229	-1.588778
35	6	0	-3.250832	3.099875	-0.902930
36	6	0	-2.385513	0.792760	-0.776983
37	6	0	-1.974556	1.100919	0.531010
38	6	0	-2.909856	3.246867	0.438549
39	8	0	-2.399735	2.198390	1.172441
40	8	0	-3.422046	1.616769	-2.742574
41	6	0	-2.071798	-0.458597	-1.349595
42	6	0	-1.239186	-1.412908	-0.816519
43	1	0	-1.753516	0.305186	1.230360
44	1	0	-2.536139	-0.663991	-2.310274
45	6	0	-0.975462	-2.649504	-1.555418
46	8	0	-1.119428	-2.902241	-2.717778
47	1	0	-0.580248	-1.192492	0.017424
48	8	0	-0.578692	-3.617251	-0.630984
49	6	0	-0.458103	-4.958478	-1.154813
50	1	0	-1.435664	-5.303303	-1.483038
51	1	0	0.243724	-4.952830	-1.983800
52	1	0	-0.087721	-5.557651	-0.329540
53	6	0	-3.793223	4.193870	-1.581725
54	6	0	-3.982650	5.399944	-0.927794
55	6	0	-3.635534	5.521337	0.421563
56	6	0	-3.099419	4.446187	1.115029
57	1	0	-4.058020	4.054015	-2.621537
58	1	0	-4.402137	6.245781	-1.455865
59	1	0	-3.786785	6.461711	0.935496
60	1	0	-2.829118	4.512754	2.160061

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trans-endo-IM1-VI

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.679339 a.u.

Enthalpy H = -4189.644420 a.u.

Entropy S = 219.459 cal/mol/K

Gibbs free energy G = -4189.748692 a.u.

Total free energy in solution E_{sol}= -4190.39806 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554025	-1.151688	1.646639
2	7	0	0.758252	-1.528911	1.556299
3	6	0	-0.240066	-0.885496	2.131533
4	6	0	-0.075797	0.030320	3.307882
5	6	0	-1.808598	-1.836620	0.468778
6	6	0	0.448446	-2.714545	0.724053
7	6	0	-0.690262	-2.498282	-0.269638

8	1	0	-0.587311	0.976638	3.129309
9	1	0	0.961612	0.213123	3.572348
10	1	0	-0.550610	-0.467200	4.159233
11	6	0	-3.187887	-1.676606	0.188449
12	6	0	-3.718348	-0.880771	1.232055
13	7	0	-2.724674	-0.602013	2.134155
14	1	0	-2.744416	0.217116	2.720948
15	1	0	0.161332	-3.498502	1.428662
16	1	0	1.363483	-3.020578	0.227364
17	1	0	-0.987851	-3.475815	-0.655165
18	1	0	-0.374420	-1.891147	-1.122618
19	6	0	-4.016283	-2.132195	-0.862396
20	6	0	-5.341395	-1.755998	-0.840723
21	6	0	-5.856402	-0.941207	0.206224
22	6	0	-5.070263	-0.501190	1.241391
23	8	0	-6.263988	-2.103415	-1.773647
24	6	0	-5.819144	-2.907121	-2.851705
25	1	0	-3.603964	-2.746020	-1.649774
26	1	0	-6.905345	-0.681731	0.154544
27	1	0	-5.478868	0.115876	2.030329
28	1	0	-5.437340	-3.865937	-2.491727
29	1	0	-6.688565	-3.073486	-3.481252
30	1	0	-5.042118	-2.395448	-3.425246
31	6	0	2.616665	-1.170650	-1.188500
32	6	0	3.592015	-2.200590	-0.745319
33	6	0	2.027100	-0.383212	-0.113720
34	6	0	2.105190	-0.873013	1.297224
35	6	0	3.806822	-2.438411	0.611972
36	8	0	3.115706	-1.788722	1.607357
37	8	0	2.353137	-1.012248	-2.373457
38	6	0	1.172880	0.650035	-0.425572
39	6	0	0.548425	1.498727	0.517076
40	1	0	2.192578	-0.070597	2.021241
41	1	0	0.968920	0.789440	-1.484096
42	6	0	-0.806536	2.012258	0.313827
43	8	0	-1.705150	2.016196	1.127476
44	1	0	0.793171	1.396543	1.559801
45	8	0	-0.932180	2.577653	-0.922508
46	6	0	-2.182537	3.246824	-1.174054
47	1	0	-3.001887	2.540521	-1.062845
48	1	0	-2.292973	4.069752	-0.470930
49	1	0	-2.111534	3.609687	-2.193801
50	6	0	4.325161	-2.926875	-1.686462
51	6	0	5.261031	-3.864704	-1.281476
52	6	0	5.467166	-4.083243	0.082871
53	6	0	4.743055	-3.377192	1.034002
54	1	0	4.135903	-2.716191	-2.730958
55	1	0	5.831542	-4.419588	-2.013984
56	1	0	6.198961	-4.811113	0.409543
57	1	0	4.886519	-3.534081	2.094448
58	30	0	1.175168	3.434415	-0.351356
59	17	0	0.500695	5.006484	1.025239
60	17	0	2.428977	3.445028	-2.126774

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trans-endo-TS2-VI

Imaginary frequency: -200.7544 cm^{-1}

Standard orientation:

Electronic energy E = -4189.671961 a.u.

Enthalpy H = -4189.638015 a.u.

Entropy S = 213.148 cal/mol/K

Gibbs free energy G = -4189.739288 a.u.

Total free energy in solution E_{sol}= -4190.38352 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.684207	-0.652116	-1.548653

2	7	0	-0.544585	-1.444508	-1.699379
3	6	0	0.347204	-0.499008	-2.083875
4	6	0	0.171006	0.173501	-3.425065
5	6	0	2.009284	-1.464539	-0.486404
6	6	0	-0.078226	-2.630921	-0.944193
7	1	0	0.634745	1.158214	-3.438151
8	1	0	-0.878610	0.272014	-3.697334
9	1	0	0.649019	-0.461065	-4.176258
10	6	0	3.381182	-1.223810	-0.186789
11	6	0	3.828246	-0.247309	-1.106230
12	7	0	2.790199	0.066036	-1.953968
13	1	0	2.727602	0.933215	-2.463267
14	1	0	0.351723	-3.301830	-1.690977
15	1	0	-0.953878	-3.120070	-0.526575
16	6	0	4.263033	-1.746957	0.781532
17	6	0	5.555182	-1.260179	0.808511
18	6	0	5.985623	-0.271150	-0.112076
19	6	0	5.142083	0.238600	-1.071794
20	8	0	6.514479	-1.660176	1.687951
21	6	0	6.144981	-2.637921	2.640470
22	1	0	3.917298	-2.496045	1.479006
23	1	0	7.010131	0.066452	-0.032710
24	1	0	5.485401	0.988713	-1.772346
25	1	0	5.835592	-3.565519	2.151127
26	1	0	7.030492	-2.822082	3.242724
27	1	0	5.335202	-2.276824	3.280241
28	6	0	-2.289027	-1.298824	1.112090
29	6	0	-3.189380	-2.413141	0.744886
30	6	0	-1.849263	-0.471863	-0.016444
31	6	0	-1.952109	-0.989223	-1.410582
32	6	0	-3.439557	-2.705107	-0.597677
33	8	0	-2.851380	-2.038119	-1.639911
34	8	0	-1.949113	-1.081373	2.265416
35	6	0	-0.998262	0.586401	0.198774
36	6	0	-0.432040	1.283033	-0.893847
37	1	0	-2.190051	-0.225743	-2.146279
38	1	0	-0.626147	0.710084	1.215361
39	6	0	0.609878	2.300944	-0.725436
40	8	0	1.444695	2.637959	-1.528831
41	1	0	-1.004336	1.429890	-1.795823
42	8	0	0.500204	2.904255	0.502255
43	6	0	1.456940	3.943301	0.809985
44	1	0	2.457430	3.521626	0.769172
45	1	0	1.353730	4.749898	0.088535
46	1	0	1.203798	4.268547	1.813535
47	6	0	-3.815036	-3.172114	1.738443
48	6	0	-4.683424	-4.195715	1.400626
49	6	0	-4.928109	-4.469313	0.051549
50	6	0	-4.310561	-3.733194	-0.949123
51	1	0	-3.598422	-2.918161	2.767963
52	1	0	-5.171532	-4.776347	2.171546
53	1	0	-5.607842	-5.265914	-0.222881
54	1	0	-4.484742	-3.933566	-1.997425
55	6	0	0.977840	-2.357034	0.127436
56	1	0	1.409233	-3.315755	0.425967
57	1	0	0.539812	-1.906975	1.022826
58	30	0	-1.647672	2.939058	0.671095
59	17	0	-2.436552	3.978851	-1.072124
60	17	0	-1.947919	2.912111	2.809822

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trans-endo-IM2-VI Imaginary frequency: none

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.384174	-0.975821	1.275503
2	7	0	-0.112902	0.710723	2.246717
3	6	0	0.073397	-0.741045	1.986450
4	6	0	0.003139	-1.484144	3.326394
5	6	0	2.290172	-0.014067	0.914160
6	6	0	1.139713	1.436164	2.488211
7	1	0	0.179996	-2.551185	3.199931
8	1	0	-0.976607	-1.327521	3.780492
9	1	0	0.761836	-1.082871	3.997981
10	6	0	3.366395	-0.684574	0.243560
11	6	0	3.048881	-2.058145	0.241861
12	7	0	1.833052	-2.213360	0.872688
13	1	0	1.354684	-3.082182	1.041801
14	1	0	1.619095	0.950087	3.340547
15	1	0	0.886951	2.447659	2.793622
16	6	0	4.563963	-0.235984	-0.343676
17	6	0	5.402217	-1.177989	-0.913372
18	6	0	5.071207	-2.552317	-0.905129
19	6	0	3.902129	-3.005806	-0.333516
20	8	0	6.591113	-0.887742	-1.519626
21	6	0	6.959731	0.473631	-1.587222
22	1	0	4.803532	0.817968	-0.346220
23	1	0	5.770195	-3.236452	-1.366931
24	1	0	3.658741	-4.060833	-0.333544
25	1	0	7.079009	0.901134	-0.587572
26	1	0	7.912026	0.504035	-2.110339
27	1	0	6.218479	1.055644	-2.142336
28	6	0	-0.701831	1.869579	-1.191570
29	6	0	-0.491053	3.262008	-0.786616
30	6	0	-0.974467	0.940085	-0.056261
31	6	0	-1.092224	1.403477	1.368812
32	6	0	-0.632431	3.640223	0.554801
33	8	0	-0.984050	2.796435	1.561037
34	8	0	-0.656846	1.466053	-2.336719
35	6	0	-1.027370	-0.391185	-0.215090
36	6	0	-1.108447	-1.179078	1.069721
37	1	0	-2.094625	1.145131	1.722383
38	1	0	-0.754172	-0.841976	-1.167534
39	6	0	-1.293010	-2.642635	0.759538
40	8	0	-0.688775	-3.606657	1.143145
41	1	0	-2.025072	-0.906666	1.613614
42	8	0	-2.353961	-2.748057	-0.090235
43	6	0	-2.691827	-4.081651	-0.557355
44	1	0	-1.807092	-4.534311	-0.994372
45	1	0	-3.047776	-4.666263	0.285967
46	1	0	-3.462519	-3.930223	-1.304525
47	6	0	-0.146797	4.224700	-1.745757
48	6	0	0.052714	5.541004	-1.380184
49	6	0	-0.096286	5.906376	-0.036234
50	6	0	-0.436323	4.971356	0.926813
51	1	0	-0.048617	3.893375	-2.771321
52	1	0	0.317377	6.282744	-2.121144
53	1	0	0.054575	6.936444	0.260769
54	1	0	-0.562020	5.241170	1.966444
55	6	0	2.115261	1.417174	1.308107
56	1	0	3.069784	1.853150	1.617456
57	1	0	1.742836	2.034605	0.482960

Electronic energy E = -4189.703343 a.u.
Enthalpy H = -4189.669619 a.u.
Entropy S = 209.792 cal/mol/K
Gibbs free energy G = -4189.769298 a.u.
Total free energy in solution E_{sol}= -4190.40954 a.u.

58	30	0	-3.232445	-0.892352	-0.829850
59	17	0	-4.459109	-0.088696	0.778802
60	17	0	-3.368203	-1.433771	-2.915918

trans-exo-TS1-VI

Imaginary frequency: -216.7781 cm^{-1}

Standard orientation:

Electronic energy E = -4189.676057 a.u.

Enthalpy H = -4189.640699 a.u.

Entropy S = 224.109 cal/mol/K

Gibbs free energy G = -4189.747180 a.u.

Total free energy in solution E_{sol}= -4190.85969 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.174091	-1.658898	-0.443902
2	7	0	-0.096527	-1.564143	0.661019
3	6	0	-0.736436	-1.811309	-0.435367
4	6	0	-0.008451	-2.205733	-1.687058
5	6	0	-2.844304	-0.958773	0.539048
6	6	0	-0.856982	-1.333447	1.897701
7	6	0	-2.084230	-0.438195	1.718120
8	1	0	0.260753	-1.320715	-2.268231
9	1	0	-0.644328	-2.839751	-2.305653
10	1	0	0.897896	-2.756460	-1.449775
11	6	0	-4.196024	-0.836631	0.115924
12	6	0	-4.289455	-1.500871	-1.129553
13	7	0	-3.048213	-1.981024	-1.460291
14	1	0	-2.832352	-2.506272	-2.288219
15	1	0	-0.173506	-0.921749	2.639671
16	1	0	-1.182133	-2.317648	2.248059
17	1	0	-1.795176	0.609204	1.574698
18	1	0	-2.680314	-0.479705	2.631657
19	6	0	-5.335457	-0.229723	0.687428
20	6	0	-6.526239	-0.314839	-0.003528
21	6	0	-6.605252	-0.994540	-1.248093
22	6	0	-5.507670	-1.589756	-1.820397
23	1	0	-5.255910	0.283151	1.634924
24	1	0	-5.584798	-2.100298	-2.771535
25	1	0	-7.571389	-1.023561	-1.733549
26	8	0	-7.705495	0.218737	0.413216
27	6	0	-7.697500	0.910578	1.647727
28	1	0	-7.405001	0.247282	2.466236
29	1	0	-7.019015	1.766879	1.612178
30	1	0	-8.714867	1.257468	1.805334
31	30	0	2.087044	2.618273	0.522902
32	17	0	0.759159	2.597457	2.285777
33	17	0	4.219383	2.952918	0.304684
34	6	0	3.160263	-1.275454	-1.152311
35	6	0	3.539134	-2.509973	-0.420127
36	6	0	2.185583	-0.457629	-0.465068
37	6	0	1.659034	-0.862556	0.787484
38	6	0	3.077921	-2.728726	0.876570
39	8	0	2.278390	-1.814710	1.522730
40	8	0	3.615906	-1.015565	-2.261262
41	6	0	1.744956	0.749056	-1.069996
42	6	0	0.557133	1.384310	-0.792358
43	1	0	1.285125	-0.075741	1.435843
44	1	0	2.407185	1.152135	-1.833281
45	6	0	0.194444	2.684352	-1.379655
46	8	0	-0.855408	3.041360	-1.833773
47	1	0	-0.219645	0.910323	-0.209525
48	8	0	1.277012	3.535756	-1.260693
49	6	0	1.109598	4.874222	-1.771414
50	1	0	0.885425	4.822668	-2.833465

51	1	0	0.297106	5.363494	-1.240142
52	1	0	2.058956	5.367470	-1.592071
53	6	0	4.375649	-3.462240	-1.007324
54	6	0	4.738518	-4.602646	-0.309704
55	6	0	4.269400	-4.797172	0.993142
56	6	0	3.438866	-3.862890	1.595364
57	1	0	4.727336	-3.264098	-2.011413
58	1	0	5.387700	-5.337828	-0.766325
59	1	0	4.555014	-5.684635	1.543147
60	1	0	3.068914	-3.987772	2.603784

trans-exo-IM1-VI

Imaginary frequency: -6.2506 cm^{-1}

Standard orientation:

Electronic energy E = -4189.687058 a.u.

Enthalpy H = -4189.652526 a.u.

Entropy S = 214.926 cal/mol/K

Gibbs free energy G = -4189.754645 a.u.

Total free energy in solution E_{sol}= -4190.87369 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.453669	-2.002606	0.473581
2	7	0	-0.567582	-1.274774	-0.451915
3	6	0	0.043996	-1.836272	0.567851
4	6	0	-0.672035	-2.192122	1.831975
5	6	0	2.230618	-1.339767	-0.468524
6	6	0	0.156680	-1.038325	-1.727268
7	6	0	1.572630	-0.511851	-1.517812
8	1	0	-0.681246	-1.310380	2.478277
9	1	0	-0.144220	-2.994221	2.345399
10	1	0	-1.694652	-2.497533	1.641309
11	6	0	3.583261	-1.543810	-0.113325
12	6	0	3.577672	-2.359739	1.044699
13	7	0	2.282200	-2.610872	1.399892
14	1	0	1.997605	-3.196090	2.164618
15	1	0	-0.431451	-0.329096	-2.304514
16	1	0	0.186110	-2.000098	-2.247934
17	1	0	1.582439	0.544631	-1.228650
18	1	0	2.099328	-0.577287	-2.471395
19	6	0	4.800681	-1.098887	-0.678115
20	6	0	5.969393	-1.501200	-0.072366
21	6	0	5.947564	-2.340054	1.079745
22	6	0	4.777738	-2.775570	1.647146
23	1	0	4.789386	-0.456530	-1.546264
24	1	0	4.784620	-3.403298	2.528262
25	1	0	6.905106	-2.616922	1.500187
26	8	0	7.215637	-1.162299	-0.482439
27	6	0	7.311913	-0.291625	-1.597959
28	1	0	6.875449	-0.750443	-2.488710
29	1	0	6.814343	0.659077	-1.392757
30	1	0	8.373118	-0.124048	-1.756354
31	30	0	-0.311717	2.519064	-0.664896
32	17	0	1.712765	3.310063	-1.098409
33	17	0	-1.804250	2.086341	-2.242442
34	6	0	-3.942548	-0.053228	0.804661
35	6	0	-4.685824	-1.178811	0.168499
36	6	0	-2.491085	-0.060160	0.597650
37	6	0	-2.014054	-1.019744	-0.457202
38	6	0	-4.004231	-2.264488	-0.381146
39	8	0	-2.628616	-2.308627	-0.401827
40	8	0	-4.534070	0.781962	1.474826
41	6	0	-1.783752	0.993131	1.106010
42	6	0	-0.388644	1.311506	1.089614
43	1	0	-2.234881	-0.591849	-1.438335
44	1	0	-2.430789	1.720190	1.593501

45	6	0	0.028855	2.504313	1.838523
46	8	0	0.895747	2.633397	2.660964
47	1	0	0.361768	0.533704	1.099741
48	8	0	-0.682406	3.593784	1.344511
49	6	0	-0.281483	4.870237	1.871141
50	1	0	-0.372434	4.863039	2.954566
51	1	0	0.748880	5.069301	1.583859
52	1	0	-0.957663	5.594330	1.428097
53	6	0	-6.081576	-1.197217	0.186461
54	6	0	-6.779029	-2.275986	-0.334398
55	6	0	-6.076928	-3.358815	-0.868693
56	6	0	-4.688463	-3.360825	-0.895161
57	1	0	-6.584856	-0.347768	0.629156
58	1	0	-7.860751	-2.282945	-0.323129
59	1	0	-6.615837	-4.205883	-1.274001
60	1	0	-4.125398	-4.185405	-1.311243

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trans-exo-TS2-VI

Imaginary frequency: -362.7156 cm^{-1}

Standard orientation:

Electronic energy E = -4189.660681 a.u.

Enthalpy H = -4189.626224 a.u.

Entropy S = 218.978 cal/mol/K

Gibbs free energy G = -4189.730267 a.u.

Total free energy in solution E_{sol}= -4190.84290 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.591440	-1.315118	0.804841
2	7	0	-0.488762	-1.752715	-0.221143
3	6	0	0.148501	-1.269467	0.880020
4	6	0	-0.507271	-1.364238	2.228699
5	6	0	2.301195	-1.552179	-0.352448
6	6	0	0.256105	-2.517947	-1.237798
7	6	0	1.576776	-1.858907	-1.622991
8	1	0	-0.055033	-0.665131	2.929865
9	1	0	-0.349616	-2.386912	2.583765
10	1	0	-1.577900	-1.190224	2.174384
11	6	0	3.680164	-1.404836	-0.033131
12	6	0	3.735794	-1.071984	1.339026
13	7	0	2.457619	-1.060223	1.848804
14	1	0	2.195110	-0.480801	2.630717
15	1	0	-0.398682	-2.633394	-2.098904
16	1	0	0.457260	-3.511027	-0.827689
17	1	0	1.406649	-0.940552	-2.197745
18	1	0	2.143253	-2.542525	-2.258483
19	6	0	4.864609	-1.524279	-0.789586
20	6	0	6.063168	-1.282775	-0.149174
21	6	0	6.103211	-0.935935	1.226521
22	6	0	4.958663	-0.830386	1.980208
23	1	0	4.815004	-1.781623	-1.837668
24	1	0	5.004177	-0.568803	3.029246
25	1	0	7.077081	-0.757316	1.662068
26	8	0	7.285991	-1.347197	-0.741813
27	6	0	7.317690	-1.656960	-2.121666
28	1	0	6.892795	-2.646419	-2.311554
29	1	0	6.773382	-0.908557	-2.703683
30	1	0	8.365763	-1.650288	-2.407958
31	30	0	-0.669058	2.922523	-0.801274
32	17	0	-2.615439	3.826732	-1.035795
33	17	0	1.176068	2.816237	-1.973491
34	6	0	-3.899173	-0.190452	0.364294
35	6	0	-4.647208	-1.432650	0.050049
36	6	0	-2.445530	-0.252700	0.132994
37	6	0	-1.890937	-1.506927	-0.482232
38	6	0	-3.956864	-2.629124	-0.146081

39	8	0	-2.590477	-2.684096	-0.058109
40	8	0	-4.461659	0.805516	0.790223
41	6	0	-1.686854	0.806713	0.522619
42	6	0	-0.256571	0.899009	0.462855
43	1	0	-1.985253	-1.444712	-1.571970
44	1	0	-2.239151	1.575463	1.060529
45	6	0	0.411975	1.837211	1.388800
46	8	0	1.305252	1.618760	2.167048
47	1	0	0.351033	0.554851	-0.354827
48	8	0	-0.136823	3.093418	1.269851
49	6	0	0.412800	4.136873	2.105122
50	1	0	0.306372	3.848068	3.146992
51	1	0	1.461062	4.278891	1.855215
52	1	0	-0.174515	5.020261	1.878910
53	6	0	-6.042475	-1.431495	0.010202
54	6	0	-6.736348	-2.607235	-0.229503
55	6	0	-6.030178	-3.798173	-0.417880
56	6	0	-4.641996	-3.817710	-0.378755
57	1	0	-6.548615	-0.489949	0.178730
58	1	0	-7.817502	-2.605546	-0.265642
59	1	0	-6.567358	-4.720328	-0.600080
60	1	0	-4.078663	-4.730210	-0.519416

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trans-exo-IM2-VI

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.712898 a.u.

Enthalpy H = -4189.678682 a.u.

Entropy S = 214.137 cal/mol/K

Gibbs free energy G = -4189.780426 a.u.

Total free energy in solution E_{sol}= -4190.89438 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.022689	0.481427	-0.591946
2	7	0	0.083234	1.506798	0.353023
3	6	0	0.527672	0.611953	-0.739475
4	6	0	0.169720	1.128344	-2.141584
5	6	0	2.812136	1.139124	0.314398
6	6	0	0.944643	2.644478	0.685676
7	6	0	2.261080	2.147000	1.269406
8	1	0	0.571168	0.464627	-2.907130
9	1	0	0.605900	2.118164	-2.276810
10	1	0	-0.908584	1.209138	-2.273339
11	6	0	4.162216	0.723558	0.071424
12	6	0	4.118815	-0.183816	-1.005988
13	7	0	2.805708	-0.311759	-1.399497
14	1	0	2.455554	-0.916317	-2.122916
15	1	0	0.400234	3.257278	1.405710
16	1	0	1.137176	3.266481	-0.195657
17	1	0	2.086435	1.714314	2.258504
18	1	0	2.951476	2.986139	1.389121
19	6	0	5.393015	1.052141	0.669584
20	6	0	6.537917	0.455939	0.171413
21	6	0	6.478006	-0.455825	-0.907451
22	6	0	5.280156	-0.784516	-1.504315
23	1	0	5.424139	1.747102	1.496716
24	1	0	5.246205	-1.482309	-2.331432
25	1	0	7.409703	-0.886684	-1.248339
26	8	0	7.796745	0.678540	0.652858
27	6	0	7.916248	1.566249	1.744415
28	1	0	7.560714	2.566552	1.480885
29	1	0	7.358430	1.202175	2.611981
30	1	0	8.975284	1.609662	1.985367
31	30	0	-2.037292	-2.769953	0.838359

32	17	0	-3.609003	-3.908889	-0.097184
33	17	0	-1.048642	-2.286935	2.686064
34	6	0	-3.636950	0.881584	0.115339
35	6	0	-4.001407	2.303355	-0.005131
36	6	0	-2.165861	0.626373	0.095722
37	6	0	-1.291945	1.781531	0.471736
38	6	0	-3.006138	3.254951	-0.277959
39	8	0	-1.691092	2.918046	-0.370257
40	8	0	-4.435871	-0.031378	0.200617
41	6	0	-1.667243	-0.533861	-0.318692
42	6	0	-0.170102	-0.734094	-0.393071
43	1	0	-1.508011	2.097270	1.498994
44	1	0	-2.367484	-1.246514	-0.760512
45	6	0	0.089091	-1.929022	-1.272010
46	8	0	0.719329	-2.021332	-2.289947
47	1	0	0.195812	-1.006716	0.605277
48	8	0	-0.557073	-3.010475	-0.737082
49	6	0	-0.445506	-4.251666	-1.490069
50	1	0	-0.880298	-4.106510	-2.474250
51	1	0	0.604737	-4.516015	-1.565239
52	1	0	-1.010649	-4.982202	-0.923763
53	6	0	-5.342658	2.697132	0.065081
54	6	0	-5.691691	4.020308	-0.132071
55	6	0	-4.692423	4.958752	-0.415939
56	6	0	-3.358278	4.588112	-0.487581
57	1	0	-6.082913	1.933730	0.267383
58	1	0	-6.726680	4.328699	-0.074689
59	1	0	-4.960984	5.995103	-0.577792
60	1	0	-2.576737	5.304890	-0.699487

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trans-COM-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -3501.484056 a.u.

Enthalpy H = -3501.463069 a.u.

Entropy S = 159.063 cal/mol/K

Gibbs free energy G = -3501.538645 a.u.

Total free energy in solution E_{sol}= -3502.22527 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.482291	0.930765	-0.192105
2	6	0	4.853292	0.406925	-0.054685
3	6	0	2.425996	-0.087555	-0.038537
4	6	0	2.772483	-1.380416	0.167461
5	6	0	5.069011	-0.949223	0.177138
6	8	0	4.022519	-1.833996	0.277828
7	8	0	3.238751	2.105088	-0.413867
8	6	0	1.046059	0.360999	-0.154654
9	6	0	-0.056904	-0.346064	0.139107
10	1	0	2.059326	-2.188738	0.250953
11	1	0	0.945379	1.382297	-0.503382
12	6	0	-1.395760	0.203739	-0.035269
13	8	0	-2.398721	-0.461998	0.248362
14	1	0	-0.045883	-1.353932	0.530511
15	8	0	-1.456604	1.432780	-0.502048
16	6	0	-2.762842	2.015884	-0.676081
17	1	0	-3.324213	1.448188	-1.419112
18	1	0	-3.282999	2.055624	0.281289
19	1	0	-2.577839	3.019880	-1.040874
20	30	0	-4.373199	-0.387521	0.144678
21	17	0	-4.999854	-0.989535	-1.833112
22	17	0	-5.181299	0.445027	1.964415
23	6	0	5.960393	1.257472	-0.154497
24	6	0	7.240109	0.751482	-0.022201
25	6	0	7.430201	-0.617165	0.211200

26	6	0	6.349646	-1.477465	0.312149
27	1	0	5.771916	2.307366	-0.335029
28	1	0	8.095626	1.408949	-0.097860
29	1	0	8.432589	-1.011570	0.314227
30	1	0	6.470241	-2.537057	0.490420

trans-endo-TS1-VII

Imaginary frequency: -276.3986 cm^{-1}

Standard orientation:

Electronic energy E = -4189.698022 a.u.

Enthalpy H = -4189.663701 a.u.

Entropy S = 213.858 cal/mol/K

Gibbs free energy G = -4189.765312 a.u.

Total free energy in solution E_{sol}= -4190.87594 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.463246	0.133122	-1.210792
2	7	0	1.878033	-0.233829	-1.317752
3	6	0	0.681104	-0.719291	-1.471136
4	6	0	0.464199	-2.080246	-2.065617
5	6	0	-0.357837	1.363497	-0.630137
6	6	0	2.036651	1.210754	-1.078830
7	6	0	0.980482	1.852077	-0.175970
8	1	0	-0.298405	-2.655132	-1.540726
9	1	0	1.389911	-2.646044	-2.138662
10	1	0	0.097208	-1.937880	-3.087249
11	6	0	-1.673217	1.932602	-0.569034
12	6	0	-2.542936	0.993437	-1.142790
13	7	0	-1.823103	-0.187848	-1.434082
14	1	0	-2.078483	-0.725323	-2.260145
15	1	0	1.984093	1.675029	-2.068243
16	1	0	3.036927	1.378614	-0.687935
17	1	0	1.057400	2.937625	-0.261999
18	1	0	1.142622	1.594700	0.875028
19	6	0	-2.152255	3.175054	-0.119352
20	6	0	-3.498773	3.442661	-0.301224
21	6	0	-4.354885	2.496916	-0.912738
22	6	0	-3.897916	1.266208	-1.330215
23	1	0	-4.571551	0.536911	-1.759948
24	1	0	-1.479368	3.885687	0.337683
25	1	0	-5.396218	2.766696	-1.021256
26	8	0	-4.108426	4.597172	0.068796
27	6	0	-3.313615	5.568221	0.723316
28	1	0	-3.979402	6.394760	0.954761
29	1	0	-2.507710	5.919055	0.073071
30	1	0	-2.890241	5.167730	1.647902
31	6	0	4.025419	0.122788	1.450289
32	6	0	5.176457	0.421299	0.561739
33	6	0	3.066752	-0.819986	0.902954
34	6	0	3.175155	-1.251139	-0.451517
35	6	0	5.265510	-0.170700	-0.695867
36	8	0	4.315130	-1.054244	-1.156681
37	8	0	3.917883	0.643798	2.556049
38	6	0	1.896774	-1.103195	1.643671
39	6	0	0.852667	-1.867606	1.207959
40	1	0	2.745272	-2.202381	-0.727005
41	1	0	1.815252	-0.582900	2.592429
42	6	0	-0.443746	-1.864542	1.819588
43	8	0	-1.451958	-2.302773	1.222325
44	1	0	0.899913	-2.458871	0.308938
45	8	0	-0.536001	-1.363086	3.034861
46	6	0	-1.859440	-1.307875	3.613057
47	1	0	-2.508019	-0.675652	3.012077
48	1	0	-2.279499	-2.309514	3.662685
49	1	0	-1.711488	-0.896098	4.605499

50	30	0	-2.817452	-1.774615	-0.087065
51	17	0	-2.996617	-3.087028	-1.881323
52	17	0	-4.481993	-0.916941	1.073665
53	6	0	6.186573	1.296886	0.966762
54	6	0	7.259827	1.564815	0.132560
55	6	0	7.329797	0.955245	-1.123617
56	6	0	6.334560	0.085363	-1.546797
57	1	0	6.093313	1.743227	1.948129
58	1	0	8.042149	2.240740	0.450804
59	1	0	8.167241	1.160468	-1.778034
60	1	0	6.367105	-0.398923	-2.513209

trans-endo-IM1-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.703107 a.u.

Enthalpy H = -4189.668615 a.u.

Entropy S = 213.509cal/mol/K

Gibbs free energy G = -4189.770060 a.u.

Total free energy in solution E_{sol}= -4190.88490 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.445576	0.261332	-1.178862
2	7	0	1.879029	-0.107298	-1.155968
3	6	0	0.682001	-0.585977	-1.434384
4	6	0	0.457231	-1.859479	-2.194730
5	6	0	-0.372701	1.446134	-0.488382
6	6	0	2.036293	1.330199	-0.840717
7	6	0	0.943195	1.885825	0.068136
8	1	0	-0.401163	-2.410386	-1.810685
9	1	0	1.324862	-2.510262	-2.235456
10	1	0	0.221327	-1.570220	-3.224418
11	6	0	-1.689820	1.989654	-0.424169
12	6	0	-2.529554	1.083224	-1.096789
13	7	0	-1.786795	-0.044349	-1.466110
14	1	0	-2.050984	-0.588048	-2.284150
15	1	0	2.005148	1.851260	-1.800885
16	1	0	3.021635	1.467761	-0.406889
17	1	0	1.028009	2.973616	0.087192
18	1	0	1.057204	1.523604	1.094135
19	6	0	-2.206879	3.185544	0.112688
20	6	0	-3.550428	3.441099	-0.083823
21	6	0	-4.374879	2.528741	-0.791198
22	6	0	-3.887550	1.346682	-1.295389
23	1	0	-4.534508	0.639065	-1.796493
24	1	0	-1.561282	3.868446	0.644849
25	1	0	-5.418508	2.789332	-0.901039
26	8	0	-4.196142	4.549283	0.355880
27	6	0	-3.440858	5.486513	1.101272
28	1	0	-4.131465	6.279221	1.374291
29	1	0	-2.627131	5.900566	0.499699
30	1	0	-3.032401	5.027300	2.004963
31	6	0	4.108090	-0.169367	1.438221
32	6	0	5.190970	0.335645	0.552990
33	6	0	3.066270	-0.924388	0.769548
34	6	0	3.020716	-1.013058	-0.716782
35	6	0	5.171292	0.071445	-0.815878
36	8	0	4.171059	-0.646364	-1.424606
37	8	0	4.127108	0.049657	2.645793
38	6	0	1.969632	-1.358412	1.501355
39	6	0	0.878820	-2.038854	0.976947
40	1	0	2.755239	-2.004656	-1.066739
41	1	0	1.952987	-1.056806	2.544046
42	6	0	-0.382311	-2.128090	1.611946
43	8	0	-1.412949	-2.536125	1.004569

44	1	0	0.914081	-2.525094	0.018414
45	8	0	-0.455918	-1.749462	2.879168
46	6	0	-1.749710	-1.818993	3.510139
47	1	0	-2.443414	-1.129713	3.035036
48	1	0	-2.141373	-2.831363	3.442136
49	1	0	-1.569970	-1.542711	4.544065
50	30	0	-2.799651	-1.799276	-0.131586
51	17	0	-3.075188	-2.828449	-2.093406
52	17	0	-4.366879	-0.872191	1.099851
53	6	0	6.251987	1.071255	1.085322
54	6	0	7.274288	1.530164	0.269949
55	6	0	7.239171	1.249888	-1.098135
56	6	0	6.191961	0.522669	-1.647470
57	1	0	6.239386	1.256355	2.151480
58	1	0	8.095006	2.097082	0.688537
59	1	0	8.034723	1.600489	-1.743227
60	1	0	6.146444	0.293577	-2.703569

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trans-endo-TS2-VII

Imaginary frequency: -190.4885 cm^{-1}

Standard orientation:

Electronic energy E = -4189.700414 a.u.

Enthalpy H = -4189.667095 a.u.

Entropy S = 206.109 cal/mol/K

Gibbs free energy G = -4189.765024 a.u.

Total free energy in solution E_{sol}= -4190.87905 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.547729	0.422430	-0.723666
2	7	0	1.807515	0.291472	-0.945213
3	6	0	0.621297	-0.279791	-1.215646
4	6	0	0.389373	-1.090275	-2.469148
5	6	0	-0.506717	1.672137	-0.181984
6	1	0	-0.467025	-1.754532	-2.343955
7	1	0	1.238948	-1.688341	-2.783193
8	1	0	0.162212	-0.386944	-3.275769
9	6	0	-1.859730	2.148762	-0.073976
10	6	0	-2.680043	1.137414	-0.586599
11	7	0	-1.888679	0.017371	-0.957860
12	1	0	-2.090546	-0.348299	-1.891845
13	6	0	-2.406098	3.357286	0.384089
14	6	0	-3.780905	3.510426	0.289241
15	6	0	-4.593697	2.484431	-0.243567
16	6	0	-4.062196	1.288117	-0.678307
17	1	0	-4.695597	0.499650	-1.062438
18	1	0	-1.767167	4.128027	0.789495
19	1	0	-5.658871	2.665404	-0.285150
20	8	0	-4.456652	4.619098	0.682738
21	6	0	-3.699249	5.683209	1.227649
22	1	0	-4.413549	6.462438	1.477901
23	1	0	-2.980101	6.065809	0.498552
24	1	0	-3.171948	5.366129	2.131111
25	6	0	4.413994	-0.799287	1.088638
26	6	0	5.357218	0.151762	0.458531
27	6	0	3.264056	-1.184756	0.265051
28	6	0	3.034523	-0.564714	-1.076013
29	6	0	5.138671	0.607832	-0.841221
30	8	0	4.070189	0.222984	-1.605534
31	8	0	4.588679	-1.221922	2.222486
32	6	0	2.222482	-1.839834	0.863373
33	6	0	1.011396	-2.178625	0.212115

34	1	0	2.806845	-1.302070	-1.837742
35	1	0	2.310077	-2.000080	1.933560
36	6	0	-0.170566	-2.459199	0.964016
37	8	0	-1.241287	-2.842321	0.434970
38	1	0	1.013424	-2.597739	-0.780455
39	8	0	-0.089164	-2.262390	2.270086
40	6	0	-1.259426	-2.572620	3.056637
41	1	0	-2.069537	-1.887987	2.818550
42	1	0	-1.576384	-3.593947	2.858841
43	1	0	-0.939469	-2.457173	4.086816
44	30	0	-2.816863	-1.907934	-0.239819
45	6	0	6.482617	0.596612	1.157695
46	6	0	7.375817	1.476890	0.570897
47	6	0	7.144337	1.918495	-0.734895
48	6	0	6.032195	1.489729	-1.444915
49	1	0	6.622643	0.221154	2.162914
50	1	0	8.246684	1.817233	1.114675
51	1	0	7.838823	2.603680	-1.204373
52	1	0	5.837321	1.818589	-2.456620
53	6	0	1.850513	1.227195	0.197761
54	1	0	2.860373	1.630755	0.247209
55	6	0	0.809878	2.330070	0.056124
56	1	0	1.641626	0.672420	1.117075
57	1	0	0.805911	2.928975	0.968683
58	1	0	1.048224	2.997072	-0.778364
59	17	0	-4.304673	-1.493328	1.325008
60	17	0	-3.224449	-2.395487	-2.393163

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trans-endo-IM2-VII

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.720695 a.u.

Enthalpy H = -4189.687209a.u.

Entropy S = 205.667 cal/mol/K

Gibbs free energy G = -4190.89627 a.u.

Total free energy in solution E_{sol}= -4190.85265 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.352138	0.037172	-1.208882
2	7	0	2.019802	0.271464	-1.271873
3	6	0	0.945747	-0.712511	-1.127811
4	6	0	1.030101	-1.767810	-2.235357
5	6	0	-0.577319	1.183408	-0.493665
6	6	0	1.820726	1.647127	-0.742777
7	6	0	0.588066	1.865874	0.147186
8	1	0	0.194480	-2.467151	-2.151298
9	1	0	1.941975	-2.359905	-2.161340
10	1	0	1.005935	-1.277250	-3.207840
11	6	0	-1.983073	1.438473	-0.555398
12	6	0	-2.545181	0.396693	-1.339348
13	7	0	-1.506675	-0.418662	-1.770623
14	1	0	-1.655800	-1.320423	-2.201381
15	1	0	1.739673	2.311735	-1.604114
16	1	0	2.715389	1.935509	-0.193248
17	1	0	0.419632	2.941791	0.233200
18	1	0	0.773588	1.486627	1.155336
19	6	0	-2.811146	2.453572	-0.042283
20	6	0	-4.160322	2.417630	-0.353175
21	6	0	-4.696261	1.412403	-1.193837
22	6	0	-3.906429	0.414053	-1.715807
23	1	0	-4.316504	-0.344691	-2.368980
24	1	0	-2.388319	3.237382	0.569412
25	1	0	-5.755809	1.449594	-1.403951
26	8	0	-5.069840	3.320241	0.085808
27	6	0	-4.626600	4.292180	1.014240

28	1	0	-5.505988	4.868089	1.287753
29	1	0	-3.881502	4.954657	0.565487
30	1	0	-4.207397	3.814382	1.903197
31	6	0	4.612758	-0.609458	1.301935
32	6	0	5.729502	0.014562	0.570228
33	6	0	3.347610	-0.701089	0.524651
34	6	0	3.307722	-0.291288	-0.926199
35	6	0	5.512543	0.613137	-0.677099
36	8	0	4.295639	0.667788	-1.286466
37	8	0	4.708162	-1.020067	2.444157
38	6	0	2.252654	-1.228471	1.073490
39	6	0	0.988330	-1.469975	0.299601
40	1	0	3.481282	-1.169026	-1.555079
41	1	0	2.296714	-1.547968	2.108528
42	6	0	-0.256883	-1.203903	1.122376
43	8	0	-1.354486	-1.657905	0.808857
44	1	0	0.925484	-2.541466	0.079256
45	8	0	-0.056703	-0.501852	2.210773
46	6	0	-1.232434	-0.172739	2.993805
47	1	0	-1.868914	0.494785	2.417672
48	1	0	-1.782960	-1.077629	3.234088
49	1	0	-0.847525	0.311652	3.884080
50	30	0	-3.261165	-1.356075	0.137438
51	17	0	-3.462646	-2.969603	-1.378917
52	17	0	-4.482984	-0.653547	1.813811
53	6	0	7.008431	0.047886	1.137894
54	6	0	8.056956	0.661317	0.477954
55	6	0	7.824719	1.260279	-0.765276
56	6	0	6.565637	1.240303	-1.343828
57	1	0	7.136803	-0.418393	2.106090
58	1	0	9.045048	0.682024	0.917052
59	1	0	8.638441	1.745417	-1.289468
60	1	0	6.370592	1.697869	-2.304040

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trans-exo-TS1-VII

Imaginary frequency: -285.3974 cm^{-1}

Standard orientation:

Electronic energy E = -4189.700880 a.u.

Enthalpy H = -4189.667007 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.198935	-1.223246	1.472462
2	7	0	-2.131501	-1.431303	0.134088
3	6	0	-1.579014	-0.914125	1.193707
4	6	0	-2.336029	0.010019	2.097148
5	6	0	0.635310	-1.741984	0.497160
6	6	0	-1.438181	-2.551353	-0.519531
7	6	0	0.057946	-2.318725	-0.754430
8	1	0	-1.988554	1.039585	1.996571
9	1	0	-2.170203	-0.317250	3.127818
10	1	0	-3.402137	-0.032985	1.896151
11	6	0	1.965537	-1.464897	0.907912
12	6	0	1.879612	-0.823217	2.164052
13	7	0	0.558042	-0.681820	2.489260
14	1	0	0.206483	-0.208406	3.302553
15	1	0	-1.965548	-2.763291	-1.449060
16	1	0	-1.565673	-3.412760	0.140561
17	1	0	0.263755	-1.665757	-1.606695
18	1	0	0.518228	-3.280070	-0.994438
19	6	0	3.234013	-1.667262	0.292120
20	6	0	4.364312	-1.286698	1.005436
21	6	0	4.250061	-0.655377	2.278474

Entropy S = 210.512 cal/mol/K

Gibbs free energy G = -4189.767028 a.u.

Total free energy in solution E_{sol} = -4190.88069 a.u.

22	6	0	3.033053	-0.426354	2.864495
23	1	0	3.302443	-2.212076	-0.638673
24	1	0	2.966603	0.067370	3.825281
25	1	0	5.170707	-0.347674	2.753621
26	8	0	5.623672	-1.462397	0.586398
27	6	0	5.817907	-1.924719	-0.745919
28	1	0	5.440508	-2.943527	-0.860340
29	1	0	5.329234	-1.254768	-1.455975
30	1	0	6.890678	-1.907452	-0.908736
31	30	0	3.024621	0.467503	-0.854699
32	17	0	2.303840	-0.470983	-2.744869
33	17	0	4.901771	1.595760	-0.569875
34	6	0	-4.335744	1.457308	-0.107789
35	6	0	-5.450231	0.471984	-0.097162
36	6	0	-3.090152	0.945402	-0.634890
37	6	0	-3.002337	-0.427533	-1.048087
38	6	0	-5.299427	-0.776312	-0.697090
39	8	0	-4.133333	-1.132804	-1.333569
40	8	0	-4.487287	2.588352	0.346989
41	6	0	-1.925923	1.725211	-0.496605
42	6	0	-0.629081	1.305716	-0.654110
43	1	0	-2.267694	-0.631838	-1.822386
44	1	0	-2.102735	2.728492	-0.121650
45	6	0	0.488915	2.078344	-0.209254
46	8	0	1.646715	1.626292	-0.073907
47	1	0	-0.364747	0.326563	-1.021622
48	8	0	0.247410	3.336325	0.140989
49	6	0	1.382165	4.092661	0.599714
50	1	0	1.779525	3.655099	1.513275
51	1	0	2.160855	4.100177	-0.159619
52	1	0	0.999720	5.091822	0.780497
53	6	0	-6.672310	0.786644	0.501671
54	6	0	-7.713957	-0.127156	0.496946
55	6	0	-7.541764	-1.370568	-0.118197
56	6	0	-6.335666	-1.702999	-0.719261
57	1	0	-6.766068	1.765481	0.953552
58	1	0	-8.659138	0.120922	0.961140
59	1	0	-8.354181	-2.085902	-0.128252
60	1	0	-6.179761	-2.656915	-1.204452

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trans-exo-IM1-VII

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.701051 a.u.

Enthalpy H = -4189.666484 a.u.

Entropy S = 212.264 cal/mol/K

Gibbs free energy G = -4189.767338 a.u.

Total free energy in solution E_{sol}= -4190.85265 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.311287	-2.227989	0.204481
2	7	0	-1.244563	-0.784099	-0.791395
3	6	0	-0.983493	-1.629495	0.181652
4	6	0	-1.955084	-1.948365	1.274797
5	6	0	1.382421	-1.702821	-0.505745
6	6	0	-0.318015	-0.721717	-1.945610
7	6	0	1.139779	-0.641473	-1.516796
8	1	0	-1.937125	-1.164705	2.034133
9	1	0	-1.683458	-2.893410	1.741375
10	1	0	-2.971182	-2.032975	0.897816
11	6	0	2.561040	-2.281660	0.015166
12	6	0	2.151781	-3.198138	1.013321
13	7	0	0.790029	-3.138801	1.132710
14	1	0	0.240402	-3.729363	1.730332

15	1	0	-0.584403	0.143922	-2.545773
16	1	0	-0.481374	-1.629897	-2.532222
17	1	0	1.388492	0.337295	-1.107366
18	1	0	1.769920	-0.760605	-2.399785
19	6	0	3.929283	-2.072722	-0.264347
20	6	0	4.844211	-2.807127	0.455252
21	6	0	4.417997	-3.762906	1.421893
22	6	0	3.093142	-3.971401	1.714270
23	1	0	4.220218	-1.322960	-0.984929
24	1	0	2.794554	-4.687542	2.468431
25	1	0	5.192362	-4.312551	1.940336
26	8	0	6.189627	-2.697581	0.335107
27	6	0	6.669552	-1.670406	-0.521135
28	1	0	6.382777	-1.863519	-1.557888
29	1	0	6.285403	-0.695649	-0.211077
30	1	0	7.751949	-1.689881	-0.432740
31	30	0	1.902436	2.740992	-0.687473
32	17	0	0.846386	2.726239	-2.618863
33	17	0	3.788938	1.702878	-0.281375
34	6	0	-4.152489	0.314545	1.034526
35	6	0	-4.986219	-0.633882	0.245386
36	6	0	-2.901397	0.687618	0.420247
37	6	0	-2.474015	0.108721	-0.882637
38	6	0	-4.585975	-1.047057	-1.025237
39	8	0	-3.438178	-0.599418	-1.625205
40	8	0	-4.530574	0.711204	2.135434
41	6	0	-2.092462	1.627980	1.035240
42	6	0	-0.856142	2.076028	0.585847
43	1	0	-2.120875	0.906550	-1.536835
44	1	0	-2.485539	2.038337	1.959635
45	6	0	-0.122753	3.095181	1.218953
46	8	0	1.003357	3.526188	0.810950
47	1	0	-0.431334	1.716205	-0.340636
48	8	0	-0.636231	3.636225	2.319516
49	6	0	0.145901	4.651179	2.963013
50	1	0	1.109646	4.248383	3.267836
51	1	0	0.299441	5.492280	2.290452
52	1	0	-0.437634	4.951840	3.827258
53	6	0	-6.184811	-1.123192	0.769206
54	6	0	-6.970197	-2.002819	0.040882
55	6	0	-6.554569	-2.401057	-1.231960
56	6	0	-5.365471	-1.928485	-1.770052
57	1	0	-6.468358	-0.779712	1.755400
58	1	0	-7.899140	-2.375471	0.451472
59	1	0	-7.162000	-3.085412	-1.810668
60	1	0	-5.028392	-2.219780	-2.755611

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trans-exo-TS2-VII

Imaginary frequency: -190.7999 cm^{-1}

Standard orientation:

Electronic energy E = -4189.695868 a.u.

Enthalpy H = -4189.662510 a.u.

Entropy S = 205.462 cal/mol/K

Gibbs free energy G = -4189.760132 a.u.

Total free energy in solution E_{sol}= -4190.87759 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.176616	-0.984099	1.339007
2	7	0	-1.874404	-1.313269	0.226532
3	6	0	-1.207411	-0.642607	1.168711
4	6	0	-1.916229	0.127196	2.240252
5	6	0	0.921301	-1.586149	0.342863
6	6	0	-1.221439	-2.485155	-0.392564
7	6	0	0.220884	-2.212374	-0.820077

8	1	0	-1.339451	1.004591	2.530930
9	1	0	-2.019065	-0.548817	3.095725
10	1	0	-2.909603	0.435925	1.935179
11	6	0	2.290175	-1.389349	0.684105
12	6	0	2.305707	-0.738608	1.943832
13	7	0	1.012225	-0.484592	2.313642
14	1	0	0.729367	0.001315	3.146040
15	1	0	-1.835623	-2.796559	-1.233492
16	1	0	-1.230672	-3.282459	0.354299
17	1	0	0.286231	-1.574962	-1.705716
18	1	0	0.685481	-3.163490	-1.089753
19	6	0	3.511271	-1.697564	0.026822
20	6	0	4.691731	-1.396261	0.684783
21	6	0	4.679929	-0.799372	1.975114
22	6	0	3.510709	-0.464822	2.609723
23	1	0	3.496883	-2.174812	-0.941929
24	1	0	3.523840	0.024937	3.574381
25	1	0	5.639877	-0.571240	2.416449
26	8	0	5.919148	-1.602111	0.175930
27	6	0	6.001119	-1.901068	-1.212852
28	1	0	5.592795	-2.892566	-1.423192
29	1	0	5.471900	-1.142973	-1.794141
30	1	0	7.058883	-1.883186	-1.456776
31	30	0	2.858786	0.647300	-0.877515
32	17	0	2.212583	-0.232828	-2.811898
33	17	0	4.744423	1.711226	-0.468744
34	6	0	-4.567980	1.290023	-0.421987
35	6	0	-5.689775	0.320560	-0.332684
36	6	0	-3.222488	0.711461	-0.413716
37	6	0	-3.100770	-0.791965	-0.397038
38	6	0	-5.438461	-1.005568	0.013506
39	8	0	-4.167613	-1.439903	0.295660
40	8	0	-4.780509	2.492554	-0.511457
41	6	0	-2.151477	1.564621	-0.383224
42	6	0	-0.790997	1.185460	-0.417806
43	1	0	-3.075824	-1.182873	-1.419349
44	1	0	-2.401484	2.610629	-0.232726
45	6	0	0.257814	2.004875	0.061238
46	8	0	1.477836	1.710783	0.023675
47	1	0	-0.457726	0.330415	-0.979607
48	8	0	-0.106575	3.125378	0.693265
49	6	0	0.966421	3.960477	1.157015
50	1	0	1.560650	3.433018	1.900858
51	1	0	1.610130	4.244939	0.327712
52	1	0	0.482305	4.829895	1.590358
53	6	0	-7.005450	0.731020	-0.550388
54	6	0	-8.050844	-0.171759	-0.428951
55	6	0	-7.780763	-1.496096	-0.076558
56	6	0	-6.476970	-1.921445	0.145655
57	1	0	-7.170006	1.769267	-0.807459
58	1	0	-9.070116	0.146811	-0.601709
59	1	0	-8.593157	-2.204885	0.022592
60	1	0	-6.247077	-2.941867	0.421207

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trans-exo-IM2-VII

Imaginary frequency: -470.2858 cm^{-1}

Standard orientation:

Electronic energy E = -4189.729754 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Enthalpy H = -4189.695734 a.u.

Entropy S = 209.809 cal/mol/K

Gibbs free energy G = -4189.795421 a.u.

Total free energy in solution E_{sol}= -4190.90935 a.u.

1	6	0	-0.466806	-0.651239	-0.991706
2	7	0	1.688151	-1.181195	-0.087279
3	6	0	0.938587	-0.167055	-0.820573
4	6	0	1.580433	0.176951	-2.168540
5	6	0	-1.126462	-1.374153	-0.037070
6	6	0	1.035709	-2.403451	0.378159
7	6	0	-0.341200	-2.119761	0.997775
8	1	0	1.075690	1.025794	-2.640279
9	1	0	1.516209	-0.691279	-2.824668
10	1	0	2.628814	0.438314	-2.051417
11	6	0	-2.524130	-1.335926	-0.388502
12	6	0	-2.610640	-0.632969	-1.617018
13	7	0	-1.337176	-0.247055	-1.972546
14	1	0	-1.121571	0.384567	-2.723555
15	1	0	1.699772	-2.860937	1.111873
16	1	0	0.914598	-3.112728	-0.446056
17	1	0	-0.245534	-1.549452	1.924322
18	1	0	-0.833607	-3.065011	1.239342
19	6	0	-3.689485	-1.887930	0.199847
20	6	0	-4.886129	-1.727409	-0.471406
21	6	0	-4.942781	-1.062311	-1.724949
22	6	0	-3.826589	-0.521333	-2.309221
23	1	0	-3.619038	-2.393345	1.151901
24	1	0	-3.893196	0.004950	-3.251956
25	1	0	-5.915551	-0.964086	-2.186126
26	8	0	-6.083071	-2.167513	-0.018907
27	6	0	-6.120142	-2.694416	1.296627
28	1	0	-5.533039	-3.613886	1.367466
29	1	0	-5.747171	-1.960990	2.015292
30	1	0	-7.163948	-2.913682	1.501617
31	30	0	-2.647462	0.827736	0.674312
32	17	0	-1.789748	0.529818	2.701947
33	17	0	-4.536603	1.848114	0.213242
34	6	0	4.668074	0.991779	0.767900
35	6	0	5.664705	-0.034670	0.397504
36	6	0	3.254744	0.597405	0.510759
37	6	0	2.995661	-0.875723	0.325031
38	6	0	5.267799	-1.177744	-0.312092
39	8	0	3.968026	-1.423469	-0.626175
40	8	0	4.968143	2.085053	1.211148
41	6	0	2.283296	1.508027	0.466881
42	6	0	0.882324	1.076064	0.158355
43	1	0	3.208133	-1.384976	1.272188
44	1	0	2.521540	2.548569	0.650756
45	6	0	-0.041215	2.152660	-0.330482
46	8	0	-1.265825	2.053808	-0.292895
47	1	0	0.397810	0.701841	1.068509
48	8	0	0.544545	3.215173	-0.838225
49	6	0	-0.335909	4.275019	-1.279537
50	1	0	-0.966886	3.913475	-2.087797
51	1	0	-0.957861	4.600208	-0.449709
52	1	0	0.323640	5.066339	-1.617004
53	6	0	7.020991	0.175703	0.670245
54	6	0	7.971378	-0.736970	0.250699
55	6	0	7.564845	-1.869448	-0.464489
56	6	0	6.226475	-2.094947	-0.746158
57	1	0	7.290465	1.075621	1.207809
58	1	0	9.019021	-0.576094	0.465944
59	1	0	8.303603	-2.585957	-0.801420
60	1	0	5.897385	-2.967749	-1.293638

5.3 (R)-5a-Zn-catalyzed reaction

5.3.1 Kumar's transition state models

cis-endo-c-TS-Re

Imaginary frequency: -433.4941 cm^{-1}

Standard orientation:

Electronic energy E = - -4188.770018 a.u.

Enthalpy H = -4188.722827 a.u.

Entropy S = 274.857 cal/mol/K

Gibbs free energy G = -4188.853420 a.u.

Total free energy in solution E_{sol}= -4190.36292 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.623988	4.359429	0.878912
2	6	0	-3.671883	4.202913	-0.065026
3	6	0	-3.934958	2.906761	-0.588143
4	6	0	-3.159123	1.781309	-0.155453
5	6	0	-1.865564	3.291176	1.255905
6	6	0	-2.103828	1.988683	0.728451
7	6	0	-3.573447	0.416140	-0.615950
8	6	0	-4.793493	-0.135030	-0.097245
9	6	0	-5.302203	-1.363179	-0.606008
10	6	0	-4.580012	-2.028721	-1.631798
11	6	0	-2.858652	-0.307567	-1.570255
12	6	0	-3.399896	-1.521848	-2.089281
13	6	0	-4.450148	5.307426	-0.489425
14	6	0	-5.457156	5.149988	-1.405812
15	6	0	-5.717709	3.867355	-1.937166
16	6	0	-4.982325	2.778968	-1.540761
17	6	0	-5.518104	0.499057	0.949058
18	6	0	-6.670248	-0.053876	1.449332
19	6	0	-7.174443	-1.268685	0.932710
20	6	0	-6.498130	-1.905957	-0.075063
21	1	0	-2.431451	5.344587	1.289056
22	1	0	-1.053789	3.391662	1.965483
23	1	0	-4.229041	6.283948	-0.072856
24	1	0	-6.046921	5.999712	-1.725620
25	1	0	-6.505740	3.741348	-2.669324
26	1	0	-5.187442	1.804991	-1.963874
27	1	0	-5.138585	1.426509	1.355706
28	1	0	-7.199213	0.447649	2.250245
29	1	0	-8.087130	-1.690819	1.333666
30	1	0	-6.865703	-2.841141	-0.482602
31	1	0	-4.974246	-2.955609	-2.032886
32	1	0	-2.822881	-2.027661	-2.853501
33	8	0	-1.639076	0.066158	-2.007218
34	8	0	-1.270244	1.008695	1.129167
35	30	0	-0.728406	0.090510	-0.380183
36	6	0	3.302980	0.304541	-0.604338
37	7	0	1.163569	-0.697803	-0.233294
38	6	0	2.135012	-0.374584	-1.128907
39	6	0	3.343216	0.863705	0.653129
40	6	0	1.589178	-0.719641	1.190736
41	6	0	2.212598	0.612444	1.596301
42	6	0	4.538799	1.638806	0.721637
43	6	0	5.180159	1.501953	-0.530986
44	7	0	4.396595	0.707093	-1.334876
45	1	0	4.635878	0.355728	-2.246150
46	1	0	2.335259	-1.505962	1.328910
47	1	0	0.705254	-0.939879	1.789924
48	1	0	2.559422	0.529355	2.628165
49	1	0	1.459911	1.407626	1.563492
50	6	0	5.118890	2.429770	1.734023
51	6	0	6.325329	3.045531	1.463337
52	6	0	6.962001	2.887742	0.206639

53	6	0	6.406895	2.124762	-0.794473
54	8	0	7.004072	3.837099	2.338401
55	6	0	6.417828	4.039706	3.609632
56	1	0	4.621876	2.536922	2.687283
57	1	0	7.905948	3.395581	0.062560
58	1	0	6.902514	2.018195	-1.751003
59	1	0	6.308997	3.093603	4.146762
60	1	0	7.095599	4.691548	4.153941
61	1	0	5.440386	4.520995	3.518757
62	6	0	1.685898	0.003783	-2.521491
63	1	0	1.433646	1.068386	-2.511590
64	1	0	2.480503	-0.152932	-3.249636
65	1	0	0.788756	-0.530666	-2.834639
66	6	0	0.964730	-4.024482	1.137311
67	6	0	-0.373352	-3.735913	1.702075
68	6	0	1.275417	-3.313111	-0.111763
69	6	0	0.369003	-2.360572	-0.634057
70	6	0	-1.229140	-2.829772	1.082434
71	8	0	-0.879748	-2.201198	-0.108089
72	8	0	1.752172	-4.787933	1.670895
73	6	0	2.580528	-3.269755	-0.592648
74	6	0	2.963858	-2.481301	-1.670395
75	1	0	0.327589	-2.175043	-1.698704
76	1	0	3.347516	-3.763440	-0.004104
77	6	0	4.404994	-2.371485	-1.952437
78	8	0	5.297901	-2.780192	-1.251347
79	8	0	4.638135	-1.707378	-3.117833
80	6	0	6.029562	-1.614127	-3.464172
81	1	0	6.060245	-1.093330	-4.416535
82	1	0	6.458878	-2.609393	-3.553644
83	1	0	6.574190	-1.065540	-2.695412
84	6	0	-0.799944	-4.346473	2.885290
85	6	0	-2.046394	-4.052203	3.413036
86	6	0	-2.881196	-3.136853	2.763709
87	6	0	-2.480703	-2.514720	1.589187
88	1	0	-0.124178	-5.045512	3.360160
89	1	0	-2.374003	-4.527526	4.327861
90	1	0	-3.855591	-2.902460	3.171916
91	1	0	-3.107972	-1.800753	1.070160
92	1	0	2.301854	-2.325562	-2.509847

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cis-endo-c-TS-Si

Imaginary frequency: -453.8089 cm^{-1}

Standard orientation:

Electronic energy E = -4188.765040 a.u.

Enthalpy H = -4188.717777 a.u.

Entropy S = 273.927 cal/mol/K

Gibbs free energy G = -4188.847929 a.u.

Total free energy in solution E_{sol} = -4190.35736 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.100531	1.827616	1.913602
2	6	0	-5.904563	1.073476	1.019990
3	6	0	-5.303687	0.014929	0.283451
4	6	0	-3.910342	-0.283919	0.449419
5	6	0	-3.767207	1.565307	2.036721
6	6	0	-3.144071	0.524989	1.285336
7	6	0	-3.369101	-1.515941	-0.215542
8	6	0	-3.795343	-2.792152	0.281939
9	6	0	-3.461180	-3.985519	-0.416561
10	6	0	-2.702602	-3.888095	-1.611109
11	6	0	-2.552435	-1.472710	-1.344593
12	6	0	-2.262010	-2.675588	-2.055056
13	6	0	-7.282657	1.356108	0.855863
14	6	0	-8.052827	0.626594	-0.011930

15	6	0	-7.460981	-0.419198	-0.754469
16	6	0	-6.129564	-0.718670	-0.611006
17	6	0	-4.555780	-2.916486	1.476384
18	6	0	-4.954141	-4.145314	1.938551
19	6	0	-4.625609	-5.325770	1.234892
20	6	0	-3.892175	-5.240100	0.080396
21	1	0	-5.563076	2.618979	2.493367
22	1	0	-3.131259	2.136221	2.702141
23	1	0	-7.715352	2.165896	1.433035
24	1	0	-9.105339	0.849156	-0.132683
25	1	0	-8.064871	-0.991071	-1.448047
26	1	0	-5.688630	-1.516818	-1.192321
27	1	0	-4.808291	-2.021226	2.027909
28	1	0	-5.526379	-4.210981	2.855623
29	1	0	-4.950409	-6.288229	1.609248
30	1	0	-3.626777	-6.133450	-0.474103
31	1	0	-2.477005	-4.793462	-2.163725
32	1	0	-1.683209	-2.581203	-2.965926
33	8	0	-2.004223	-0.332235	-1.811938
34	8	0	-1.810040	0.389248	1.419824
35	30	0	-1.158075	0.361480	-0.308927
36	6	0	2.834006	-0.951759	-0.173981
37	7	0	0.943933	0.510440	-0.383253
38	6	0	1.708712	-0.475008	-0.930667
39	6	0	3.417337	-0.268862	0.869816
40	6	0	1.331351	0.995996	0.980545
41	6	0	2.828400	1.032501	1.305694
42	6	0	4.556495	-1.018383	1.272981
43	6	0	4.609922	-2.155320	0.431722
44	7	0	3.560157	-2.089250	-0.451503
45	1	0	3.334902	-2.775483	-1.149424
46	1	0	0.838367	0.308559	1.671496
47	1	0	0.867946	1.970449	1.122349
48	1	0	2.923618	1.169126	2.385535
49	1	0	3.335600	1.875633	0.830483
50	6	0	5.531963	-0.829823	2.274122
51	6	0	6.520778	-1.784193	2.402377
52	6	0	6.554331	-2.923101	1.557004
53	6	0	5.612173	-3.124074	0.575642
54	8	0	7.526777	-1.739271	3.317330
55	6	0	7.555796	-0.621632	4.184338
56	1	0	5.491829	0.044275	2.907485
57	1	0	7.354906	-3.632939	1.715192
58	1	0	5.649140	-4.000621	-0.058738
59	1	0	6.650008	-0.575515	4.794848
60	1	0	8.421087	-0.761023	4.826635
61	1	0	7.662918	0.308817	3.620450
62	6	0	1.070855	-1.370609	-1.956706
63	1	0	1.813402	-1.776014	-2.643454
64	1	0	0.577059	-2.194925	-1.429206
65	1	0	0.286039	-0.859596	-2.514861
66	6	0	1.876883	3.884996	-0.698226
67	6	0	0.574825	4.329252	-0.140976
68	6	0	1.822204	2.661558	-1.494246
69	6	0	0.640213	1.869830	-1.513596
70	6	0	-0.574795	3.563689	-0.311606
71	8	0	-0.554686	2.381562	-1.046302
72	8	0	2.913254	4.498559	-0.489934
73	6	0	2.991726	2.030724	-1.917941
74	6	0	2.996091	0.799311	-2.543695
75	1	0	0.423073	1.269204	-2.388114
76	1	0	3.936947	2.460736	-1.601412

77	6	0	4.270279	0.076826	-2.647843
78	8	0	5.302824	0.398687	-2.107124
79	1	0	2.189301	0.469001	-3.181313
80	8	0	4.144626	-1.053669	-3.382586
81	6	0	5.351803	-1.821354	-3.476164
82	1	0	6.133917	-1.232866	-3.951497
83	1	0	5.688170	-2.114742	-2.481983
84	1	0	5.102782	-2.688618	-4.080796
85	6	0	0.480933	5.509946	0.600348
86	6	0	-0.731988	5.901888	1.143659
87	6	0	-1.866793	5.107924	0.957282
88	6	0	-1.799517	3.929133	0.225583
89	1	0	1.384339	6.091299	0.729543
90	1	0	-0.800472	6.817793	1.714955
91	1	0	-2.814776	5.405610	1.386042
92	1	0	-2.667188	3.298180	0.077756

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cis-exo-c-TS-Re

Standard orientation:

Imaginary frequency: -422.4492 cm^{-1}

Electronic energy E = -4188.771118 a.u.

Enthalpy H = -4188.724355 a.u.

Entropy S = 265.848 cal/mol/K

Gibbs free energy G = -4188.850668 a.u.

Total free energy in solution E_{sol}= -4190.36150 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.950029	-0.255398	-0.240031
2	7	0	1.088425	-1.316534	0.860075
3	6	0	1.968073	-1.331744	-0.190224
4	6	0	2.907607	0.846867	0.575700
5	6	0	1.516474	-0.510488	2.036500
6	6	0	1.879098	0.921778	1.654644
7	6	0	3.900003	1.756766	0.092219
8	6	0	4.508861	1.132002	-1.025845
9	7	0	3.899125	-0.087382	-1.224340
10	1	0	4.165645	-0.782884	-1.902819
11	1	0	2.405351	-0.970514	2.483841
12	1	0	0.693642	-0.532368	2.750490
13	1	0	2.256956	1.430446	2.544198
14	1	0	0.993616	1.476780	1.324061
15	6	0	4.325480	3.026854	0.497010
16	6	0	5.347194	3.643506	-0.206383
17	6	0	5.950259	3.008667	-1.314249
18	6	0	5.537526	1.753380	-1.731566
19	8	0	5.719187	4.876781	0.243759
20	6	0	6.701104	5.581324	-0.489923
21	1	0	3.880058	3.542142	1.337420
22	1	0	6.744014	3.499981	-1.857761
23	1	0	5.998116	1.282442	-2.590789
24	1	0	6.382041	5.746843	-1.522463
25	1	0	6.816614	6.539230	0.010024
26	1	0	7.658654	5.053343	-0.483947
27	6	0	1.436058	-1.805335	-1.516605
28	1	0	0.921741	-0.961782	-1.985742
29	1	0	2.242692	-2.154240	-2.161063
30	1	0	0.701591	-2.598805	-1.396429
31	6	0	-4.804710	-0.736177	-2.273237
32	6	0	-5.483846	0.098476	-1.347194
33	6	0	-4.715406	0.873147	-0.432658
34	6	0	-3.281529	0.805713	-0.448276
35	6	0	-3.445136	-0.838034	-2.242455

36	6	0	-2.663988	-0.104553	-1.301427
37	6	0	-2.514624	1.782085	0.390022
38	6	0	-2.574622	3.171539	0.034349
39	6	0	-2.002023	4.157782	0.885131
40	6	0	-1.364523	3.741757	2.081864
41	6	0	-1.810209	1.410636	1.531683
42	6	0	-1.269404	2.415975	2.388471
43	6	0	-6.898286	0.173867	-1.323058
44	6	0	-7.546581	0.979967	-0.423386
45	6	0	-6.791232	1.744902	0.493044
46	6	0	-5.419617	1.697034	0.487245
47	6	0	-3.197218	3.616270	-1.163875
48	6	0	-3.251186	4.949358	-1.483886
49	6	0	-2.691681	5.923523	-0.627365
50	6	0	-2.078120	5.527496	0.532341
51	1	0	-5.385379	-1.300491	-2.995133
52	1	0	-2.906555	-1.492278	-2.916829
53	1	0	-7.458562	-0.421914	-2.035338
54	1	0	-8.627951	1.031166	-0.411346
55	1	0	-7.300453	2.376711	1.210205
56	1	0	-4.854248	2.284171	1.198056
57	1	0	-3.622798	2.882228	-1.834122
58	1	0	-3.726595	5.257933	-2.406754
59	1	0	-2.745265	6.972378	-0.890441
60	1	0	-1.636422	6.257374	1.201867
61	1	0	-0.950518	4.493617	2.744604
62	1	0	-0.780426	2.075114	3.293572
63	8	0	-1.615887	0.131824	1.896137
64	8	0	-1.342642	-0.351175	-1.284842
65	30	0	-0.855272	-0.787111	0.452481
66	6	0	0.055840	-4.769627	-0.050206
67	6	0	-1.285500	-4.175012	0.151371
68	6	0	1.118380	-4.054228	0.672431
69	6	0	0.772201	-3.089783	1.652095
70	6	0	-1.493876	-3.241716	1.170695
71	8	0	-0.498586	-2.967611	2.094441
72	8	0	0.267483	-5.678129	-0.833683
73	6	0	2.382779	-3.982066	0.100688
74	6	0	3.284425	-2.981546	0.443443
75	1	0	1.463110	-2.882116	2.457846
76	1	0	2.568574	-4.584136	-0.782804
77	6	0	4.518959	-2.814913	-0.342115
78	8	0	4.619255	-3.049037	-1.532420
79	1	0	3.330142	-2.578981	1.446699
80	8	0	5.504160	-2.297682	0.397687
81	6	0	6.715841	-2.001496	-0.309888
82	1	0	7.056439	-2.877788	-0.856557
83	1	0	6.546453	-1.177516	-1.002348
84	1	0	7.432569	-1.710475	0.450990
85	6	0	-2.333642	-4.449490	-0.727979
86	6	0	-3.546901	-3.790227	-0.595570
87	6	0	-3.728173	-2.850660	0.420509
88	6	0	-2.709784	-2.581920	1.331736
89	1	0	-2.153293	-5.168767	-1.516154
90	1	0	-4.347547	-3.979335	-1.297452
91	1	0	-4.659904	-2.305443	0.496796
92	1	0	-2.826811	-1.858660	2.127654

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cis-exo-c-TS-Si Imaginary frequency: -464.4711 cm^{-1}

Standard orientation: Electronic energy E = -4188.770155 a.u.

Enthalpy H = -4188.723648 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.144743	-4.052311	-1.020656
2	6	0	1.344003	-3.661195	-0.241767
3	6	0	-1.112395	-3.549897	-0.440326
4	6	0	-1.104946	-2.981471	0.859263
5	6	0	1.196600	-3.120875	1.041295
6	8	0	-0.034700	-3.120020	1.673643
7	8	0	0.205074	-4.635320	-2.087284
8	6	0	-2.178348	-3.231840	-1.270963
9	6	0	-3.199005	-2.394459	-0.834988
10	1	0	-2.011622	-2.980389	1.447711
11	1	0	-2.096190	-3.472739	-2.325676
12	6	0	-4.221536	-1.921714	-1.787591
13	8	0	-4.051328	-1.792920	-2.982472
14	1	0	-3.511509	-2.380564	0.199222
15	8	0	-5.355019	-1.594660	-1.155236
16	6	0	-6.382841	-1.048790	-1.991227
17	1	0	-5.995843	-0.202418	-2.554995
18	1	0	-7.168785	-0.728779	-1.314720
19	1	0	-6.742560	-1.809070	-2.682362
20	6	0	2.615119	-3.680388	-0.812625
21	6	0	3.702915	-3.162586	-0.122691
22	6	0	3.531785	-2.607487	1.144370
23	6	0	2.275164	-2.597240	1.747636
24	1	0	2.708860	-4.072206	-1.816411
25	1	0	4.679964	-3.146593	-0.585506
26	1	0	4.367555	-2.157702	1.664540
27	1	0	2.121903	-2.186762	2.737089
28	6	0	2.076220	2.247378	-3.260028
29	6	0	2.737647	3.160346	-2.399693
30	6	0	3.151062	2.712782	-1.113595
31	6	0	2.909942	1.359511	-0.705424
32	6	0	1.810937	0.974603	-2.846424
33	6	0	2.192875	0.516149	-1.549389
34	6	0	3.494172	0.890889	0.590271
35	6	0	4.917756	0.767799	0.703245
36	6	0	5.520208	0.475690	1.960077
37	6	0	4.684411	0.311494	3.095365
38	6	0	2.705235	0.626427	1.707168
39	6	0	3.326727	0.379066	2.968174
40	8	0	1.852503	-0.740544	-1.224088
41	8	0	1.367349	0.562776	1.659904
42	1	0	1.784693	2.577715	-4.250911
43	1	0	1.311443	0.261034	-3.490653
44	6	0	2.992747	4.495018	-2.799754
45	6	0	3.802327	3.651402	-0.267154
46	6	0	6.928842	0.353660	2.058129
47	6	0	5.776326	0.915051	-0.421150
48	1	0	5.141000	0.124053	4.061145
49	1	0	2.669446	0.245203	3.819353
50	6	0	3.629426	5.373167	-1.961973
51	6	0	4.031370	4.940022	-0.678575
52	6	0	7.136355	0.783687	-0.298103
53	6	0	7.727745	0.504395	0.954770
54	1	0	5.336066	1.124816	-1.386401
55	1	0	7.765009	0.895365	-1.172993
56	1	0	8.803046	0.408961	1.037749
57	1	0	7.361323	0.137010	3.028859
58	1	0	2.670440	4.807467	-3.786941
59	1	0	3.820313	6.391737	-2.275412

Entropy S = 262.800 cal/mol/K
Gibbs free energy G = -4188.848512 a.u.
Total free energy in solution E_{sol}= -4190.36215 a.u.

60	1	0	4.524852	5.634397	-0.009731
61	1	0	4.108972	3.337185	0.720961
62	30	0	0.899768	-0.722169	0.378499
63	6	0	-3.015060	0.264332	-0.168724
64	7	0	-1.139662	-1.048902	0.597870
65	6	0	-1.915610	-0.641957	-0.463418
66	6	0	-1.236090	-0.517478	-1.799454
67	6	0	-3.594886	0.399823	1.067047
68	6	0	-1.509399	-0.513656	1.943359
69	6	0	-3.008650	-0.356288	2.214846
70	1	0	-1.951383	-0.593859	-2.618861
71	1	0	-0.733297	0.456008	-1.842006
72	1	0	-0.464157	-1.274476	-1.929094
73	6	0	-4.715928	1.266785	0.909035
74	6	0	-4.752373	1.628449	-0.458270
75	7	0	-3.713245	0.994556	-1.100734
76	1	0	-3.471757	1.092679	-2.071701
77	1	0	-1.033251	-1.161489	2.679585
78	1	0	-1.026383	0.462211	2.022008
79	1	0	-3.504930	-1.324954	2.348526
80	1	0	-3.124118	0.184486	3.156650
81	6	0	-5.731924	2.494175	-0.960356
82	6	0	-5.685989	1.770634	1.799217
83	6	0	-6.654230	2.616877	1.293458
84	6	0	-6.673072	2.973428	-0.077998
85	8	0	-7.653755	3.176799	2.029751
86	6	0	-7.677288	2.882897	3.412629
87	1	0	-6.758916	3.219838	3.901043
88	1	0	-8.526683	3.423379	3.821455
89	1	0	-5.657566	1.492666	2.843023
90	1	0	-5.753660	2.779702	-2.004624
91	1	0	-7.455890	3.643844	-0.405738
92	1	0	-7.808602	1.811037	3.584947

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trans-endo-c-TS-Re

Imaginary frequency: -431.4868 cm^{-1}

Standard orientation:

Electronic energy E = -4188.774567 a.u.

Enthalpy H = -4188.727645 a.u.

Entropy S = 269.085 cal/mol/K

Gibbs free energy G = -4188.855496 a.u.

Total free energy in solution E_{sol}= -4190.36584 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.658904	4.325233	0.923958
2	6	0	-3.735881	4.165889	0.014097
3	6	0	-3.996904	2.873451	-0.519062
4	6	0	-3.189317	1.754340	-0.129910
5	6	0	-1.871416	3.263795	1.258723
6	6	0	-2.107492	1.965449	0.720027
7	6	0	-3.600990	0.390195	-0.595479
8	6	0	-4.794062	-0.184471	-0.041047
9	6	0	-5.308770	-1.408812	-0.552828
10	6	0	-4.619260	-2.047017	-1.617919
11	6	0	-2.912828	-0.310192	-1.586296
12	6	0	-3.461136	-1.520193	-2.108147
13	6	0	-4.545466	5.263794	-0.366872
14	6	0	-5.581088	5.103115	-1.250387
15	6	0	-5.839985	3.824185	-1.791393
16	6	0	-5.074223	2.742337	-1.436844

17	6	0	-5.481630	0.419601	1.047034
18	6	0	-6.604586	-0.158517	1.584350
19	6	0	-7.115719	-1.368868	1.064230
20	6	0	-6.475241	-1.976771	0.015505
21	1	0	-2.467579	5.307276	1.342058
22	1	0	-1.037344	3.367119	1.941572
23	1	0	-4.325296	6.237790	0.056044
24	1	0	-6.194580	5.947739	-1.537321
25	1	0	-6.650801	3.696065	-2.497825
26	1	0	-5.278380	1.771164	-1.866804
27	1	0	-5.096170	1.343379	1.456503
28	1	0	-7.104788	0.319584	2.417380
29	1	0	-8.005517	-1.810658	1.494298
30	1	0	-6.848463	-2.908219	-0.395399
31	1	0	-5.019238	-2.970112	-2.022029
32	1	0	-2.907794	-2.005483	-2.902547
33	8	0	-1.713278	0.083344	-2.059118
34	8	0	-1.245420	0.992883	1.076077
35	30	0	-0.749377	0.099142	-0.464702
36	6	0	3.282592	0.352871	-0.729242
37	7	0	1.154188	-0.676007	-0.346050
38	6	0	2.116877	-0.336045	-1.247354
39	6	0	3.320938	0.910988	0.530912
40	6	0	1.584328	-0.685685	1.077851
41	6	0	2.193490	0.654269	1.475461
42	6	0	4.511683	1.690695	0.600861
43	6	0	5.152082	1.558106	-0.653209
44	7	0	4.371416	0.768647	-1.463200
45	1	0	4.645896	0.375715	-2.352108
46	1	0	2.338965	-1.463262	1.217669
47	1	0	0.704166	-0.911090	1.680278
48	1	0	2.541033	0.581316	2.507899
49	1	0	1.431806	1.440380	1.438357
50	6	0	5.090968	2.480381	1.615643
51	6	0	6.298051	3.095027	1.347180
52	6	0	6.936271	2.938980	0.090217
53	6	0	6.381007	2.180717	-0.914044
54	8	0	6.977325	3.884144	2.224160
55	6	0	6.383671	4.096509	3.490325
56	1	0	4.592756	2.586963	2.568377
57	1	0	7.879805	3.448204	-0.052125
58	1	0	6.872908	2.080288	-1.873113
59	1	0	6.268948	3.154275	4.033154
60	1	0	7.059635	4.750157	4.034709
61	1	0	5.408009	4.579395	3.389988
62	6	0	1.672750	0.021165	-2.645233
63	1	0	1.426490	1.087187	-2.653575
64	1	0	2.474014	-0.152888	-3.363008
65	1	0	0.775244	-0.516758	-2.951511
66	6	0	1.019197	-3.992190	1.045262
67	6	0	-0.314461	-3.719658	1.626192
68	6	0	1.303660	-3.286210	-0.211888
69	6	0	0.381912	-2.338630	-0.724995
70	6	0	-1.188888	-2.825728	1.014895
71	8	0	-0.862440	-2.194568	-0.180782
72	8	0	1.825916	-4.740622	1.573242
73	6	0	2.603679	-3.235060	-0.707850
74	6	0	2.943229	-2.455407	-1.805357
75	1	0	0.317347	-2.165100	-1.790651
76	1	0	3.375543	-3.711560	-0.113519
77	6	0	4.330132	-2.169390	-2.180715
78	8	0	4.637204	-1.543143	-3.184032

79	8	0	5.223158	-2.576599	-1.275074
80	6	0	6.584230	-2.211296	-1.542451
81	1	0	7.171855	-2.705159	-0.775601
82	1	0	6.697608	-1.129968	-1.468905
83	1	0	6.876422	-2.545139	-2.535263
84	6	0	-0.718848	-4.333048	2.815821
85	6	0	-1.962436	-4.053758	3.358223
86	6	0	-2.816285	-3.150074	2.717377
87	6	0	-2.437449	-2.525300	1.537171
88	1	0	-0.028643	-5.022612	3.283722
89	1	0	-2.272929	-4.531588	4.277692
90	1	0	-3.788814	-2.926270	3.136063
91	1	0	-3.079328	-1.819137	1.026030
92	1	0	2.244695	-2.317860	-2.617210

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trans-endo-c-TS-Si

Imaginary frequency: -457.6268 cm^{-1}

Standard orientation:

Electronic energy E = -4188.768195 a.u.

Enthalpy H = -4188.721140 a.u.

Entropy S = 272.020 cal/mol/K

Gibbs free energy G = -4188.850385 a.u.

Total free energy in solution E_{sol}= -4190.35896 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.036021	1.970477	1.923330
2	6	0	-5.873718	1.274541	1.013899
3	6	0	-5.331555	0.184126	0.278479
4	6	0	-3.962372	-0.203778	0.460403
5	6	0	-3.723787	1.622820	2.062423
6	6	0	-3.157542	0.550372	1.311377
7	6	0	-3.493116	-1.466628	-0.201785
8	6	0	-4.007146	-2.713433	0.287722
9	6	0	-3.741032	-3.924706	-0.408716
10	6	0	-2.957867	-3.875167	-1.590651
11	6	0	-2.660370	-1.474778	-1.319705
12	6	0	-2.433483	-2.693330	-2.025682
13	6	0	-7.228967	1.644598	0.834394
14	6	0	-8.032738	0.969203	-0.046707
15	6	0	-7.498779	-0.108106	-0.788018
16	6	0	-6.190657	-0.491401	-0.630201
17	6	0	-4.791324	-2.789885	1.471023
18	6	0	-5.276585	-3.990665	1.923206
19	6	0	-5.016136	-5.188655	1.220954
20	6	0	-4.261054	-5.149294	0.078079
21	1	0	-5.455882	2.785119	2.503357
22	1	0	-3.062326	2.147126	2.741305
23	1	0	-7.616990	2.477034	1.411149
24	1	0	-9.067593	1.258242	-0.178838
25	1	0	-8.128775	-0.637456	-1.492033
26	1	0	-5.793587	-1.312764	-1.210647
27	1	0	-4.993208	-1.881379	2.021717
28	1	0	-5.865816	-4.020492	2.831346
29	1	0	-5.409237	-6.128388	1.587596
30	1	0	-4.045943	-6.057092	-0.474659
31	1	0	-2.779274	-4.792892	-2.139927
32	1	0	-1.833264	-2.637371	-2.925630
33	8	0	-2.037897	-0.368493	-1.779029
34	8	0	-1.836180	0.331224	1.461769
35	30	0	-1.169569	0.257720	-0.259295
36	6	0	2.842674	-1.053895	-0.173677
37	7	0	0.927021	0.377349	-0.363682
38	6	0	1.680311	-0.622418	-0.906592
39	6	0	3.430262	-0.345914	0.851187
40	6	0	1.326928	0.886330	0.987530

41	6	0	2.825049	0.944035	1.298259
42	6	0	4.601413	-1.058962	1.229002
43	6	0	4.667590	-2.197743	0.390587
44	7	0	3.580658	-2.184676	-0.448719
45	1	0	3.484487	-2.745567	-1.279213
46	1	0	0.848735	0.203387	1.693243
47	1	0	0.853967	1.857116	1.122262
48	1	0	2.928514	1.079845	2.377603
49	1	0	3.313338	1.797295	0.820665
50	6	0	5.599209	-0.833419	2.200852
51	6	0	6.630108	-1.746875	2.294555
52	6	0	6.683757	-2.881913	1.444592
53	6	0	5.714878	-3.123976	0.498936
54	8	0	7.663124	-1.660840	3.176098
55	6	0	7.655556	-0.563333	4.068755
56	1	0	5.542964	0.035928	2.839749
57	1	0	7.517582	-3.558458	1.574608
58	1	0	5.762496	-3.999715	-0.135649
59	1	0	6.760685	-0.575493	4.696518
60	1	0	8.539298	-0.674935	4.691037
61	1	0	7.706603	0.384509	3.526208
62	6	0	1.006052	-1.564962	-1.864817
63	1	0	1.715497	-1.984385	-2.578152
64	1	0	0.559613	-2.377540	-1.280303
65	1	0	0.185313	-1.079168	-2.393994
66	6	0	1.970205	3.705597	-0.794434
67	6	0	0.711592	4.213999	-0.196413
68	6	0	1.833338	2.469921	-1.563177
69	6	0	0.620490	1.726641	-1.515260
70	6	0	-0.474188	3.492543	-0.307299
71	8	0	-0.529662	2.293187	-1.008461
72	8	0	3.040291	4.276394	-0.639461
73	6	0	2.957711	1.795253	-2.036402
74	6	0	2.869867	0.550579	-2.633333
75	1	0	0.340174	1.112579	-2.362099
76	1	0	3.926293	2.210577	-1.781189
77	6	0	4.032604	-0.318168	-2.845001
78	8	0	3.962389	-1.421944	-3.357610
79	1	0	1.999224	0.250988	-3.197484
80	8	0	5.165836	0.186240	-2.343525
81	6	0	6.318846	-0.656512	-2.467905
82	1	0	6.184154	-1.559069	-1.874324
83	1	0	6.477730	-0.922759	-3.510813
84	1	0	7.147907	-0.071012	-2.083812
85	6	0	0.693851	5.413414	0.520568
86	6	0	-0.480625	5.867342	1.098475
87	6	0	-1.653608	5.118181	0.970131
88	6	0	-1.662042	3.921793	0.264784
89	1	0	1.624061	5.959811	0.603159
90	1	0	-0.490400	6.797161	1.650888
91	1	0	-2.572300	5.465223	1.424753
92	1	0	-2.559383	3.324462	0.162655

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trans-exo-c-TS-Re

Imaginary frequency: -425.0754 cm^{-1}

Standard orientation:

Electronic energy E = -4188.764449 a.u.

Enthalpy H = -4188.717556 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.052941	-0.041282	-0.059230
2	7	0	1.233300	-1.232815	0.974075
3	6	0	2.127633	-1.162762	-0.071127
4	6	0	2.839500	1.077575	0.712879
5	6	0	1.567681	-0.380007	2.152019
6	6	0	1.767610	1.071426	1.745095
7	6	0	3.745272	2.083704	0.257215
8	6	0	4.495454	1.495423	-0.787616
9	7	0	4.022209	0.217169	-1.016212
10	1	0	4.633016	-0.508887	-1.358116
11	1	0	2.500411	-0.739580	2.601678
12	1	0	0.748246	-0.486667	2.861341
13	1	0	2.055425	1.647953	2.626810
14	1	0	0.837844	1.511985	1.369045
15	6	0	3.990576	3.405958	0.644343
16	6	0	4.998847	4.105585	0.002977
17	6	0	5.763906	3.499111	-1.018269
18	6	0	5.519636	2.196481	-1.420616
19	8	0	5.196868	5.387680	0.424268
20	6	0	6.172327	6.161680	-0.245912
21	1	0	3.421621	3.894874	1.423719
22	1	0	6.552892	4.052279	-1.506097
23	1	0	6.106154	1.747026	-2.211241
24	1	0	5.943795	6.251827	-1.311230
25	1	0	6.139846	7.145539	0.214627
26	1	0	7.172226	5.737293	-0.121556
27	6	0	1.654667	-1.655807	-1.410439
28	1	0	1.007497	-0.885986	-1.841743
29	1	0	2.495020	-1.837874	-2.078473
30	1	0	1.058273	-2.561419	-1.316437
31	6	0	-4.628019	-1.107350	-2.253288
32	6	0	-5.371280	-0.268399	-1.381556
33	6	0	-4.665419	0.606892	-0.509034
34	6	0	-3.229991	0.634866	-0.510970
35	6	0	-3.265261	-1.120873	-2.202977
36	6	0	-2.545618	-0.286991	-1.297929
37	6	0	-2.543242	1.720456	0.259092
38	6	0	-2.702840	3.071863	-0.198454
39	6	0	-2.219019	4.158350	0.582299
40	6	0	-1.570655	3.880155	1.812647
41	6	0	-1.824338	1.487860	1.427550
42	6	0	-1.376833	2.591227	2.214535
43	6	0	-6.787773	-0.286917	-1.370419
44	6	0	-7.497107	0.522949	-0.521621
45	6	0	-6.803731	1.387676	0.353907
46	6	0	-5.432011	1.433031	0.357908
47	6	0	-3.338079	3.379960	-1.432596
48	6	0	-3.485100	4.678440	-1.851283
49	6	0	-3.013089	5.752035	-1.063887
50	6	0	-2.390717	5.488917	0.128364
51	1	0	-5.161936	-1.747284	-2.947721
52	1	0	-2.677660	-1.776987	-2.833111
53	1	0	-7.299939	-0.958774	-2.050588
54	1	0	-8.579512	0.501574	-0.518593
55	1	0	-7.361147	2.022975	1.031075
56	1	0	-4.913965	2.097086	1.036486
57	1	0	-3.696585	2.569421	-2.052107
58	1	0	-3.966918	4.881691	-2.799613
59	1	0	-3.139188	6.771687	-1.404953

Entropy S = 268.712cal/mol/K
Gibbs free energy G = -4188.845230 a.u.
Total free energy in solution E_{sol}= -4190.35519 a.u.

60	1	0	-2.014463	6.296567	0.746423
61	1	0	-1.226384	4.707299	2.423515
62	1	0	-0.877166	2.355538	3.146627
63	8	0	-1.530686	0.258879	1.884604
64	8	0	-1.211109	-0.450485	-1.247328
65	30	0	-0.744440	-0.756304	0.523916
66	6	0	0.238229	-4.678632	0.173914
67	6	0	-1.104503	-4.098874	0.410801
68	6	0	1.315437	-3.930816	0.830857
69	6	0	1.000514	-2.908099	1.770395
70	6	0	-1.286121	-3.135143	1.407817
71	8	0	-0.257356	-2.810665	2.277693
72	8	0	0.426693	-5.613292	-0.586616
73	6	0	2.570659	-3.919482	0.243413
74	6	0	3.522209	-2.933227	0.476046
75	1	0	1.719081	-2.713236	2.556405
76	1	0	2.714850	-4.600140	-0.587295
77	6	0	4.728420	-2.858548	-0.360715
78	8	0	5.637761	-2.069931	-0.186010
79	1	0	3.616960	-2.410263	1.418451
80	8	0	4.703594	-3.708089	-1.404591
81	6	0	5.859507	-3.663558	-2.249962
82	1	0	5.933636	-2.693140	-2.739510
83	1	0	6.760255	-3.837551	-1.665269
84	1	0	5.712677	-4.449553	-2.983508
85	6	0	-2.186127	-4.433606	-0.403071
86	6	0	-3.412185	-3.807618	-0.228574
87	6	0	-3.570693	-2.841056	0.764724
88	6	0	-2.514751	-2.510655	1.611306
89	1	0	-2.023937	-5.176353	-1.173128
90	1	0	-4.241751	-4.045492	-0.879927
91	1	0	-4.515223	-2.324606	0.874426
92	1	0	-2.614579	-1.764459	2.387552

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trans-exo-c-TS-Si

Imaginary frequency: -464.5850 cm^{-1}

Standard orientation:

Electronic energy E = -4188.764743 a.u.

Enthalpy H = -4188.717889 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 266.575 cal/mol/K

Gibbs free energy G = -4188.844547 a.u.

Total free energy in solution E_{sol} = -4190.35737 a.u.

1	6	0	-0.093448	-4.109168	0.780408
2	6	0	-1.303680	-3.680420	0.038334
3	6	0	1.154231	-3.578945	0.209361
4	6	0	1.130338	-2.938429	-1.057377
5	6	0	-1.173346	-3.074012	-1.216833
6	8	0	0.048426	-3.043073	-1.865290
7	8	0	-0.140860	-4.742883	1.819447
8	6	0	2.236699	-3.315790	1.038826
9	6	0	3.250541	-2.454057	0.635874
10	1	0	2.028799	-2.920594	-1.658512
11	1	0	2.167320	-3.634535	2.072780
12	6	0	4.366647	-2.058571	1.516020
13	8	0	5.445899	-1.696731	1.111674
14	1	0	3.528295	-2.370293	-0.404768
15	8	0	4.040183	-2.097323	2.824820
16	6	0	5.106963	-1.719546	3.706174
17	1	0	5.952189	-2.393380	3.581405
18	1	0	4.697965	-1.792331	4.708914
19	1	0	5.430092	-0.703157	3.485650
20	6	0	-2.566929	-3.730444	0.624397
21	6	0	-3.664078	-3.177220	-0.022170

22	6	0	-3.509948	-2.554579	-1.259575
23	6	0	-2.261708	-2.513506	-1.879355
24	1	0	-2.647224	-4.175210	1.607133
25	1	0	-4.634706	-3.186917	0.454122
26	1	0	-4.352121	-2.076953	-1.743294
27	1	0	-2.122318	-2.052428	-2.848472
28	6	0	-1.974534	2.076712	3.354184
29	6	0	-2.627152	3.041938	2.546029
30	6	0	-3.057551	2.665465	1.242827
31	6	0	-2.840579	1.331408	0.764384
32	6	0	-1.730167	0.823392	2.873540
33	6	0	-2.126239	0.437061	1.556965
34	6	0	-3.450300	0.933783	-0.543464
35	6	0	-4.876985	0.832100	-0.638087
36	6	0	-5.502830	0.603241	-1.896792
37	6	0	-4.686976	0.479465	-3.051712
38	6	0	-2.682562	0.711554	-1.683828
39	6	0	-3.326742	0.526139	-2.944114
40	8	0	-1.800871	-0.803332	1.163793
41	8	0	-1.344771	0.633286	-1.661293
42	1	0	-1.672952	2.351802	4.358947
43	1	0	-1.237794	0.070048	3.476866
44	6	0	-2.857365	4.358787	3.014403
45	6	0	-3.700816	3.655195	0.450095
46	6	0	-6.914275	0.502708	-1.977249
47	6	0	-5.716013	0.938276	0.505629
48	1	0	-5.160882	0.339475	-4.017156
49	1	0	-2.684789	0.423037	-3.811130
50	6	0	-3.485797	5.287740	2.226732
51	6	0	-3.905233	4.925224	0.926997
52	6	0	-7.079323	0.828653	0.398883
53	6	0	-7.693850	0.613543	-0.855614
54	1	0	-5.258426	1.098487	1.472243
55	1	0	-7.692637	0.907994	1.288081
56	1	0	-8.771438	0.535021	-0.925290
57	1	0	-7.364648	0.334932	-2.949499
58	1	0	-2.522418	4.616303	4.013199
59	1	0	-3.657229	6.292459	2.591753
60	1	0	-4.392201	5.659933	0.297707
61	1	0	-4.019697	3.395033	-0.549844
62	30	0	-0.872888	-0.717707	-0.452013
63	6	0	3.030180	0.262473	0.101158
64	7	0	1.167530	-1.042054	-0.710115
65	6	0	1.949983	-0.670934	0.362238
66	6	0	1.279970	-0.617089	1.707453
67	6	0	3.601237	0.455992	-1.131922
68	6	0	1.524272	-0.443199	-2.033103
69	6	0	3.021225	-0.266046	-2.304397
70	1	0	2.009841	-0.684785	2.513677
71	1	0	0.735018	0.330873	1.787339
72	1	0	0.545779	-1.412225	1.825333
73	6	0	4.688830	1.358920	-0.952875
74	6	0	4.718503	1.680145	0.423940
75	7	0	3.710572	0.986219	1.053232
76	1	0	3.429310	1.107475	2.009982
77	1	0	1.045534	-1.058820	-2.794588
78	1	0	1.036836	0.533297	-2.062343
79	1	0	3.526114	-1.224173	-2.474770
80	1	0	3.129509	0.310447	-3.225643
81	6	0	5.659407	2.576619	0.944730
82	6	0	5.628101	1.931098	-1.834490
83	6	0	6.557872	2.807522	-1.310313

84	6	0	6.568036	3.126260	0.070598
85	8	0	7.524845	3.435105	-2.035616
86	6	0	7.568089	3.161360	-3.421875
87	1	0	6.637464	3.462437	-3.910804
88	1	0	8.393495	3.745754	-3.819398
89	1	0	5.607365	1.679015	-2.884941
90	1	0	5.679698	2.828559	1.997296
91	1	0	7.322643	3.821127	0.413237
92	1	0	7.749116	2.099065	-3.607135

5.3.2 models of activation of ester carbonyl group of diene 2a

trans-2a as diene

(R)-5a-trans-2a

Imaginary frequency: none

Standard orientation:

Electronic energy E = -2698.517722 a.u.

Enthalpy H = -2698.500052 a.u.

Entropy S = 131.696 cal/mol/K

Gibbs free energy G = -2698.562626 a.u.

Total free energy in solution E_{sol} = -2699.25145 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.827666	-2.654181	-1.708326
2	6	0	-5.188057	-2.693902	-1.785758
3	6	0	-5.981618	-1.776316	-1.049124
4	6	0	-5.332915	-0.798378	-0.245790
5	6	0	-3.901571	-0.742674	-0.196238
6	6	0	-3.162461	-1.688822	-0.900082
7	6	0	6.291123	0.739887	-0.560770
8	6	0	7.720321	0.396952	-0.443132
9	6	0	5.374701	-0.310173	-0.076725
10	6	0	5.882090	-1.483323	0.368560
11	6	0	8.107533	-0.841623	0.062458
12	8	0	7.181258	-1.778838	0.451301
13	8	0	5.896336	1.800283	-1.015730
14	6	0	3.946215	-0.036416	-0.145039
15	6	0	2.971029	-0.726171	0.467840
16	1	0	5.274096	-2.316835	0.691960
17	1	0	3.689474	0.830135	-0.743104
18	6	0	1.561806	-0.375338	0.315410
19	8	0	0.689215	-1.020954	0.920961
20	1	0	3.147713	-1.567702	1.123820
21	8	0	1.308698	0.643319	-0.463987
22	6	0	-0.068370	1.077347	-0.615767
23	1	0	-0.652213	0.291867	-1.093524
24	1	0	-0.473804	1.344667	0.359586
25	1	0	-0.015948	1.955981	-1.248682
26	30	0	-1.233432	-1.387870	0.842387
27	8	0	-2.352954	-1.005325	2.288289
28	8	0	-1.817304	-1.745466	-0.869375
29	6	0	8.711742	1.305403	-0.831475
30	6	0	10.047673	0.971286	-0.708705
31	6	0	10.411000	-0.280917	-0.195398
32	6	0	9.447148	-1.196425	0.192394
33	1	0	8.390880	2.261801	-1.222544
34	1	0	10.813815	1.673859	-1.007545
35	1	0	11.457210	-0.540344	-0.099543
36	1	0	9.701732	-2.169539	0.589098
37	6	0	-3.263456	0.388785	0.553554

38	6	0	-3.354647	1.713325	0.007596
39	6	0	-2.898919	2.834354	0.756639
40	6	0	-2.650065	0.212500	1.798645
41	6	0	-2.238369	1.355264	2.554516
42	6	0	-2.366990	2.618847	2.057265
43	1	0	-5.682971	-3.433901	-2.404695
44	1	0	-3.204369	-3.353431	-2.250601
45	6	0	-7.395910	-1.821776	-1.100398
46	6	0	-6.150294	0.099141	0.492703
47	6	0	-3.866136	1.951054	-1.297062
48	6	0	-2.972175	4.133376	0.198132
49	1	0	-2.047396	3.475746	2.640001
50	1	0	-1.812650	1.164516	3.531572
51	6	0	-3.917719	3.220851	-1.816415
52	6	0	-3.469844	4.329709	-1.064582
53	6	0	-8.157030	-0.936649	-0.381583
54	6	0	-7.519301	0.030351	0.426227
55	1	0	-7.864591	-2.577189	-1.721408
56	1	0	-9.237941	-0.979378	-0.425452
57	1	0	-8.117510	0.723564	1.004630
58	1	0	-5.676885	0.837345	1.125751
59	1	0	-4.209657	1.107910	-1.881086
60	1	0	-4.307450	3.373873	-2.815073
61	1	0	-3.520974	5.325825	-1.485269
62	1	0	-2.622806	4.971086	0.791418

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trans-endo-TS1-Re

Imaginary frequency: -272.0706 cm^{-1}

Standard orientation:

Electronic energy E = -4188.794797 a.u.

Enthalpy H = -4188.747695 a.u.

Entropy S = 271.649 cal/mol/K

Gibbs free energy G = -4188.876764a.u.

Total free energy in solution E_{sol}= -4190.39004 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.427352	0.377510	0.804063
2	7	0	3.506399	-0.706861	1.187784
3	6	0	2.213616	-0.812677	1.079681
4	6	0	1.513654	-2.105759	1.379250
5	6	0	1.990584	1.552144	0.397490
6	6	0	4.097070	0.641528	1.229471
7	6	0	3.474972	1.667248	0.277614
8	1	0	0.573282	-2.220861	0.838495
9	1	0	2.150682	-2.973145	1.220308
10	1	0	1.270555	-2.091557	2.446906
11	6	0	0.929406	2.476334	0.119844
12	6	0	-0.269958	1.804362	0.395630
13	7	0	0.012227	0.454189	0.729879
14	1	0	-0.527802	0.064113	1.508795
15	1	0	3.955407	0.989348	2.257089
16	1	0	5.166193	0.546425	1.058249
17	1	0	3.814871	2.663481	0.568285
18	1	0	3.788747	1.507583	-0.758048
19	6	0	0.926167	3.819452	-0.294509
20	6	0	-0.301721	4.454967	-0.374707
21	6	0	-1.499663	3.772025	-0.057755
22	6	0	-1.507392	2.447301	0.322376
23	1	0	-2.430880	1.925084	0.529230
24	1	0	1.854292	4.323671	-0.520051
25	1	0	-2.424021	4.327503	-0.136591
26	8	0	-0.471452	5.749737	-0.746297
27	6	0	0.692601	6.494523	-1.051057
28	1	0	0.350830	7.491149	-1.315493
29	1	0	1.358358	6.552647	-0.185818

30	1	0	1.229649	6.055302	-1.895962
31	6	0	6.156128	-0.581313	-1.104523
32	6	0	7.152982	-0.832002	-0.034785
33	6	0	4.889940	-1.271263	-0.927026
34	6	0	4.608616	-1.944651	0.297012
35	6	0	6.829317	-1.643808	1.049836
36	8	0	5.597197	-2.247994	1.168357
37	8	0	6.402480	0.158148	-2.051950
38	6	0	3.837392	-0.988200	-1.823077
39	6	0	2.567645	-1.489077	-1.738735
40	1	0	3.871160	-2.732244	0.306020
41	1	0	4.060250	-0.233768	-2.571252
42	6	0	1.436486	-0.863704	-2.348084
43	8	0	0.268919	-1.253946	-2.121026
44	1	0	2.307419	-2.327828	-1.110827
45	8	0	1.660616	0.189287	-3.116510
46	6	0	0.492797	0.881497	-3.605973
47	1	0	-0.065114	1.315325	-2.776347
48	1	0	-0.147968	0.194663	-4.152782
49	1	0	0.880565	1.658333	-4.256091
50	30	0	-1.105013	-0.746236	-0.829334
51	6	0	8.425603	-0.259074	-0.091318
52	6	0	9.350126	-0.503120	0.911138
53	6	0	9.004756	-1.327201	1.986514
54	6	0	7.743744	-1.901503	2.064492
55	1	0	8.651159	0.369043	-0.943181
56	1	0	10.336211	-0.061028	0.862571
57	1	0	9.724917	-1.522287	2.770668
58	1	0	7.453112	-2.541157	2.886555
59	8	0	-2.414325	0.374112	-1.551709
60	8	0	-1.688838	-2.043497	0.418925
61	6	0	-4.248012	-0.348572	-2.857855
62	6	0	-5.437800	-0.998991	-3.000503
63	6	0	-6.054516	-1.630119	-1.888772
64	6	0	-5.419804	-1.550708	-0.618031
65	6	0	-4.189808	-0.832172	-0.472521
66	6	0	-3.587768	-0.271117	-1.595345
67	6	0	-3.603375	-0.671645	0.892717
68	6	0	-4.260561	0.172764	1.843431
69	6	0	-3.786143	0.265321	3.183551
70	6	0	-2.450703	-1.359411	1.277313
71	6	0	-2.018569	-1.291338	2.639894
72	6	0	-2.660475	-0.507248	3.560373
73	6	0	-7.276444	-2.332156	-2.024694
74	6	0	-7.861921	-2.946153	-0.947721
75	6	0	-7.232040	-2.880743	0.314874
76	6	0	-6.049281	-2.203774	0.476667
77	6	0	-5.387604	0.966217	1.486026
78	6	0	-5.997127	1.783461	2.403226
79	6	0	-5.527357	1.859452	3.735176
80	6	0	-4.442365	1.113212	4.110849
81	1	0	-5.926427	-1.049295	-3.967318
82	1	0	-3.758425	0.130479	-3.696570
83	1	0	-7.738989	-2.375714	-3.004646
84	1	0	-8.795961	-3.481694	-1.061067
85	1	0	-7.686086	-3.373677	1.165739
86	1	0	-5.573909	-2.171279	1.447678
87	1	0	-5.754203	0.916943	0.469852
88	1	0	-6.851123	2.378301	2.103751
89	1	0	-6.023231	2.505426	4.448342
90	1	0	-4.063538	1.158869	5.125874
91	1	0	-2.317998	-0.470755	4.588759

92	1	0	-1.172042	-1.909298	2.917851

trans-endo-IM1-Re

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4189.695868 a.u.

Enthalpy H = -4189.662510 a.u.

Entropy S = 205.462 cal/mol/K

Gibbs free energy G = -4189.760132 a.u.

Total free energy in solution E_{sol} = -4190.87759 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.447667	0.407419	0.698270
2	7	0	3.541528	-0.631175	1.019808
3	6	0	2.227171	-0.774408	0.946091
4	6	0	1.526471	-2.036078	1.352561
5	6	0	1.989975	1.579027	0.234378
6	6	0	4.114942	0.731827	1.056874
7	6	0	3.468530	1.696620	0.064618
8	1	0	0.548057	-2.134233	0.879893
9	1	0	2.104419	-2.939862	1.186587
10	1	0	1.360512	-1.956749	2.432879
11	6	0	0.917086	2.481158	-0.033866
12	6	0	-0.268065	1.804700	0.300749
13	7	0	0.034979	0.475136	0.663150
14	1	0	-0.498993	0.080885	1.443237
15	1	0	3.947015	1.101647	2.071180
16	1	0	5.185447	0.647656	0.897428
17	1	0	3.811608	2.708110	0.290667
18	1	0	3.750594	1.471198	-0.967449
19	6	0	0.887245	3.812856	-0.490858
20	6	0	-0.347300	4.432632	-0.548346
21	6	0	-1.529019	3.747260	-0.168343
22	6	0	-1.514337	2.436133	0.249942
23	1	0	-2.425319	1.912172	0.501847
24	1	0	1.802022	4.317080	-0.765247
25	1	0	-2.460130	4.293211	-0.234136
26	8	0	-0.547061	5.711441	-0.953757
27	6	0	0.590582	6.447726	-1.362862
28	1	0	0.224542	7.427163	-1.656969
29	1	0	1.304241	6.554376	-0.541628
30	1	0	1.081192	5.968214	-2.213874
31	6	0	6.196349	-0.793919	-1.102089
32	6	0	7.151104	-0.866066	0.032555
33	6	0	4.875689	-1.343171	-0.837690
34	6	0	4.475201	-1.730777	0.547782
35	6	0	6.759714	-1.411440	1.255012
36	8	0	5.496526	-1.891960	1.492583
37	8	0	6.522507	-0.303285	-2.177639
38	6	0	3.882319	-1.187561	-1.784419
39	6	0	2.571977	-1.650028	-1.638257
40	1	0	3.892267	-2.644224	0.580103
41	1	0	4.142861	-0.588708	-2.652276
42	6	0	1.458573	-1.043731	-2.249919
43	8	0	0.275687	-1.451720	-2.074901
44	1	0	2.332307	-2.498219	-1.016225
45	8	0	1.686837	0.049958	-2.978608
46	6	0	0.531941	0.709791	-3.526196
47	1	0	-0.072282	1.149907	-2.731970
48	1	0	-0.074062	0.008055	-4.093843
49	1	0	0.930666	1.487541	-4.169655
50	30	0	-1.108604	-0.835806	-0.878782
51	6	0	8.460491	-0.402135	-0.116281
52	6	0	9.363222	-0.485892	0.931134
53	6	0	8.954472	-1.042245	2.145907

54	6	0	7.656773	-1.504671	2.315511
55	1	0	8.732188	0.012998	-1.078063
56	1	0	10.376926	-0.128786	0.809740
57	1	0	9.653400	-1.115941	2.969333
58	1	0	7.321039	-1.938372	3.247696
59	8	0	-2.411856	0.319766	-1.556247
60	8	0	-1.673828	-2.012782	0.491720
61	6	0	-4.258107	-0.443275	-2.825283
62	6	0	-5.450772	-1.095021	-2.934847
63	6	0	-6.061179	-1.682818	-1.796186
64	6	0	-5.417896	-1.557928	-0.533364
65	6	0	-4.185693	-0.836632	-0.423547
66	6	0	-3.589877	-0.320780	-1.570678
67	6	0	-3.586759	-0.624735	0.928818
68	6	0	-4.236034	0.254130	1.853270
69	6	0	-3.746918	0.400907	3.183498
70	6	0	-2.427052	-1.292522	1.326697
71	6	0	-1.978799	-1.167672	2.679891
72	6	0	-2.613295	-0.350666	3.576793
73	6	0	-7.285027	-2.387384	-1.897666
74	6	0	-7.863561	-2.960743	-0.794769
75	6	0	-7.224512	-2.850622	0.460183
76	6	0	-6.039889	-2.169847	0.588768
77	6	0	-5.369862	1.029952	1.478005
78	6	0	-5.973024	1.879034	2.369802
79	6	0	-5.489817	2.007340	3.693118
80	6	0	-4.397257	1.280998	4.084990
81	1	0	-5.946174	-1.180084	-3.895718
82	1	0	-3.772756	0.002174	-3.684637
83	1	0	-7.754554	-2.466329	-2.872032
84	1	0	-8.798938	-3.498826	-0.881866
85	1	0	-7.672850	-3.312206	1.331351
86	1	0	-5.557102	-2.103252	1.554424
87	1	0	-5.747484	0.940910	0.468652
88	1	0	-6.832626	2.458834	2.057108
89	1	0	-5.981368	2.677722	4.386507
90	1	0	-4.007829	1.366719	5.093366
91	1	0	-2.259152	-0.273013	4.598846
92	1	0	-1.128272	-1.773119	2.973785

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trans-endo-TS2-Re

Imaginary frequency: -176.0712 cm^{-1}

Standard orientation:

Electronic energy E = -4188.788003 a.u.

Enthalpy H = -4188.741833 a.u.

Entropy S = 265.436 cal/mol/K

Gibbs free energy G = -4188.867950 a.u.

Total free energy in solution E_{sol}= -4190.37992 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.594057	0.811433	-0.341028
2	7	0	-3.771789	0.114924	-0.966934
3	6	0	-2.447151	-0.133284	-1.036999
4	6	0	-1.820151	-0.766552	-2.257834
5	6	0	-2.040972	1.971336	0.217941
6	6	0	-4.240424	0.955598	0.155923
7	6	0	-3.498595	2.282892	0.209950
8	1	0	-0.835387	-1.171711	-2.018910
9	1	0	-2.414544	-1.553523	-2.711668
10	1	0	-1.690648	0.024790	-3.002064
11	6	0	-0.892498	2.732467	0.626349
12	6	0	0.233740	1.977585	0.273863
13	7	0	-0.177849	0.748151	-0.309605
14	1	0	0.280581	0.517913	-1.197679
15	1	0	-5.311981	1.097422	0.023350

16	1	0	-4.062700	0.427979	1.096727
17	1	0	-3.742028	2.910297	-0.653123
18	6	0	-0.759511	3.988874	1.238875
19	6	0	0.527517	4.452243	1.462927
20	6	0	1.653662	3.680854	1.095559
21	6	0	1.529160	2.439053	0.508561
22	1	0	2.398755	1.844455	0.263356
23	1	0	-1.634725	4.558202	1.516380
24	1	0	2.631360	4.094974	1.301172
25	8	0	0.823230	5.645598	2.039121
26	6	0	-0.261420	6.460034	2.440514
27	1	0	0.178156	7.352532	2.876780
28	1	0	-0.881358	6.738774	1.584154
29	1	0	-0.877535	5.952774	3.187876
30	6	0	3.785455	-2.232176	2.320750
31	6	0	4.834813	-3.073967	2.095133
32	6	0	5.539080	-3.037361	0.863433
33	6	0	5.150176	-2.086435	-0.120374
34	6	0	4.072431	-1.180418	0.140603
35	6	0	3.369588	-1.285044	1.338426
36	6	0	-6.262572	-1.694412	0.655472
37	6	0	-7.330800	-1.025027	-0.117691
38	6	0	-4.947191	-1.735266	0.005927
39	6	0	-4.698329	-1.018310	-1.285777
40	6	0	-7.057714	-0.473942	-1.369771
41	8	0	-5.820918	-0.498306	-1.954368
42	8	0	-6.469206	-2.178108	1.758880
43	6	0	-3.862898	-2.125214	0.737566
44	6	0	-2.541557	-2.138515	0.217741
45	1	0	-4.182677	-1.638626	-2.011729
46	1	0	-4.032078	-2.342739	1.787713
47	6	0	-1.400591	-2.153104	1.069431
48	8	0	-0.242869	-2.396131	0.643979
49	1	0	-2.354906	-2.548716	-0.762324
50	8	0	-1.606506	-1.845617	2.341390
51	6	0	-0.459126	-1.900709	3.217167
52	1	0	0.296013	-1.173803	2.920598
53	1	0	-0.028988	-2.900004	3.194325
54	1	0	-0.851233	-1.670130	4.201930
55	30	0	1.102004	-1.043501	0.270416
56	8	0	1.659787	-0.987022	-1.540110
57	8	0	2.295928	-0.521653	1.615226
58	6	0	-8.629627	-0.949631	0.393959
59	6	0	-9.639242	-0.339872	-0.330451
60	6	0	-9.349103	0.202453	-1.585764
61	6	0	-8.066263	0.139740	-2.109922
62	1	0	-8.806032	-1.389387	1.366857
63	1	0	-10.643349	-0.285488	0.067716
64	1	0	-10.131986	0.678833	-2.162229
65	1	0	-7.823460	0.552576	-3.079587
66	6	0	3.785813	-0.089545	-0.842210
67	6	0	4.719759	0.991779	-0.957758
68	6	0	4.532111	2.006968	-1.938241
69	6	0	3.408984	1.923708	-2.799181
70	6	0	2.658486	-0.099059	-1.661836
71	6	0	2.508459	0.906617	-2.663949
72	1	0	3.231163	-2.250387	3.251173
73	1	0	5.141296	-3.788012	2.851587
74	6	0	6.612509	-3.923190	0.602100
75	6	0	5.864880	-2.073169	-1.348611
76	6	0	5.845622	1.105596	-0.095812
77	6	0	5.458886	3.074302	-2.037756

78	1	0	3.273822	2.682785	-3.561414
79	1	0	1.646859	0.825312	-3.317895
80	6	0	7.284909	-3.883259	-0.591968
81	6	0	6.898526	-2.946508	-1.576277
82	6	0	6.723706	2.153064	-0.211912
83	6	0	6.536932	3.151138	-1.195577
84	1	0	6.889691	-4.637639	1.369425
85	1	0	8.103607	-4.565088	-0.784246
86	1	0	7.422805	-2.919007	-2.523552
87	1	0	5.573455	-1.365620	-2.113173
88	1	0	5.996556	0.351838	0.664705
89	1	0	7.570571	2.216623	0.460041
90	1	0	7.240553	3.969763	-1.277228
91	1	0	5.294197	3.831523	-2.796268
92	1	0	-3.804527	2.821331	1.108755

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trans-endo-TS1-Si

Imaginary frequency: -276.9824 cm^{-1}

Standard orientation:

Electronic energy E = -4188.790617 a.u.

Enthalpy H = -4188.743623 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Entropy S = 205.462 cal/mol/K

Gibbs free energy G = -4188.872347 a.u.

Total free energy in solution E_{sol}= -4190.38228 a.u.

1	6	0	1.848756	0.314099	-1.504051
2	7	0	3.962638	-0.759113	-1.396851
3	6	0	2.675062	-0.874418	-1.512744
4	6	0	1.999578	-2.207550	-1.655949
5	6	0	2.323421	1.526351	-1.044750
6	6	0	4.539722	0.590765	-1.522604
7	6	0	3.784233	1.709148	-0.789758
8	1	0	1.189724	-2.321410	-0.932006
9	1	0	2.700333	-3.035539	-1.581513
10	1	0	1.551721	-2.246724	-2.653519
11	6	0	1.185661	2.339260	-0.790517
12	6	0	0.051038	1.562208	-1.144171
13	7	0	0.479373	0.340690	-1.599933
14	1	0	-0.163174	-0.434973	-1.755955
15	1	0	4.533950	0.811908	-2.593276
16	1	0	5.575864	0.542549	-1.196273
17	1	0	4.140547	2.663961	-1.183766
18	1	0	3.996083	1.706856	0.283089
19	6	0	1.023442	3.646752	-0.284848
20	6	0	-0.263721	4.129554	-0.135133
21	6	0	-1.388593	3.343819	-0.495217
22	6	0	-1.256522	2.072116	-1.010262
23	1	0	-2.124206	1.502913	-1.324645
24	1	0	1.891449	4.235001	-0.023364
25	1	0	-2.370648	3.775246	-0.358683
26	8	0	-0.574133	5.360775	0.349729
27	6	0	0.502705	6.203782	0.712113
28	1	0	0.055331	7.128908	1.064338
29	1	0	1.145245	6.411010	-0.147812
30	1	0	1.099026	5.756944	1.512627
31	6	0	-4.337521	2.263302	1.047623
32	6	0	-5.371830	2.658616	0.250445
33	6	0	-5.917112	1.772338	-0.714579
34	6	0	-5.392682	0.452966	-0.805688
35	6	0	-4.333273	0.031487	0.064642
36	6	0	-3.776777	0.954565	0.948613
37	6	0	6.274207	-0.320850	1.213272
38	6	0	7.388628	-0.749036	0.331490
39	6	0	5.013596	-0.995758	0.966967

40	6	0	4.870438	-1.849783	-0.166864
41	6	0	7.179024	-1.717025	-0.647713
42	8	0	5.953830	-2.321575	-0.824837
43	8	0	6.431686	0.542751	2.071134
44	6	0	3.867718	-0.550368	1.662891
45	6	0	2.593074	-1.009458	1.479788
46	1	0	4.104119	-2.610159	-0.150930
47	1	0	4.036642	0.292929	2.325492
48	6	0	1.429116	-0.265771	1.842506
49	8	0	0.289043	-0.644183	1.485540
50	1	0	2.373707	-1.906351	0.922256
51	8	0	1.605263	0.856182	2.520463
52	6	0	0.429530	1.633887	2.813407
53	1	0	0.045588	2.086238	1.898038
54	1	0	-0.334965	1.017724	3.281285
55	1	0	0.766305	2.411053	3.491370
56	30	0	-1.357734	-0.012391	0.685269
57	8	0	-1.761616	-0.939134	-0.911461
58	8	0	-2.714232	0.690673	1.722621
59	6	0	8.661617	-0.189803	0.463314
60	6	0	9.696593	-0.597486	-0.362732
61	6	0	9.463308	-1.574494	-1.335089
62	6	0	8.204755	-2.140088	-1.484928
63	1	0	8.797940	0.560483	1.231007
64	1	0	10.682072	-0.164240	-0.256093
65	1	0	10.269209	-1.896872	-1.981718
66	1	0	7.999800	-2.897059	-2.229643
67	6	0	-3.916053	-1.406593	0.033265
68	6	0	-4.827879	-2.400730	0.521363
69	6	0	-4.527515	-3.783208	0.374124
70	6	0	-2.709351	-1.820284	-0.518993
71	6	0	-2.426512	-3.207336	-0.669547
72	6	0	-3.308894	-4.158096	-0.247634
73	1	0	-5.786396	3.656816	0.339043
74	1	0	-3.898195	2.927160	1.782055
75	6	0	-6.964967	2.177945	-1.576605
76	6	0	-5.950411	-0.412129	-1.786605
77	6	0	-6.048116	-2.052060	1.160639
78	6	0	-5.440622	-4.758022	0.846516
79	1	0	-3.086097	-5.211923	-0.371207
80	1	0	-1.484937	-3.473962	-1.134319
81	6	0	-6.911838	-3.017383	1.612624
82	6	0	-6.613116	-4.388954	1.452543
83	6	0	-7.483566	1.318200	-2.509557
84	6	0	-6.961888	0.009402	-2.612720
85	1	0	-7.347665	3.188211	-1.482427
86	1	0	-8.283868	1.636682	-3.165318
87	1	0	-7.363905	-0.670117	-3.354071
88	1	0	-5.557655	-1.415297	-1.880643
89	1	0	-6.285133	-1.005666	1.295361
90	1	0	-7.832953	-2.723944	2.100607
91	1	0	-7.305405	-5.139813	1.811780
92	1	0	-5.189011	-5.805052	0.719400

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trans-endo-IM1-Si

Imaginary frequency: -190.7999 cm^{-1}

Standard orientation:

Electronic energy E = -4188.798160 a.u.

Enthalpy H = -4188.751220 a.u.

Entropy S = 205.462 cal/mol/K

Gibbs free energy G = -4188.880474 a.u.

Total free energy in solution E_{sol}= -4190.39423 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.749807	0.042867	-1.252318

2	7	0	3.874953	-0.954673	-1.122392
3	6	0	2.558833	-1.119476	-1.099859
4	6	0	1.892741	-2.463138	-1.061033
5	6	0	2.242151	1.333752	-1.078189
6	6	0	4.405570	0.345660	-1.590523
7	6	0	3.714961	1.561375	-0.972782
8	1	0	1.065038	-2.467596	-0.351298
9	1	0	2.575339	-3.278696	-0.841563
10	1	0	1.478964	-2.638006	-2.059194
11	6	0	1.124195	2.187777	-0.961608
12	6	0	-0.022317	1.361906	-1.090187
13	7	0	0.372841	0.068607	-1.268491
14	1	0	-0.292055	-0.709766	-1.263704
15	1	0	4.241082	0.359713	-2.670235
16	1	0	5.475703	0.352785	-1.408405
17	1	0	4.021536	2.442614	-1.541112
18	1	0	4.017220	1.718580	0.065940
19	6	0	0.980604	3.579668	-0.740623
20	6	0	-0.297680	4.083641	-0.656399
21	6	0	-1.439454	3.239658	-0.791195
22	6	0	-1.325142	1.890952	-1.009758
23	1	0	-2.196598	1.256800	-1.099855
24	1	0	1.856001	4.204772	-0.640665
25	1	0	-2.415076	3.701224	-0.715296
26	8	0	-0.602019	5.391678	-0.441842
27	6	0	0.482382	6.289688	-0.310249
28	1	0	0.044326	7.271161	-0.151575
29	1	0	1.092693	6.302388	-1.217292
30	1	0	1.109335	6.025121	0.545625
31	6	0	-3.634912	1.554726	2.301275
32	6	0	-4.240373	2.572519	1.625974
33	6	0	-4.759824	2.362505	0.321828
34	6	0	-4.666945	1.063300	-0.252959
35	6	0	-4.063007	-0.011415	0.480463
36	6	0	-3.509288	0.251808	1.731534
37	6	0	6.202804	-0.116042	1.154390
38	6	0	7.305827	-0.477525	0.227766
39	6	0	4.986435	-0.895387	0.997800
40	6	0	4.786342	-1.750718	-0.215052
41	6	0	7.121667	-1.460044	-0.745844
42	8	0	5.933618	-2.120381	-0.932071
43	8	0	6.339498	0.770394	1.991796
44	6	0	3.889243	-0.606338	1.781176
45	6	0	2.684415	-1.315915	1.729033
46	1	0	4.261830	-2.674861	0.000351
47	1	0	3.974578	0.262293	2.427527
48	6	0	1.434017	-0.789380	2.069027
49	8	0	0.374327	-1.487837	1.992607
50	1	0	2.653275	-2.335127	1.376690
51	8	0	1.380651	0.500109	2.411928
52	6	0	0.093489	1.091355	2.620686
53	1	0	-0.414683	1.245060	1.662979
54	1	0	-0.518763	0.494241	3.294618
55	1	0	0.292280	2.063830	3.059575
56	30	0	-1.412574	-1.196742	1.426276
57	8	0	-1.685172	-1.459508	-0.409421
58	8	0	-2.850727	-0.668135	2.454615
59	6	0	8.549532	0.149559	0.332856
60	6	0	9.591719	-0.200121	-0.510254
61	6	0	9.390556	-1.191659	-1.473899
62	6	0	8.160794	-1.823209	-1.598094
63	1	0	8.658663	0.906339	1.098639

64	1	0	10.553725	0.286578	-0.422314
65	1	0	10.199000	-1.474334	-2.136121
66	1	0	7.984042	-2.590077	-2.340019
67	6	0	-4.072466	-1.385255	-0.112527
68	6	0	-5.321996	-2.076119	-0.249973
69	6	0	-5.379355	-3.326285	-0.925567
70	6	0	-2.918445	-1.998705	-0.581506
71	6	0	-2.988983	-3.245629	-1.261119
72	6	0	-4.181024	-3.885221	-1.438611
73	1	0	-4.325841	3.557277	2.071731
74	1	0	-3.228175	1.694067	3.295521
75	6	0	-5.346907	3.421178	-0.414621
76	6	0	-5.164982	0.889698	-1.573913
77	6	0	-6.533001	-1.550031	0.276005
78	6	0	-6.620815	-3.994006	-1.069288
79	1	0	-4.226230	-4.834147	-1.960782
80	1	0	-2.059377	-3.664432	-1.626580
81	6	0	-7.720182	-2.221405	0.127174
82	6	0	-7.772429	-3.455968	-0.557955
83	6	0	-5.818933	3.219617	-1.686231
84	6	0	-5.719368	1.936328	-2.267829
85	1	0	-5.410850	4.398862	0.050510
86	1	0	-6.262855	4.034905	-2.243037
87	1	0	-6.084462	1.775458	-3.274524
88	1	0	-5.093207	-0.086026	-2.034789
89	1	0	-6.504611	-0.610636	0.810627
90	1	0	-8.627383	-1.801507	0.543384
91	1	0	-8.716701	-3.973350	-0.670011
92	1	0	-6.638055	-4.944612	-1.590436

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trans-endo-TS2-Si

Imaginary frequency: -197.9714 cm^{-1}

Standard orientation:

Electronic energy E = -4188.788640 a.u.

Enthalpy H = -4188.743562 a.u.

Entropy S = 255.478 cal/mol/K

Gibbs free energy G = -4188.864948 a.u.

Total free energy in solution E_{sol}= -4190.38213 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659363	0.572457	-0.919310
2	7	0	3.984497	0.120045	-0.994143
3	6	0	2.748872	-0.276596	-1.352982
4	6	0	2.487103	-0.997208	-2.656815
5	6	0	1.839588	1.802781	-0.351312
6	1	0	1.572667	-1.584999	-2.572392
7	1	0	3.285898	-1.660444	-2.973328
8	1	0	2.354395	-0.240301	-3.434395
9	6	0	0.576887	2.484054	-0.365721
10	6	0	-0.339085	1.618457	-0.977968
11	7	0	0.298606	0.381875	-1.251797
12	1	0	0.046673	-0.054519	-2.134671
13	6	0	0.182221	3.770426	0.042996
14	6	0	-1.123948	4.147317	-0.221060
15	6	0	-2.017988	3.279118	-0.891308
16	6	0	-1.650032	2.004266	-1.263466
17	1	0	-2.341171	1.320575	-1.735841
18	1	0	0.884638	4.425758	0.536894
19	1	0	-3.022258	3.637717	-1.072204
20	8	0	-1.658962	5.347453	0.122219
21	6	0	-0.824904	6.253009	0.817773
22	1	0	-1.433716	7.130281	1.018383
23	1	0	0.038584	6.538893	0.210964
24	1	0	-0.480647	5.821687	1.761631

25	6	0	-2.589490	1.440625	2.064754
26	6	0	-3.492759	2.450498	1.917243
27	6	0	-4.542033	2.341749	0.967555
28	6	0	-4.662798	1.141224	0.212511
29	6	0	-3.742123	0.060283	0.413839
30	6	0	-2.676227	0.245039	1.291983
31	6	0	6.270857	-1.406077	1.154488
32	6	0	7.382629	-0.579271	0.633040
33	6	0	5.141232	-1.590695	0.238614
34	6	0	5.092370	-0.888237	-1.080934
35	6	0	7.319527	-0.039414	-0.651307
36	8	0	6.258692	-0.223310	-1.496637
37	8	0	6.303873	-1.894504	2.274748
38	6	0	3.984904	-2.137480	0.724288
39	6	0	2.800064	-2.271991	-0.037617
40	1	0	4.828881	-1.556787	-1.893940
41	1	0	3.966107	-2.365537	1.785336
42	6	0	1.525120	-2.439748	0.587011
43	8	0	0.462845	-2.521978	-0.083118
44	1	0	2.838306	-2.615564	-1.057020
45	8	0	1.521720	-2.469577	1.905757
46	6	0	0.270921	-2.743959	2.581764
47	1	0	-0.386344	-1.879241	2.533391
48	1	0	-0.206660	-3.607722	2.124337
49	1	0	0.558109	-2.961702	3.605169
50	30	0	-0.937303	-1.142216	-0.175784
51	8	0	-2.045029	-1.059257	-1.697934
52	8	0	-1.696332	-0.654113	1.455273
53	6	0	8.513313	-0.340936	1.419134
54	6	0	9.563338	0.419627	0.933260
55	6	0	9.484870	0.949336	-0.357891
56	6	0	8.370259	0.725391	-1.153000
57	1	0	8.529901	-0.777093	2.409346
58	1	0	10.437569	0.600457	1.544015
59	1	0	10.301476	1.543004	-0.748807
60	1	0	8.292175	1.125578	-2.154680
61	6	0	-3.988538	-1.236533	-0.293752
62	6	0	-5.132399	-2.016994	0.081754
63	6	0	-5.476913	-3.186106	-0.652322
64	6	0	-3.182529	-1.684251	-1.337801
65	6	0	-3.551720	-2.849485	-2.071846
66	6	0	-4.661926	-3.571531	-1.747814
67	1	0	-3.406820	3.361339	2.499799
68	1	0	-1.762845	1.512590	2.760642
69	6	0	-5.442395	3.411862	0.742583
70	6	0	-5.700545	1.073883	-0.757643
71	6	0	-5.955688	-1.665314	1.186391
72	6	0	-6.614703	-3.944009	-0.281338
73	1	0	-4.930986	-4.455050	-2.315940
74	1	0	-2.907496	-3.135502	-2.893829
75	6	0	-7.049015	-2.421188	1.526641
76	6	0	-7.392149	-3.573600	0.784756
77	6	0	-6.429712	3.316692	-0.204377
78	6	0	-6.552759	2.130461	-0.961924
79	1	0	-5.324876	4.315762	1.330336
80	1	0	-7.110154	4.141559	-0.373969
81	1	0	-7.327911	2.053606	-1.714466
82	1	0	-5.802403	0.173127	-1.347673
83	1	0	-5.701437	-0.789914	1.768221
84	1	0	-7.655043	-2.131568	2.376275
85	1	0	-8.259630	-4.159037	1.062121
86	1	0	-6.855417	-4.828820	-0.860252

87	6	0	4.074083	1.006300	0.184515
88	1	0	5.124451	1.258215	0.320569
89	6	0	3.215112	2.251862	0.009263
90	1	0	3.719386	0.462728	1.065318
91	1	0	3.225242	2.819666	0.941551
92	1	0	3.612755	2.900031	-0.778139

trans-exo-TS1-Re

Imaginary frequency: -283.8582 cm^{-1}

Standard orientation:

Electronic energy E = -4188.787657 a.u.

Enthalpy H = -4188.741447 a.u.

Entropy S = 264.139 cal/mol/K

Gibbs free energy G = -4188.866948 a.u.

Total free energy in solution E_{sol} = -4190.38164 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.444160	-2.535435	-0.231472
2	7	0	-3.783092	-0.894141	-1.272581
3	6	0	-3.621618	-1.702398	-0.264821
4	6	0	-4.611255	-1.756413	0.858634
5	6	0	-1.356869	-2.276651	-1.044244
6	6	0	-2.955970	-1.105808	-2.470579
7	6	0	-1.465783	-1.325985	-2.189291
8	1	0	-4.218097	-1.284091	1.760244
9	1	0	-4.819008	-2.808270	1.074790
10	1	0	-5.545070	-1.277524	0.579654
11	6	0	-0.242326	-2.925455	-0.452261
12	6	0	-0.716404	-3.597455	0.696938
13	7	0	-2.059876	-3.354883	0.811607
14	1	0	-2.640562	-3.648802	1.576990
15	1	0	-3.124338	-0.259485	-3.135845
16	1	0	-3.358830	-1.996420	-2.958849
17	1	0	-0.904142	-0.414007	-1.962763
18	1	0	-1.010430	-1.742849	-3.090788
19	6	0	1.138842	-2.942004	-0.783638
20	6	0	1.990950	-3.677556	0.029408
21	6	0	1.490903	-4.348875	1.183127
22	6	0	0.159722	-4.327608	1.519417
23	1	0	1.481647	-2.442095	-1.678395
24	1	0	-0.192486	-4.840539	2.404825
25	1	0	2.210650	-4.880665	1.789632
26	8	0	3.305550	-3.823604	-0.188496
27	6	0	3.839899	-3.240659	-1.378433
28	1	0	3.365520	-3.686467	-2.256089
29	1	0	3.705034	-2.157273	-1.374955
30	1	0	4.900217	-3.467344	-1.365607
31	30	0	1.279795	-0.935964	0.547924
32	8	0	1.150237	0.051292	-1.060064
33	8	0	2.854925	-0.917612	1.551666
34	6	0	-5.653047	1.399919	0.862050
35	6	0	-6.735548	1.289003	-0.151752
36	6	0	-4.322580	1.174897	0.341812
37	6	0	-4.146123	0.834500	-1.040145
38	6	0	-6.429341	1.138095	-1.502484
39	8	0	-5.127430	1.105316	-1.945921
40	8	0	-5.910699	1.620832	2.042560
41	6	0	-3.250967	1.056610	1.248584
42	6	0	-2.008011	0.536428	0.994164
43	1	0	-3.191725	1.128556	-1.469541
44	1	0	-3.502840	1.311644	2.273127
45	6	0	-1.093011	0.199500	2.042041
46	8	0	-0.102189	-0.549917	1.895522
47	1	0	-1.679845	0.234443	0.011311
48	8	0	-1.371691	0.668824	3.250450

49	6	0	-0.438198	0.334096	4.292345
50	1	0	-0.425551	-0.741966	4.452896
51	1	0	0.559306	0.671282	4.020870
52	1	0	-0.801802	0.853419	5.172824
53	6	0	-8.077632	1.353840	0.229883
54	6	0	-9.083605	1.270609	-0.719221
55	6	0	-8.751841	1.126885	-2.069533
56	6	0	-7.424660	1.060940	-2.470114
57	1	0	-8.288234	1.480348	1.283767
58	1	0	-10.121860	1.322730	-0.419333
59	1	0	-9.534458	1.065907	-2.814975
60	1	0	-7.143277	0.954269	-3.508898
61	6	0	3.909708	-0.609153	0.798572
62	6	0	5.086112	-1.402262	0.971398
63	6	0	6.191975	-1.219420	0.194977
64	6	0	6.199220	-0.237224	-0.830281
65	6	0	5.055821	0.596704	-0.984783
66	6	0	3.920774	0.441080	-0.122300
67	6	0	2.851100	1.490979	-0.156015
68	6	0	3.181726	2.801138	0.329541
69	6	0	2.251078	3.870709	0.209401
70	6	0	0.988335	3.615194	-0.384113
71	6	0	1.578086	1.269235	-0.675830
72	6	0	0.664597	2.358368	-0.801814
73	1	0	5.044548	-2.169087	1.734469
74	1	0	7.075814	-1.831877	0.339807
75	6	0	7.316549	-0.069161	-1.683825
76	6	0	5.090137	1.577655	-2.013411
77	6	0	4.429510	3.082113	0.950997
78	6	0	2.589692	5.161833	0.683154
79	1	0	0.281947	4.431300	-0.487656
80	1	0	-0.302723	2.143813	-1.240965
81	6	0	3.805109	5.401148	1.269276
82	6	0	4.729016	4.341360	1.406817
83	6	0	6.184658	1.714562	-2.829946
84	6	0	7.317442	0.886383	-2.667199
85	1	0	1.861159	5.957771	0.574239
86	1	0	4.056286	6.390518	1.630087
87	1	0	5.685702	4.523565	1.880686
88	1	0	5.143901	2.279848	1.072279
89	1	0	4.227205	2.215313	-2.150250
90	1	0	6.179296	2.467122	-3.609084
91	1	0	8.176350	1.007744	-3.315175
92	1	0	8.175914	-0.715358	-1.540122

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trans-exo-IM1-Re

Imaginary frequency: -6.5286 cm^{-1}

Standard orientation:

Electronic energy E = -4188.788771 a.u.

Enthalpy H = -4188.742210 a.u.

Entropy S = 265.800 cal/mol/K

Gibbs free energy G = -4188.868500 a.u.

Total free energy in solution E_{sol}= -4190.38696 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.505606	-2.381415	-0.341400
2	7	0	-3.710965	-0.596891	-1.267721
3	6	0	-3.629336	-1.498766	-0.313515
4	6	0	-4.643748	-1.627520	0.780036
5	6	0	-1.377905	-2.096824	-1.099334

6	6	0	-2.907117	-0.808489	-2.486601
7	6	0	-1.432357	-1.089949	-2.196670
8	1	0	-4.268648	-1.213768	1.716836
9	1	0	-4.839914	-2.694789	0.915734
10	1	0	-5.578943	-1.141220	0.521490
11	6	0	-0.300595	-2.801727	-0.511640
12	6	0	-0.831650	-3.532293	0.577268
13	7	0	-2.172785	-3.278141	0.658547
14	1	0	-2.776475	-3.587544	1.399728
15	1	0	-3.047838	0.065160	-3.119334
16	1	0	-3.343173	-1.670980	-2.994312
17	1	0	-0.840936	-0.212385	-1.917554
18	1	0	-0.978442	-1.482045	-3.109985
19	6	0	1.087730	-2.840503	-0.806945
20	6	0	1.890176	-3.649593	-0.019498
21	6	0	1.337080	-4.368265	1.083519
22	6	0	-0.000599	-4.331067	1.385007
23	1	0	1.472582	-2.287281	-1.651225
24	1	0	-0.393616	-4.885276	2.227147
25	1	0	2.024521	-4.956583	1.675592
26	8	0	3.202185	-3.838773	-0.215315
27	6	0	3.779539	-3.240396	-1.378017
28	1	0	3.298476	-3.638051	-2.275133
29	1	0	3.688956	-2.153493	-1.341374
30	1	0	4.828900	-3.512495	-1.358330
31	30	0	1.220848	-0.796085	0.638654
32	8	0	1.180854	0.116714	-1.017257
33	8	0	2.807947	-0.890411	1.610960
34	6	0	-5.714921	1.467111	0.848393
35	6	0	-6.785686	1.269634	-0.169489
36	6	0	-4.373640	1.241686	0.364407
37	6	0	-4.148193	0.874120	-1.050257
38	6	0	-6.465080	1.100331	-1.515769
39	8	0	-5.166259	1.158601	-1.961194
40	8	0	-6.001393	1.728738	2.014864
41	6	0	-3.337335	1.127582	1.284080
42	6	0	-2.062693	0.629852	1.053811
43	1	0	-3.261659	1.383533	-1.435072
44	1	0	-3.622591	1.343993	2.309100
45	6	0	-1.216294	0.203313	2.105596
46	8	0	-0.175741	-0.491366	1.956075
47	1	0	-1.684732	0.416069	0.065140
48	8	0	-1.597221	0.502618	3.347404
49	6	0	-0.719655	0.080745	4.401869
50	1	0	-0.655874	-1.005491	4.430516
51	1	0	0.274743	0.494925	4.252716
52	1	0	-1.168158	0.464991	5.312438
53	6	0	-8.128542	1.251149	0.211577
54	6	0	-9.127966	1.069953	-0.732331
55	6	0	-8.785480	0.910987	-2.076975
56	6	0	-7.455325	0.925797	-2.476469
57	1	0	-8.347350	1.393488	1.261839
58	1	0	-10.167268	1.058143	-0.431598
59	1	0	-9.560590	0.774477	-2.820360
60	1	0	-7.167849	0.811086	-3.512866
61	6	0	3.884869	-0.662440	0.862692
62	6	0	5.010595	-1.518579	1.070467
63	6	0	6.135025	-1.419828	0.306290
64	6	0	6.211645	-0.467673	-0.744611
65	6	0	5.121390	0.427809	-0.934614
66	6	0	3.969595	0.363122	-0.082171
67	6	0	2.967630	1.475331	-0.152626

68	6	0	3.379349	2.777577	0.292761
69	6	0	2.518055	3.898554	0.135963
70	6	0	1.241005	3.703792	-0.450632
71	6	0	1.683696	1.318826	-0.668007
72	6	0	0.838701	2.457179	-0.827790
73	1	0	4.915572	-2.261184	1.852263
74	1	0	6.979199	-2.079093	0.479017
75	6	0	7.345055	-0.391400	-1.590358
76	6	0	5.224647	1.375688	-1.989871
77	6	0	4.640999	2.998767	0.910278
78	6	0	2.936640	5.180610	0.569101
79	1	0	0.586399	4.558501	-0.579658
80	1	0	-0.142189	2.289433	-1.257143
81	6	0	4.163788	5.361319	1.151437
82	6	0	5.018464	4.250625	1.326581
83	6	0	6.332590	1.423027	-2.798039
84	6	0	7.412204	0.533601	-2.600259
85	1	0	2.259582	6.016710	0.432888
86	1	0	4.476173	6.343903	1.481686
87	1	0	5.983533	4.387215	1.798797
88	1	0	5.302506	2.157252	1.061519
89	1	0	4.403377	2.060256	-2.154804
90	1	0	6.379769	2.151862	-3.597941
91	1	0	8.282708	0.584625	-3.242068
92	1	0	8.162603	-1.083314	-1.418867

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trans-exo-TS2-Re

Imaginary frequency: -87.4201 cm^{-1}

Standard orientation:

Electronic energy E = -4188.785104 a.u.

Enthalpy H = -4188.738336 a.u.

Entropy S = 205.462 cal/mol/K

Gibbs free energy G = -4188.865687 a.u.

Total free energy in solution E_{sol} = -4190.38190 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.019517	3.782979	-0.520853
2	6	0	2.323724	4.010249	-0.010425
3	6	0	3.201847	2.902410	0.148919
4	6	0	2.779935	1.580173	-0.222816
5	6	0	0.607953	2.519248	-0.823990
6	6	0	1.471744	1.394664	-0.662970
7	6	0	2.752484	5.311887	0.347385
8	6	0	4.005319	5.525409	0.860197
9	6	0	4.876283	4.428344	1.040623
10	6	0	4.489434	3.157783	0.695750
11	6	0	3.789133	0.475053	-0.159318
12	6	0	4.914191	0.527868	-1.047963
13	6	0	6.021420	-0.348733	-0.866675
14	6	0	3.741524	-0.527993	0.811703
15	6	0	4.878131	-1.374524	0.997113
16	6	0	5.982404	-1.280339	0.203722
17	6	0	4.975272	1.447567	-2.131297
18	6	0	6.058263	1.486096	-2.973190
19	6	0	7.154582	0.615423	-2.783699
20	6	0	7.128295	-0.282618	-1.747784
21	1	0	2.062423	6.137105	0.209741
22	1	0	4.325239	6.523168	1.132787
23	1	0	5.861493	4.590323	1.460397
24	1	0	5.164402	2.327831	0.850897
25	1	0	4.140705	2.117012	-2.291071
26	1	0	6.072175	2.193073	-3.793704
27	1	0	8.005034	0.659083	-3.452401
28	1	0	7.958637	-0.960786	-1.582214
29	1	0	6.835385	-1.930776	0.366192

30	1	0	4.814793	-2.100214	1.798129
31	1	0	0.352022	4.627544	-0.651111
32	1	0	-0.392415	2.324949	-1.191694
33	8	0	2.706144	-0.732823	1.622455
34	6	0	-1.896355	-2.359731	0.270094
35	7	0	-3.493087	-1.135769	-0.946643
36	6	0	-3.144209	-1.657939	0.226995
37	6	0	-4.112574	-1.778140	1.360143
38	6	0	-0.930835	-2.227946	-0.710828
39	6	0	-2.763400	-1.558706	-2.162445
40	6	0	-1.248341	-1.530360	-1.989729
41	1	0	-3.599427	-1.703923	2.317597
42	1	0	-4.582198	-2.763062	1.269329
43	1	0	-4.893211	-1.026959	1.312704
44	6	0	0.268496	-2.791770	-0.189736
45	6	0	-0.048826	-3.298244	1.098166
46	7	0	-1.366105	-3.024960	1.358196
47	1	0	-1.822590	-3.175440	2.240243
48	1	0	-3.083712	-0.915022	-2.976840
49	1	0	-3.086340	-2.579426	-2.381908
50	1	0	-0.821953	-0.523077	-1.962846
51	1	0	-0.795146	-2.045383	-2.839565
52	6	0	1.559369	-2.974375	-0.746158
53	6	0	2.486712	-3.663833	0.005711
54	6	0	2.153494	-4.160436	1.299481
55	6	0	0.911107	-3.992381	1.856133
56	1	0	1.792054	-2.541276	-1.706980
57	1	0	0.687262	-4.371117	2.844263
58	1	0	2.937950	-4.670351	1.842136
59	8	0	3.747060	-3.928548	-0.387926
60	6	0	4.166614	-3.349427	-1.619456
61	1	0	3.611669	-3.789584	-2.452560
62	1	0	4.032175	-2.266729	-1.599078
63	1	0	5.223226	-3.579459	-1.713389
64	30	0	1.049322	-0.607518	0.790399
65	6	0	-5.752300	1.685300	0.246030
66	6	0	-6.905012	1.259195	-0.591671
67	6	0	-4.507929	0.940347	0.045200
68	6	0	-4.491601	-0.068062	-1.077670
69	6	0	-6.849660	0.057784	-1.295515
70	8	0	-5.738160	-0.747312	-1.237347
71	8	0	-5.865804	2.606040	1.045412
72	6	0	-3.471913	1.174223	0.912572
73	6	0	-2.184489	0.595285	0.894537
74	1	0	-4.254681	0.421446	-2.027079
75	1	0	-3.731274	1.811218	1.753241
76	6	0	-1.407232	0.456573	2.061206
77	8	0	-0.292258	-0.133844	2.121821
78	1	0	-1.681905	0.312161	-0.014429
79	8	0	-1.950974	0.891710	3.201953
80	6	0	-1.127768	0.802272	4.373755
81	1	0	-0.903908	-0.237786	4.602741
82	1	0	-0.196939	1.344502	4.223418
83	1	0	-1.714961	1.253769	5.167235
84	6	0	-8.073792	2.020237	-0.635388
85	6	0	-9.164611	1.587896	-1.374355
86	6	0	-9.092561	0.377782	-2.068267
87	6	0	-7.937564	-0.393782	-2.034599
88	1	0	-8.092507	2.941694	-0.068160
89	1	0	-10.069031	2.180482	-1.409764
90	1	0	-9.943077	0.033876	-2.643220
91	1	0	-7.861924	-1.334361	-2.563302

92	8	0	0.962441	0.176012	-0.930670

trans-exo-TS1-Si

Imaginary frequency: -287.7373 cm^{-1}

Standard orientation:

Electronic energy E = -4188.790934 a.u.

Enthalpy H = -4188.744004 a.u.

Entropy S = 267.754 cal/mol/K

Gibbs free energy G = -4188.871222 a.u.

Total free energy in solution E_{sol}= -4190.38429 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.574534	1.769776	-0.366558
2	6	0	-6.633934	1.441157	0.624535
3	6	0	-4.240885	1.378493	0.033216
4	6	0	-4.043852	0.695367	1.278621
5	6	0	-6.298372	0.946010	1.882762
6	8	0	-4.987504	0.765701	2.258540
7	8	0	-5.854573	2.288157	-1.444407
8	6	0	-3.196156	1.476165	-0.906909
9	6	0	-1.963273	0.878205	-0.844500
10	1	0	-3.065463	0.831542	1.730840
11	1	0	-3.465004	2.005183	-1.815850
12	6	0	-1.071776	0.854468	-1.963367
13	8	0	-1.359753	1.663294	-2.973188
14	1	0	-1.616163	0.318579	0.011047
15	8	0	-0.083025	0.090873	-2.064180
16	6	0	-7.982385	1.637301	0.317134
17	6	0	-8.965743	1.343451	1.248031
18	6	0	-8.604430	0.853808	2.506483
19	6	0	-7.270373	0.653462	2.832810
20	1	0	-8.216027	2.031492	-0.663285
21	1	0	-10.008966	1.497524	1.006369
22	1	0	-9.369272	0.627219	3.238281
23	1	0	-6.965777	0.280833	3.801314
24	6	0	-0.429742	1.668176	-4.070743
25	1	0	-0.405674	0.689904	-4.546726
26	1	0	0.564942	1.924113	-3.710885
27	1	0	-0.806162	2.422590	-4.753681
28	6	0	3.402010	0.372349	1.010003
29	6	0	2.231334	-0.173471	1.536117
30	6	0	3.393486	1.212359	-0.226691
31	6	0	3.645862	2.617262	-0.135231
32	6	0	3.208444	0.628780	-1.479045
33	6	0	3.346564	1.427915	-2.654447
34	8	0	1.038559	-0.068494	0.935989
35	8	0	2.893875	-0.664457	-1.626197
36	30	0	1.189429	-0.737818	-0.822365
37	6	0	2.289469	-0.910945	2.757510
38	6	0	4.648681	0.115420	1.666423
39	6	0	3.616973	2.763742	-2.577545
40	6	0	3.761637	3.401461	-1.317269
41	6	0	4.688292	-0.644087	2.870314
42	6	0	3.471112	-1.138315	3.403601
43	1	0	1.352067	-1.282173	3.155774
44	1	0	3.494669	-1.701511	4.330157
45	6	0	5.928803	-0.894177	3.508670
46	6	0	5.885312	0.582549	1.139774
47	6	0	3.788644	3.277692	1.115160
48	6	0	4.019848	4.790222	-1.218150

49	1	0	3.726039	3.357784	-3.478758
50	1	0	3.231027	0.921568	-3.605182
51	6	0	7.100964	-0.422947	2.978852
52	6	0	7.071532	0.319856	1.776082
53	6	0	4.034519	4.626099	1.180745
54	6	0	4.156353	5.397546	0.003258
55	1	0	5.876318	1.147216	0.217700
56	1	0	7.998044	0.685436	1.350777
57	1	0	8.044616	-0.618426	3.472166
58	1	0	5.928970	-1.469976	4.427716
59	1	0	3.691177	2.697394	2.022939
60	1	0	4.134747	5.105358	2.146866
61	1	0	4.353222	6.460099	0.069282
62	1	0	4.106295	5.365020	-2.133829
63	6	0	-2.524503	-2.428218	-0.404296
64	7	0	-3.765780	-1.054460	1.057739
65	6	0	-3.664036	-1.589288	-0.123932
66	6	0	-4.673834	-1.312456	-1.195162
67	6	0	-1.395707	-2.395771	0.395524
68	6	0	-2.919470	-1.595676	2.131239
69	6	0	-1.445705	-1.766269	1.749235
70	1	0	-4.281534	-0.617915	-1.939880
71	1	0	-4.916269	-2.257700	-1.688590
72	1	0	-5.588305	-0.906624	-0.772615
73	6	0	-0.323190	-2.897556	-0.390693
74	6	0	-0.871299	-3.266864	-1.641071
75	7	0	-2.209892	-2.977978	-1.629434
76	1	0	-2.830456	-3.070555	-2.414066
77	1	0	-3.041160	-0.948831	2.999619
78	1	0	-3.338295	-2.573311	2.381824
79	1	0	-0.871630	-0.834532	1.749580
80	1	0	-0.977819	-2.413117	2.496187
81	6	0	-0.066209	-3.811284	-2.656604
82	6	0	1.077335	-3.011273	-0.156304
83	6	0	1.861826	-3.554053	-1.169062
84	6	0	1.277887	-3.937114	-2.412401
85	8	0	3.178462	-3.762372	-1.086418
86	6	0	3.866711	-3.248187	0.057992
87	1	0	3.514658	-3.737026	0.969146
88	1	0	4.913394	-3.484536	-0.104446
89	1	0	1.488663	-2.781912	0.819029
90	1	0	-0.483257	-4.099872	-3.612718
91	1	0	1.948516	-4.329503	-3.164053
92	1	0	3.733236	-2.168173	0.114982

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trans-exo-IM1-Si

Imaginary frequency: none

Standard orientation:

Electronic energy E = -4188.791786 a.u.

Enthalpy H = -4188.744709 a.u.

Entropy S = 268.080 cal/mol/K

Gibbs free energy G = -4188.872082 a.u.

Total free energy in solution E_{sol} = -4190.38979 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.614360	1.824756	-0.269597
2	6	0	-6.673736	1.397848	0.688433
3	6	0	-4.279239	1.405692	0.081352
4	6	0	-4.046353	0.628492	1.317976
5	6	0	-6.336502	0.827044	1.914859
6	8	0	-5.028281	0.678923	2.308081
7	8	0	-5.910284	2.427265	-1.299812
8	6	0	-3.257623	1.556219	-0.850469
9	6	0	-2.001012	0.969971	-0.823594
10	1	0	-3.124675	0.960232	1.800895

11	1	0	-3.541376	2.110749	-1.739630
12	6	0	-1.139123	0.965387	-1.946952
13	8	0	-1.482227	1.735716	-2.977589
14	1	0	-1.631127	0.413631	0.024589
15	8	0	-0.105918	0.249985	-2.061533
16	6	0	-8.022656	1.568931	0.371943
17	6	0	-9.011877	1.180811	1.262700
18	6	0	-8.652258	0.618016	2.489238
19	6	0	-7.315841	0.438581	2.822633
20	1	0	-8.253137	2.022954	-0.583072
21	1	0	-10.055674	1.318240	1.013583
22	1	0	-9.418829	0.317257	3.192139
23	1	0	-7.014685	0.012248	3.770079
24	6	0	-0.566320	1.765828	-4.082583
25	1	0	-0.493439	0.781732	-4.541707
26	1	0	0.418503	2.081009	-3.743123
27	1	0	-0.987253	2.485532	-4.777446
28	6	0	3.480858	0.277816	0.999619
29	6	0	2.298715	-0.256146	1.512057
30	6	0	3.481539	1.195203	-0.180266
31	6	0	3.788699	2.581169	-0.004868
32	6	0	3.245175	0.701209	-1.461824
33	6	0	3.378180	1.570618	-2.586761
34	8	0	1.101145	-0.072419	0.941704
35	8	0	2.882979	-0.570708	-1.680980
36	30	0	1.177292	-0.587279	-0.872370
37	6	0	2.348732	-1.068979	2.685207
38	6	0	4.726790	-0.066594	1.615376
39	6	0	3.698130	2.888211	-2.430983
40	6	0	3.901292	3.436149	-1.136775
41	6	0	4.757483	-0.902429	2.768007
42	6	0	3.531280	-1.381834	3.293285
43	1	0	1.404695	-1.426944	3.080012
44	1	0	3.547785	-2.001774	4.183052
45	6	0	5.997769	-1.239694	3.365116
46	6	0	5.971563	0.386667	1.095784
47	6	0	3.989474	3.152349	1.281016
48	6	0	4.212573	4.805553	-0.955819
49	1	0	3.800996	3.537202	-3.294067
50	1	0	3.216055	1.132956	-3.564330
51	6	0	7.178169	-0.780259	2.843575
52	6	0	7.157246	0.039239	1.691248
53	6	0	4.287623	4.483909	1.426172
54	6	0	4.405278	5.326035	0.297803
55	1	0	5.968799	1.009272	0.211747
56	1	0	8.089954	0.396440	1.272427
57	1	0	8.121698	-1.042204	3.305232
58	1	0	5.990908	-1.872199	4.246091
59	1	0	3.895799	2.517612	2.152054
60	1	0	4.432153	4.895015	2.417766
61	1	0	4.642368	6.374501	0.426424
62	1	0	4.294126	5.436270	-1.834410
63	6	0	-2.605216	-2.345652	-0.371755
64	7	0	-3.689018	-0.861266	1.081839
65	6	0	-3.682471	-1.448418	-0.094492
66	6	0	-4.721790	-1.190995	-1.140574
67	6	0	-1.430670	-2.313634	0.372495
68	6	0	-2.865419	-1.459716	2.147866
69	6	0	-1.413094	-1.686375	1.725471
70	1	0	-4.347428	-0.509751	-1.905836
71	1	0	-4.966887	-2.150193	-1.604439
72	1	0	-5.629669	-0.780136	-0.709897

73	6	0	-0.401493	-2.816431	-0.460674
74	6	0	-1.012766	-3.186468	-1.682214
75	7	0	-2.348584	-2.909436	-1.607408
76	1	0	-2.995934	-2.977548	-2.372862
77	1	0	-2.947126	-0.813315	3.018864
78	1	0	-3.325199	-2.420119	2.388580
79	1	0	-0.797282	-0.781769	1.711823
80	1	0	-0.954813	-2.357900	2.456474
81	6	0	-0.257359	-3.721914	-2.742260
82	6	0	1.009374	-2.930602	-0.292538
83	6	0	1.740106	-3.472510	-1.342241
84	6	0	1.094855	-3.843727	-2.562523
85	8	0	3.053514	-3.702493	-1.325837
86	6	0	3.800351	-3.250396	-0.190326
87	1	0	3.462325	-3.758782	0.715389
88	1	0	4.831523	-3.516166	-0.399342
89	1	0	1.466221	-2.714383	0.665294
90	1	0	-0.720645	-4.007027	-3.677700
91	1	0	1.729842	-4.233320	-3.346085
92	1	0	3.704006	-2.169744	-0.095608

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trans-exo-TS2-Si

Imaginary frequency: -144.6322 cm^{-1}

Standard orientation:

Electronic energy E = -4188.782463 a.u.

Enthalpy H = -4188.736028 a.u.

Entropy S = 265.428 cal/mol/K

Gibbs free energy G = -4188.862141 a.u.

Total free energy in solution E_{sol}= -4190.37792 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.394413	-1.167004	0.982298
2	7	0	3.252640	-1.046322	-0.442890
3	6	0	2.739346	-0.705672	0.738650
4	6	0	3.610409	-0.351289	1.905087
5	6	0	0.855739	-2.229707	0.311035
6	6	0	2.366535	-1.641362	-1.465588
7	6	0	1.559422	-2.788289	-0.876708
8	1	0	4.478265	0.229967	1.611271
9	1	0	3.038254	0.196645	2.651201
10	1	0	3.958244	-1.292494	2.340589
11	6	0	-0.385389	-2.565953	0.937716
12	6	0	-0.580727	-1.634349	1.971890
13	7	0	0.489208	-0.702517	1.957903
14	1	0	0.816833	-0.312591	2.831639
15	1	0	1.678203	-0.869460	-1.828802
16	1	0	3.001809	-1.980830	-2.279913
17	1	0	0.842100	-3.142200	-1.617942
18	1	0	2.204073	-3.628217	-0.599583
19	6	0	-1.356147	-3.526717	0.649399
20	6	0	-2.512793	-3.532500	1.411205
21	6	0	-2.689280	-2.600248	2.458334
22	6	0	-1.737106	-1.636117	2.741795
23	1	0	-1.257622	-4.222224	-0.171799
24	1	0	-1.919604	-0.880175	3.490386
25	1	0	-3.602207	-2.608311	3.035358
26	8	0	-3.436805	-4.469761	1.089680
27	6	0	6.175377	1.373457	-0.731488
28	6	0	7.188063	0.290426	-0.856792
29	6	0	4.781838	0.926492	-0.636029

30	6	0	4.539029	-0.531349	-0.917529
31	6	0	6.824251	-1.036708	-0.631184
32	8	0	5.527948	-1.379131	-0.333409
33	8	0	6.513647	2.548938	-0.695397
34	6	0	3.841661	1.838563	-0.244090
35	6	0	2.453340	1.670088	-0.012933
36	1	0	4.541779	-0.715626	-1.996134
37	1	0	4.266978	2.799455	0.031006
38	6	0	1.778958	2.577871	0.842143
39	8	0	0.571870	2.476835	1.191174
40	1	0	1.805996	1.041036	-0.606683
41	8	0	2.502438	3.569156	1.363577
42	6	0	1.806524	4.483127	2.222574
43	1	0	1.410681	3.959752	3.090688
44	1	0	0.988780	4.957392	1.684721
45	1	0	2.551135	5.215125	2.518991
46	6	0	8.525146	0.593863	-1.118389
47	6	0	9.478381	-0.411817	-1.158409
48	6	0	9.095983	-1.734586	-0.922091
49	6	0	7.770772	-2.055589	-0.658278
50	1	0	8.780740	1.633829	-1.274025
51	1	0	10.513555	-0.174885	-1.364844
52	1	0	9.837070	-2.523521	-0.947564
53	1	0	7.454447	-3.073345	-0.473779
54	6	0	-4.766050	-4.266226	1.552072
55	1	0	-5.378870	-4.984164	1.014096
56	1	0	-4.841454	-4.456941	2.625887
57	1	0	-5.105054	-3.255477	1.318245
58	30	0	-0.614278	0.973781	0.821139
59	6	0	-1.787712	-0.321486	-1.200458
60	6	0	-2.981200	1.759113	1.161839
61	6	0	-1.665701	-1.462030	-2.051867
62	6	0	-2.711009	-2.306296	-2.286449
63	6	0	-3.968757	-2.071223	-1.674419
64	6	0	-4.131963	-0.895778	-0.888220
65	6	0	-3.046199	0.022161	-0.703628
66	6	0	-3.361346	1.368535	-0.121236
67	6	0	-3.488976	2.976185	1.710983
68	6	0	-4.299558	3.799135	0.988534
69	6	0	-4.172275	2.256496	-0.906597
70	6	0	-4.650376	3.474909	-0.348616
71	6	0	-5.057861	-2.957713	-1.861143
72	6	0	-5.413111	-0.665286	-0.311815
73	6	0	-6.282093	-2.701331	-1.299242
74	6	0	-6.453096	-1.539274	-0.512173
75	6	0	-4.523747	1.968692	-2.253952
76	6	0	-5.302363	2.830015	-2.985814
77	6	0	-5.784964	4.030204	-2.419310
78	6	0	-5.458265	4.340677	-1.124711
79	8	0	-2.141476	1.039319	1.916816
80	1	0	-4.154924	1.057924	-2.705630
81	1	0	-5.547342	2.586342	-4.012417
82	1	0	-6.401592	4.698805	-3.006690
83	1	0	-5.810673	5.260475	-0.670733
84	1	0	-4.677416	4.719883	1.419436
85	1	0	-3.191522	3.214059	2.724581
86	1	0	-5.555888	0.219706	0.293606
87	1	0	-7.417319	-1.333774	-0.062992
88	1	0	-7.111624	-3.379978	-1.454257
89	1	0	-4.902088	-3.843942	-2.466774
90	1	0	-2.595773	-3.165720	-2.938450
91	1	0	-0.699584	-1.618454	-2.517689

92	8	0	-0.670839	0.369109	-0.952771

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cis-2a as diene

cis-endo-TS-Re

Imaginary frequency: -302.3691 cm^{-1}

Standard orientation:

Electronic energy E = -4188.787327 a.u.

Enthalpy H = -4188.740476 a.u.

Entropy S = 265.359 cal/mol/K

Gibbs free energy G = -4188.866557 a.u.

Total free energy in solution E_{sol}= -4190.37820 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.637442	-2.776807	0.091995
2	7	0	-4.481495	-1.293732	-0.086076
3	6	0	-3.889132	-2.240205	0.580490
4	6	0	-4.504173	-2.862018	1.802925
5	6	0	-1.874022	-2.135580	-0.857966
6	6	0	-3.947611	-0.961436	-1.424005
7	6	0	-2.416960	-0.929714	-1.554770
8	1	0	-3.786377	-2.914252	2.622759
9	1	0	-5.401259	-2.341247	2.126861
10	1	0	-4.804142	-3.882388	1.544204
11	6	0	-0.601790	-2.774969	-0.859532
12	6	0	-0.665708	-3.818615	0.092387
13	7	0	-1.910842	-3.796667	0.670856
14	1	0	-2.238180	-4.434929	1.374021
15	1	0	-4.335939	-1.740901	-2.085315
16	1	0	-4.386502	-0.015908	-1.731424
17	1	0	-2.170925	-0.945931	-2.618716
18	1	0	-1.974276	-0.017256	-1.146507
19	6	0	0.610876	-2.515548	-1.555576
20	6	0	1.698993	-3.344767	-1.298045
21	6	0	1.595112	-4.410947	-0.361454
22	6	0	0.432395	-4.663091	0.324729
23	8	0	2.903113	-3.219788	-1.871601
24	6	0	3.123508	-2.096982	-2.731378
25	1	0	0.650963	-1.738108	-2.306500
26	1	0	2.480640	-5.010329	-0.202105
27	1	0	0.378867	-5.473289	1.040984
28	1	0	2.538044	-2.206718	-3.647492
29	1	0	4.184536	-2.110280	-2.958136
30	1	0	2.869178	-1.162989	-2.226732
31	6	0	-4.077909	2.140375	-0.242497
32	6	0	-5.395223	2.306175	-0.907070
33	6	0	-4.023535	1.072632	0.740159
34	6	0	-5.107976	0.145622	0.846265
35	6	0	-6.450517	1.450106	-0.601543
36	8	0	-6.327053	0.438184	0.326017
37	8	0	-3.126169	2.862086	-0.522422
38	6	0	-2.773635	0.726829	1.290000
39	6	0	-2.520339	-0.265469	2.201224
40	1	0	-5.241869	-0.378670	1.780463
41	1	0	-1.919550	1.247166	0.863151
42	6	0	-1.188079	-0.792750	2.274596
43	8	0	-0.316089	-0.533904	1.431415
44	1	0	-3.267443	-0.687477	2.857672
45	8	0	-0.958568	-1.639318	3.273708
46	6	0	0.375339	-2.186590	3.332672
47	1	0	1.119502	-1.395715	3.281970
48	1	0	0.534342	-2.872710	2.500927
49	1	0	0.423327	-2.714680	4.279549
50	6	0	-5.598369	3.315909	-1.850473
51	6	0	-6.831439	3.465536	-2.464456

52	6	0	-7.877314	2.597847	-2.137862
53	6	0	-7.694359	1.584351	-1.207065
54	1	0	-4.761627	3.965427	-2.071816
55	1	0	-6.986041	4.250451	-3.192565
56	1	0	-8.842672	2.711519	-2.614105
57	1	0	-8.488156	0.900591	-0.939075
58	30	0	1.118037	-0.935957	0.142407
59	6	0	4.839818	-1.702415	0.243425
60	6	0	2.707880	1.484359	0.193862
61	6	0	1.470990	1.438657	-0.447174
62	6	0	0.533226	2.499450	-0.268580
63	6	0	3.774708	0.468129	-0.079723
64	6	0	3.726538	-0.829358	0.432618
65	6	0	2.991161	2.572613	1.081431
66	6	0	4.906409	0.862630	-0.867228
67	6	0	5.935270	-1.320629	-0.472704
68	6	0	5.994929	-0.032481	-1.065916
69	6	0	2.038001	3.614085	1.263601
70	6	0	0.808545	3.550770	0.555723
71	1	0	6.770654	-1.999236	-0.607713
72	1	0	4.764822	-2.688629	0.684073
73	6	0	7.108219	0.369847	-1.843911
74	6	0	4.985226	2.142594	-1.482254
75	6	0	4.209377	2.653771	1.808523
76	6	0	2.327363	4.686261	2.141885
77	1	0	0.082448	4.345336	0.686939
78	1	0	-0.409174	2.435457	-0.799501
79	8	0	1.104679	0.389048	-1.205507
80	8	0	2.674778	-1.324568	1.099988
81	6	0	4.461150	3.703736	2.655966
82	6	0	3.514227	4.738061	2.826947
83	6	0	7.154962	1.613164	-2.419585
84	6	0	6.073931	2.503910	-2.235138
85	1	0	7.925733	-0.331070	-1.974012
86	1	0	8.010121	1.912529	-3.012492
87	1	0	6.103986	3.484327	-2.694561
88	1	0	4.161786	2.831800	-1.353939
89	1	0	4.938902	1.864097	1.688447
90	1	0	5.396724	3.739174	3.200662
91	1	0	3.726240	5.562161	3.496535
92	1	0	1.585310	5.467971	2.261925

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cis-endo-TS-Si

Imaginary frequency: -316.1013 cm^{-1}

Standard orientation:

Electronic energy E = -4188.785694 a.u.

Enthalpy H = -4188.865454 a.u.

Entropy S = 266.809 cal/mol/K

Gibbs free energy G = -4189.760132 a.u.

Total free energy in solution E_{sol}= -4190.37767 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929227	-2.416557	-0.796979
2	7	0	4.422303	-0.603776	-0.474076
3	6	0	4.092735	-1.826359	-0.172054
4	6	0	4.920521	-2.654267	0.770247
5	6	0	1.974720	-1.650115	-1.431040
6	6	0	3.766553	0.010374	-1.646681
7	6	0	2.254454	-0.223048	-1.777180
8	1	0	4.304254	-3.148341	1.522359
9	1	0	5.693484	-2.062451	1.255005
10	1	0	5.430354	-3.423217	0.180975

11	6	0	0.807713	-2.461802	-1.540318
12	6	0	1.136311	-3.727720	-1.001078
13	7	0	2.428516	-3.676378	-0.540541
14	1	0	2.924640	-4.434504	-0.106825
15	1	0	4.268804	-0.430806	-2.511686
16	1	0	3.998123	1.072477	-1.635381
17	1	0	1.980246	-0.026859	-2.817889
18	1	0	1.650430	0.448566	-1.162955
19	6	0	-0.511496	-2.200812	-2.004821
20	6	0	-1.429832	-3.247370	-1.974864
21	6	0	-1.061451	-4.519796	-1.455386
22	6	0	0.202157	-4.774550	-0.979410
23	8	0	-2.690725	-3.169267	-2.412146
24	6	0	-3.194257	-1.877592	-2.766060
25	1	0	-0.750719	-1.248102	-2.461992
26	1	0	-1.827465	-5.282698	-1.445636
27	1	0	0.456435	-5.750008	-0.583671
28	1	0	-2.661965	-1.480656	-3.633397
29	1	0	-4.239255	-2.031096	-3.016195
30	1	0	-3.110415	-1.203382	-1.914518
31	6	0	3.030982	2.413034	0.510752
32	6	0	4.197474	3.167806	-0.018895
33	6	0	3.351608	1.107677	1.070725
34	6	0	4.668107	0.567065	0.902664
35	6	0	5.472686	2.611760	0.015678
36	8	0	5.709428	1.360324	0.543544
37	8	0	1.902055	2.880739	0.475100
38	6	0	2.303805	0.262648	1.491699
39	6	0	2.491743	-0.970291	2.068393
40	1	0	5.019715	-0.165623	1.613514
41	1	0	1.296996	0.609758	1.259314
42	6	0	1.457855	-1.950729	2.159048
43	8	0	0.322440	-1.915051	1.650984
44	1	0	3.438197	-1.264019	2.498496
45	8	0	1.825132	-3.043183	2.841714
46	6	0	0.830582	-4.073282	2.947962
47	1	0	-0.049720	-3.692429	3.460957
48	1	0	0.541250	-4.421750	1.957455
49	1	0	1.299727	-4.866209	3.522266
50	6	0	4.033794	4.445570	-0.557422
51	6	0	5.125507	5.147310	-1.043862
52	6	0	6.397230	4.570120	-0.995033
53	6	0	6.580122	3.299172	-0.466915
54	1	0	3.031478	4.853406	-0.572523
55	1	0	4.995791	6.138044	-1.458420
56	1	0	7.253259	5.114841	-1.372220
57	1	0	7.554194	2.831789	-0.418140
58	30	0	-0.829194	-1.284865	0.179681
59	8	0	-2.622241	-1.751483	0.479663
60	8	0	-0.468248	0.494818	-0.301237
61	6	0	-1.268520	1.489005	-2.288494
62	6	0	-3.128334	0.551787	0.922506
63	6	0	-3.073298	-0.788901	1.298698
64	6	0	-3.515571	-1.173919	2.599734
65	6	0	-2.817575	0.976433	-0.477140
66	6	0	-1.515234	0.981399	-0.976605
67	6	0	-3.556263	1.530525	1.875436
68	6	0	-3.891586	1.394604	-1.328875
69	6	0	-2.284015	1.913712	-3.096211
70	6	0	-3.628666	1.861506	-2.647922
71	6	0	-3.981447	1.128476	3.172426
72	6	0	-3.958913	-0.252022	3.501754

73	1	0	-2.076884	2.294168	-4.090609
74	1	0	-0.235488	1.529409	-2.613205
75	6	0	-4.700435	2.260614	-3.484754
76	6	0	-5.250241	1.332327	-0.910717
77	6	0	-3.574742	2.919283	1.572904
78	6	0	-4.415491	2.102144	4.104628
79	1	0	-4.295638	-0.559801	4.485716
80	1	0	-3.483371	-2.231027	2.833098
81	6	0	-6.268340	1.718956	-1.745031
82	6	0	-5.997700	2.194946	-3.048116
83	6	0	-4.428389	3.433849	3.779975
84	6	0	-3.996594	3.840889	2.497597
85	1	0	-4.737017	1.769192	5.085463
86	1	0	-4.761085	4.171537	4.499457
87	1	0	-3.994454	4.893643	2.242756
88	1	0	-3.236305	3.243195	0.598059
89	1	0	-5.471309	0.964556	0.081739
90	1	0	-7.293247	1.657259	-1.400307
91	1	0	-6.811116	2.501155	-3.693743
92	1	0	-4.469542	2.618687	-4.482164

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cis-exo-TS1-Re

Imaginary frequency: -243.2936 cm^{-1}

Standard orientation:

Electronic energy E = -4188.756768 a.u.

Enthalpy H = -4188.709973 a.u.

Entropy S = 277.472 cal/mol/K

Gibbs free energy G = -4188.841809 a.u.

Total free energy in solution E_{sol}= -4190.35895 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.866992	3.775733	0.409471
2	6	0	1.753786	4.959791	0.262786
3	6	0	1.461703	2.660305	1.131052
4	6	0	2.810881	2.766302	1.604258
5	8	0	3.429121	3.967977	1.695805
6	8	0	-0.247120	3.753147	-0.096827
7	6	0	0.855182	1.399725	1.056844
8	6	0	1.427197	0.225588	1.509766
9	1	0	3.065123	2.184544	2.483167
10	1	0	-0.097153	1.368582	0.530083
11	6	0	1.048407	-1.052919	1.032887
12	8	0	0.312011	-1.304495	0.036540
13	1	0	2.250336	0.213680	2.210753
14	8	0	1.649471	-2.064596	1.651778
15	6	0	1.377699	-3.384063	1.158065
16	1	0	0.308574	-3.583621	1.175807
17	1	0	1.754774	-3.490439	0.142279
18	1	0	1.906204	-4.052183	1.829983
19	6	0	2.995526	4.998096	0.891115
20	6	0	1.357644	6.055077	-0.509477
21	6	0	2.187192	7.156663	-0.642873
22	6	0	3.427123	7.173420	0.002722
23	6	0	3.839396	6.096154	0.774217
24	1	0	4.791742	6.087249	1.286451
25	1	0	4.076589	8.033669	-0.096417
26	1	0	1.876612	8.003147	-1.240527
27	1	0	0.387103	6.004266	-0.985174
28	6	0	4.032608	-0.334514	-0.561952
29	7	0	3.936925	1.733631	0.579338
30	6	0	3.482075	0.988227	-0.385329
31	6	0	2.536439	1.512129	-1.422943
32	6	0	5.258707	-0.696034	-0.055481
33	6	0	4.952182	1.162699	1.479523
34	6	0	6.001260	0.316264	0.758854

35	1	0	1.585421	0.974549	-1.399058
36	1	0	2.997838	1.339444	-2.398206
37	1	0	2.352479	2.574143	-1.304839
38	6	0	5.533066	-2.010135	-0.533919
39	6	0	4.415841	-2.390588	-1.315915
40	7	0	3.527825	-1.339556	-1.355691
41	1	0	2.576177	-1.396217	-1.681319
42	1	0	4.447425	0.519507	2.211138
43	1	0	5.407820	2.000269	2.008767
44	1	0	6.646085	-0.150760	1.504855
45	1	0	6.633996	0.941895	0.121204
46	6	0	6.614459	-2.898995	-0.359714
47	6	0	6.532879	-4.141850	-0.955607
48	6	0	5.397538	-4.514604	-1.721143
49	6	0	4.338293	-3.658491	-1.909637
50	8	0	7.490680	-5.103510	-0.875966
51	6	0	8.646877	-4.802022	-0.118319
52	1	0	9.279888	-5.683341	-0.171635
53	1	0	8.389926	-4.597117	0.924342
54	1	0	9.177595	-3.943630	-0.538856
55	1	0	7.470256	-2.600828	0.228537
56	1	0	5.399612	-5.503481	-2.159234
57	1	0	3.483611	-3.953114	-2.505111
58	6	0	-4.527435	-4.126829	0.761966
59	6	0	-5.339554	-3.172857	1.428651
60	6	0	-5.232405	-1.802817	1.060032
61	6	0	-3.632407	-3.731060	-0.187832
62	6	0	-3.496553	-2.358733	-0.554947
63	6	0	-4.325549	-1.398354	0.024464
64	8	0	-2.537384	-2.051527	-1.455691
65	8	0	-2.195065	0.586063	0.434926
66	6	0	-4.362946	0.024291	-0.447601
67	6	0	-5.520712	0.476289	-1.162449
68	6	0	-5.649513	1.847235	-1.520873
69	6	0	-4.608771	2.747744	-1.173092
70	6	0	-3.348323	0.934714	-0.168647
71	6	0	-3.492641	2.306809	-0.525882
72	1	0	-4.624371	-5.173897	1.027457
73	1	0	-2.993919	-4.438489	-0.702555
74	6	0	-6.244541	-3.561622	2.446571
75	6	0	-6.046390	-0.865774	1.753250
76	6	0	-6.568844	-0.406134	-1.539975
77	6	0	-6.799367	2.288316	-2.219724
78	1	0	-4.710663	3.793054	-1.443347
79	1	0	-2.672584	2.966930	-0.272919
80	6	0	-7.018943	-2.633703	3.093071
81	6	0	-6.909397	-1.270047	2.740893
82	1	0	-6.309724	-4.613025	2.704379
83	1	0	-7.708287	-2.938751	3.870219
84	1	0	-7.513784	-0.533875	3.256364
85	1	0	-5.967889	0.181168	1.494353
86	6	0	-7.671448	0.048870	-2.219319
87	6	0	-7.797059	1.412976	-2.563405
88	1	0	-6.482488	-1.454859	-1.290945
89	1	0	-8.452771	-0.647842	-2.497457
90	1	0	-8.672512	1.759241	-3.098382
91	1	0	-6.871322	3.338602	-2.480241
92	30	0	-1.533453	-0.909303	-0.402013

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cis-exo-IM1-Re

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.031270	3.887916	0.513750
2	6	0	2.051507	4.928006	0.213356
3	6	0	1.551809	2.689219	1.161747
4	6	0	2.981820	2.631310	1.574459
5	8	0	3.691354	3.833005	1.615191
6	8	0	-0.130019	4.020012	0.153781
7	6	0	0.822464	1.527335	1.097030
8	6	0	1.295999	0.266194	1.521998
9	1	0	3.062204	2.222564	2.583659
10	1	0	-0.152129	1.595758	0.615042
11	6	0	0.925065	-0.931790	0.913638
12	8	0	0.323958	-1.057187	-0.212099
13	1	0	2.004210	0.173988	2.335484
14	8	0	1.368265	-2.044029	1.512719
15	6	0	1.010638	-3.292840	0.911196
16	1	0	-0.069925	-3.373169	0.801193
17	1	0	1.484753	-3.402813	-0.063424
18	1	0	1.380183	-4.052089	1.593173
19	6	0	3.338024	4.834684	0.742342
20	6	0	1.736543	6.006575	-0.616235
21	6	0	2.688152	6.970884	-0.908519
22	6	0	3.969421	6.862587	-0.362660
23	6	0	4.301555	5.797792	0.465041
24	1	0	5.284856	5.700073	0.904858
25	1	0	4.716171	7.614828	-0.583075
26	1	0	2.440468	7.805020	-1.551153
27	1	0	0.728925	6.055480	-1.007967
28	6	0	3.875431	-0.411635	-0.431885
29	7	0	3.817878	1.595392	0.795081
30	6	0	3.348482	0.902436	-0.224477
31	6	0	2.483458	1.478738	-1.303705
32	6	0	5.080659	-0.837467	0.080606
33	6	0	4.813800	0.963314	1.686136
34	6	0	5.842274	0.116273	0.943006
35	1	0	1.496274	1.011679	-1.295801
36	1	0	2.968473	1.231962	-2.250929
37	1	0	2.379614	2.554797	-1.230595
38	6	0	5.315857	-2.137208	-0.447894
39	6	0	4.195611	-2.444150	-1.258820
40	7	0	3.349795	-1.359669	-1.282347
41	1	0	2.371618	-1.396750	-1.537232
42	1	0	4.271368	0.322888	2.391297
43	1	0	5.287171	1.777609	2.233456
44	1	0	6.457930	-0.401504	1.679955
45	1	0	6.506206	0.745942	0.342594
46	6	0	6.363963	-3.070080	-0.293814
47	6	0	6.242169	-4.286429	-0.933757
48	6	0	5.101050	-4.588335	-1.724408
49	6	0	4.077264	-3.688466	-1.896195
50	8	0	7.159858	-5.285874	-0.879362
51	6	0	8.316402	-5.058227	-0.096025
52	1	0	8.913852	-5.962205	-0.172014
53	1	0	8.051186	-4.880157	0.949461

Imaginary frequency: none
Electronic energy E = -4188.758990 a.u.
Enthalpy H = -4188.712473 a.u.
Entropy S = 269.412 cal/mol/K
Gibbs free energy G = -4188.840479 a.u.
Total free energy in solution E_{sol} = -4190.36340 a.u.

54	1	0	8.887066	-4.207945	-0.478991
55	1	0	7.222209	-2.825468	0.314931
56	1	0	5.071668	-5.561361	-2.195895
57	1	0	3.219785	-3.929155	-2.511126
58	6	0	-4.203321	-4.104399	0.378223
59	6	0	-5.016590	-3.284327	1.203565
60	6	0	-5.025835	-1.879508	0.978463
61	6	0	-3.418383	-3.550028	-0.589659
62	6	0	-3.400449	-2.140443	-0.817392
63	6	0	-4.235780	-1.305852	-0.072470
64	8	0	-2.541268	-1.673102	-1.747098
65	8	0	-2.194017	0.746706	0.407951
66	6	0	-4.388489	0.154407	-0.376666
67	6	0	-5.619669	0.611430	-0.950889
68	6	0	-5.847064	2.002982	-1.141655
69	6	0	-4.830176	2.921599	-0.770669
70	6	0	-3.403565	1.088361	-0.069665
71	6	0	-3.646343	2.479961	-0.258854
72	1	0	-4.211515	-5.177416	0.535943
73	1	0	-2.783429	-4.153973	-1.226384
74	6	0	-5.807203	-3.839211	2.239277
75	6	0	-5.834408	-1.079099	1.830817
76	6	0	-6.645887	-0.286826	-1.350358
77	6	0	-7.070600	2.446630	-1.699796
78	1	0	-5.007229	3.982120	-0.912095
79	1	0	-2.843507	3.155783	0.010333
80	6	0	-6.580474	-3.040397	3.040690
81	6	0	-6.585363	-1.643190	2.831181
82	1	0	-5.784567	-4.913565	2.386016
83	1	0	-7.181313	-3.472429	3.831058
84	1	0	-7.188046	-1.008508	3.469142
85	1	0	-5.841002	-0.007883	1.683776
86	6	0	-7.820365	0.171212	-1.892501
87	6	0	-8.044794	1.554614	-2.067760
88	1	0	-6.483313	-1.349266	-1.229801
89	1	0	-8.582926	-0.537243	-2.192367
90	1	0	-8.976934	1.903604	-2.494226
91	1	0	-7.219031	3.512872	-1.832158
92	30	0	-1.516523	-0.636256	-0.597090

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cis-exo-TS2-Re

Imaginary frequency: -139.2525 cm^{-1}

Standard orientation:

Electronic energy E = -4188.758832 a.u.

Enthalpy H = -4188.712144 a.u.

Entropy S = 274.334 cal/mol/K

Gibbs free energy G = -4188.842489 a.u.

Total free energy in solution E_{sol}= -4190.35903 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.136905	4.073563	0.367463
2	6	0	2.242034	5.047379	0.177521
3	6	0	1.541427	2.799502	0.967081
4	6	0	2.925208	2.627230	1.498311
5	8	0	3.709675	3.779800	1.624845
6	8	0	0.006799	4.301744	-0.034349
7	6	0	0.757737	1.696043	0.775066
8	6	0	1.187950	0.389730	1.128515
9	1	0	2.869556	2.216346	2.509431
10	1	0	-0.186222	1.839857	0.252709
11	6	0	0.741951	-0.782270	0.500718
12	8	0	0.192641	-0.852461	-0.649727
13	1	0	1.798283	0.227056	2.007998
14	8	0	1.071722	-1.915467	1.118206
15	6	0	0.654901	-3.142994	0.503004

16	1	0	-0.424655	-3.152716	0.358242
17	1	0	1.157081	-3.280799	-0.453623
18	1	0	0.954613	-3.920932	1.197578
19	6	0	3.483108	4.835033	0.777220
20	6	0	2.054815	6.181712	-0.615617
21	6	0	3.088359	7.084759	-0.806758
22	6	0	4.323125	6.857039	-0.193920
23	6	0	4.527515	5.736571	0.600116
24	1	0	5.472979	5.547505	1.089988
25	1	0	5.134038	7.560051	-0.336082
26	1	0	2.940474	7.961968	-1.422238
27	1	0	1.079245	6.321994	-1.062713
28	6	0	3.737799	-0.512502	-0.368240
29	7	0	3.753846	1.551850	0.791991
30	6	0	3.239905	0.825841	-0.203221
31	6	0	2.602657	1.460623	-1.408520
32	6	0	4.890124	-0.981349	0.218504
33	6	0	4.626128	0.871062	1.771094
34	6	0	5.643915	-0.062485	1.124037
35	1	0	1.656149	0.975826	-1.651289
36	1	0	3.297340	1.292807	-2.236042
37	1	0	2.452613	2.527252	-1.297459
38	6	0	5.115621	-2.288013	-0.303864
39	6	0	4.049080	-2.550489	-1.196472
40	7	0	3.241332	-1.438280	-1.257941
41	1	0	2.309357	-1.409797	-1.646011
42	1	0	3.994592	0.283066	2.448777
43	1	0	5.115082	1.661194	2.339773
44	1	0	6.163653	-0.604914	1.915548
45	1	0	6.394475	0.507596	0.567696
46	6	0	6.117911	-3.256762	-0.087583
47	6	0	6.006033	-4.461755	-0.752527
48	6	0	4.920600	-4.716464	-1.629856
49	6	0	3.941512	-3.779739	-1.862257
50	8	0	6.886937	-5.491386	-0.641899
51	6	0	7.996389	-5.300818	0.214864
52	1	0	8.574558	-6.219269	0.167490
53	1	0	7.671250	-5.125108	1.243868
54	1	0	8.611691	-4.462177	-0.121962
55	1	0	6.936092	-3.048235	0.586274
56	1	0	4.895106	-5.681453	-2.117698
57	1	0	3.125432	-3.984462	-2.543273
58	6	0	-3.636369	-4.007420	0.351507
59	6	0	-4.319485	-3.239127	1.331335
60	6	0	-4.519001	-1.850334	1.097735
61	6	0	-3.143727	-3.415966	-0.774715
62	6	0	-3.311244	-2.016359	-1.015735
63	6	0	-4.039249	-1.237948	-0.109622
64	8	0	-2.708934	-1.491532	-2.100472
65	8	0	-2.227221	1.089688	-0.120499
66	6	0	-4.436956	0.180595	-0.398178
67	6	0	-5.813928	0.450009	-0.693602
68	6	0	-6.266311	1.791412	-0.833797
69	6	0	-5.330831	2.849930	-0.687896
70	6	0	-3.545772	1.247515	-0.317829
71	6	0	-4.015894	2.586568	-0.445430
72	1	0	-3.508679	-5.071743	0.517351
73	1	0	-2.611950	-3.978606	-1.532399
74	6	0	-4.802594	-3.832217	2.523031
75	6	0	-5.197242	-1.102504	2.097568
76	6	0	-6.768281	-0.589562	-0.861945
77	6	0	-7.629472	2.049653	-1.116834

78	1	0	-5.679260	3.872279	-0.783815
79	1	0	-3.276406	3.371592	-0.346000
80	6	0	-5.457706	-3.083676	3.466535
81	6	0	-5.649726	-1.701851	3.246307
82	1	0	-4.641861	-4.894200	2.673152
83	1	0	-5.824524	-3.544072	4.375168
84	1	0	-6.159726	-1.106735	3.993646
85	1	0	-5.345608	-0.042871	1.941702
86	6	0	-8.082655	-0.310132	-1.140143
87	6	0	-8.527430	1.024303	-1.265794
88	1	0	-6.440251	-1.616861	-0.779899
89	1	0	-8.786014	-1.123641	-1.269174
90	1	0	-9.567539	1.231864	-1.483550
91	1	0	-7.947429	3.081684	-1.216632
92	30	0	-1.632525	-0.367647	-1.069227

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cis-exo-TS1-Si

Imaginary frequency: -190.7999 cm^{-1}

Standard orientation:

Electronic energy E = -4188.759554 a.u.

Enthalpy H = -4188.712405 a.u.

Entropy S = 275.948 cal/mol/K

Gibbs free energy G = -4188.843517 a.u.

Total free energy in solution E_{sol}= -4190.35657 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.218151	-3.407438	-0.293623
2	6	0	6.822439	-2.141780	-0.510478
3	6	0	6.003279	-0.978952	-0.493098
4	6	0	4.873104	-3.509513	-0.099159
5	6	0	4.036128	-2.356556	-0.089776
6	6	0	4.594933	-1.089715	-0.247102
7	8	0	2.718294	-2.570579	0.074749
8	8	0	2.558583	-0.109142	-2.120619
9	6	0	3.808670	0.182145	-0.091881
10	6	0	4.045405	0.997248	1.068871
11	6	0	3.463311	2.291162	1.167820
12	6	0	2.648007	2.763131	0.102628
13	6	0	2.958184	0.667238	-1.097161
14	6	0	2.403446	1.981394	-0.986264
15	1	0	6.843201	-4.293523	-0.297412
16	1	0	4.389851	-4.466349	0.051191
17	6	0	8.213916	-2.022907	-0.744465
18	6	0	6.631653	0.273289	-0.732435
19	6	0	4.846133	0.545984	2.150871
20	6	0	3.697448	3.083486	2.316669
21	1	0	2.190148	3.743031	0.174198
22	1	0	1.756700	2.320113	-1.785605
23	6	0	8.791111	-0.799088	-0.962844
24	6	0	7.982253	0.358956	-0.960188
25	1	0	8.813753	-2.926425	-0.750197
26	1	0	9.855583	-0.717285	-1.142930
27	1	0	8.431982	1.326719	-1.145223
28	1	0	6.024644	1.168246	-0.745847
29	6	0	5.054045	1.335027	3.255470
30	6	0	4.479036	2.621075	3.344960
31	1	0	5.288241	-0.439337	2.094569
32	1	0	5.666913	0.964822	4.068078
33	1	0	4.654582	3.233950	4.220154
34	1	0	3.243488	4.067013	2.364761

35	6	0	-1.410420	3.871563	-0.361385
36	6	0	-2.502490	4.849582	-0.596108
37	6	0	-1.756513	2.785605	0.539334
38	6	0	-3.065815	2.734266	1.118860
39	8	0	-3.880837	3.815926	1.099193
40	8	0	-0.331038	3.974954	-0.934186
41	6	0	-0.953877	1.635222	0.546676
42	6	0	-1.230004	0.450522	1.195885
43	1	0	-3.154025	2.254104	2.086878
44	1	0	-0.091521	1.667891	-0.113667
45	6	0	-0.622503	-0.762136	0.772607
46	8	0	-0.044682	-0.900630	-0.344847
47	1	0	-1.927582	0.368033	2.017491
48	8	0	-0.804686	-1.792761	1.578745
49	6	0	-0.302671	-3.076766	1.158272
50	1	0	0.783965	-3.057949	1.084445
51	1	0	-0.750430	-3.352884	0.203632
52	1	0	-0.623647	-3.766342	1.931858
53	6	0	-3.692125	4.768971	0.123351
54	6	0	-2.356427	5.866840	-1.542991
55	6	0	-3.378851	6.776111	-1.758818
56	6	0	-4.561974	6.677756	-1.020497
57	6	0	-4.726622	5.676101	-0.074223
58	1	0	-5.630658	5.582991	0.511894
59	1	0	-5.361659	7.388391	-1.184937
60	1	0	-3.262739	7.561948	-2.493099
61	1	0	-1.421621	5.912024	-2.086112
62	30	0	1.794701	-1.266574	-0.846912
63	6	0	-3.789918	-0.816671	-0.500523
64	7	0	-4.051483	1.373378	0.349737
65	6	0	-3.526728	0.601583	-0.557314
66	6	0	-2.791462	1.146221	-1.743753
67	6	0	-4.856534	-1.343912	0.187417
68	6	0	-4.845423	0.747518	1.420388
69	6	0	-5.738113	-0.395038	0.936438
70	1	0	-1.738300	0.854207	-1.725528
71	1	0	-3.246189	0.710805	-2.636683
72	1	0	-2.868161	2.227028	-1.802711
73	6	0	-4.858701	-2.746528	-0.065553
74	6	0	-3.749140	-3.001193	-0.906886
75	7	0	-3.132790	-1.804980	-1.197910
76	1	0	-2.212151	-1.705615	-1.597313
77	1	0	-4.157436	0.337770	2.170125
78	1	0	-5.429248	1.544168	1.883088
79	1	0	-6.202913	-0.866109	1.803838
80	1	0	-6.541526	-0.016913	0.295968
81	6	0	-5.687311	-3.806037	0.358815
82	6	0	-5.366701	-5.083835	-0.054953
83	6	0	-4.241406	-5.324809	-0.884364
84	6	0	-3.428384	-4.303403	-1.316177
85	8	0	-6.065618	-6.202433	0.276324
86	6	0	-7.201216	-6.030996	1.102005
87	1	0	-7.619186	-7.022761	1.249590
88	1	0	-6.921975	-5.603421	2.068844
89	1	0	-7.942908	-5.388588	0.619582
90	1	0	-6.538166	-3.606303	0.993896
91	1	0	-4.048581	-6.349819	-1.170974
92	1	0	-2.579604	-4.502212	-1.958064

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cis-exo-IM1-Si Imaginary frequency: -190.7999 cm^{-1}

Standard orientation: Electronic energy E = -4188.762100 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.152328	-3.479065	-0.401886
2	6	0	6.792212	-2.226907	-0.592837
3	6	0	6.008540	-1.040936	-0.536402
4	6	0	4.807075	-3.545235	-0.194223
5	6	0	4.004547	-2.368518	-0.145364
6	6	0	4.600221	-1.115513	-0.276900
7	8	0	2.685125	-2.548111	0.031281
8	8	0	2.559575	-0.047105	-2.095290
9	6	0	3.852156	0.172909	-0.083500
10	6	0	4.127978	0.958571	1.088678
11	6	0	3.577502	2.263047	1.224259
12	6	0	2.755278	2.775523	0.183927
13	6	0	2.994317	0.696451	-1.062409
14	6	0	2.473895	2.021148	-0.915395
15	1	0	6.750233	-4.383158	-0.435607
16	1	0	4.296712	-4.490693	-0.062312
17	6	0	8.184182	-2.143785	-0.838925
18	6	0	6.672503	0.197470	-0.751437
19	6	0	4.935755	0.466709	2.147631
20	6	0	3.848696	3.025336	2.385536
21	1	0	2.319765	3.762991	0.284005
22	1	0	1.821758	2.390713	-1.696698
23	6	0	8.796258	-0.932735	-1.032181
24	6	0	8.022775	0.248457	-0.991536
25	1	0	8.756137	-3.064592	-0.874337
26	1	0	9.860943	-0.878499	-1.221398
27	1	0	8.499478	1.206807	-1.156991
28	1	0	6.092710	1.110207	-0.735794
29	6	0	5.179861	1.227053	3.264684
30	6	0	4.636110	2.523767	3.390683
31	1	0	5.353487	-0.527268	2.063979
32	1	0	5.796799	0.825491	4.059145
33	1	0	4.839527	3.113503	4.275662
34	1	0	3.417820	4.017413	2.461902
35	6	0	-1.357470	3.889846	-0.271009
36	6	0	-2.495155	4.779399	-0.625789
37	6	0	-1.703398	2.765960	0.582548
38	6	0	-3.088591	2.626641	1.104686
39	8	0	-3.925660	3.740120	1.027180
40	8	0	-0.240749	4.075105	-0.742188
41	6	0	-0.864032	1.674343	0.626045
42	6	0	-1.145672	0.455271	1.263580
43	1	0	-3.068558	2.359504	2.163064
44	1	0	0.038626	1.745282	0.024108
45	6	0	-0.614034	-0.751779	0.792224
46	8	0	-0.081525	-0.890998	-0.362113
47	1	0	-1.795919	0.389226	2.125679
48	8	0	-0.816169	-1.815365	1.566546
49	6	0	-0.353523	-3.091076	1.093133
50	1	0	0.731247	-3.096444	0.992532
51	1	0	-0.825898	-3.334683	0.140802
52	1	0	-0.668979	-3.800324	1.851866
53	6	0	-3.728633	4.643175	0.009909
54	6	0	-2.344709	5.760187	-1.608953
55	6	0	-3.403918	6.587983	-1.946088
56	6	0	-4.628948	6.440413	-1.291334
57	6	0	-4.798639	5.470833	-0.311613
58	1	0	-5.736337	5.345580	0.212531

Enthalpy H = -4188.714829 a.u.
Entropy S = 275.405 cal/mol/K
Gibbs free energy G = -4188.845682 a.u.
Total free energy in solution E_{sol}= -4190.36292 a.u.

59	1	0	-5.459234	7.086773	-1.545857
60	1	0	-3.282724	7.346607	-2.707596
61	1	0	-1.375135	5.845790	-2.081998
62	30	0	1.762093	-1.209111	-0.843418
63	6	0	-3.738663	-0.753954	-0.394618
64	7	0	-3.846755	1.402929	0.536198
65	6	0	-3.365932	0.627684	-0.416085
66	6	0	-2.633227	1.129413	-1.622792
67	6	0	-4.840654	-1.236940	0.275373
68	6	0	-4.706991	0.804679	1.579346
69	6	0	-5.664085	-0.257048	1.046637
70	1	0	-1.588877	0.807780	-1.605196
71	1	0	-3.115224	0.670925	-2.489186
72	1	0	-2.681853	2.207421	-1.723904
73	6	0	-4.930322	-2.624159	-0.026147
74	6	0	-3.831891	-2.917991	-0.871090
75	7	0	-3.144990	-1.755317	-1.131079
76	1	0	-2.194989	-1.707444	-1.472369
77	1	0	-4.052368	0.346206	2.329313
78	1	0	-5.245280	1.634628	2.035842
79	1	0	-6.166606	-0.723209	1.895175
80	1	0	-6.434593	0.194182	0.413767
81	6	0	-5.828046	-3.643103	0.358720
82	6	0	-5.579562	-4.923714	-0.090775
83	6	0	-4.459747	-5.206548	-0.917979
84	6	0	-3.583286	-4.225693	-1.314089
85	8	0	-6.344944	-6.007879	0.197013
86	6	0	-7.474747	-5.799742	1.023571
87	1	0	-7.946312	-6.771396	1.138658
88	1	0	-7.177145	-5.418017	2.003803
89	1	0	-8.177353	-5.103775	0.557597
90	1	0	-6.671525	-3.411761	0.992792
91	1	0	-4.325245	-6.232957	-1.231394
92	1	0	-2.740757	-4.455865	-1.953217

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cis-exo-TS2-Si

Imaginary frequency: -190.7999 cm^{-1}

Standard orientation:

Electronic energy E = -4188.761583 a.u.

Enthalpy H = -4188.715073 a.u.

Entropy S = 269.734cal/mol/K

Gibbs free energy G = -4188.843232 a.u.

Total free energy in solution E_{sol}= -4190.35956 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.122300	-3.521945	-0.371307
2	6	0	6.788646	-2.276448	-0.506429
3	6	0	6.021601	-1.079413	-0.460697
4	6	0	4.768232	-3.570816	-0.226226
5	6	0	3.983068	-2.382464	-0.189060
6	6	0	4.601589	-1.136555	-0.266792
7	8	0	2.652845	-2.544967	-0.076667
8	8	0	2.662731	0.007205	-2.153304
9	6	0	3.864467	0.158777	-0.077616
10	6	0	4.099512	0.912810	1.123483
11	6	0	3.560620	2.221320	1.266490
12	6	0	2.789387	2.768779	0.205537
13	6	0	3.056138	0.716383	-1.078467
14	6	0	2.545074	2.043127	-0.922099
15	1	0	6.707577	-4.434449	-0.397309

16	1	0	4.237927	-4.510390	-0.138274
17	6	0	8.191581	-2.210988	-0.687298
18	6	0	6.713113	0.152288	-0.618200
19	6	0	4.856078	0.386033	2.203461
20	6	0	3.793437	2.953706	2.455050
21	1	0	2.363933	3.759926	0.310551
22	1	0	1.933590	2.439343	-1.723171
23	6	0	8.829999	-1.006052	-0.826061
24	6	0	8.073661	0.186389	-0.795255
25	1	0	8.750557	-3.139871	-0.716567
26	1	0	9.902950	-0.965123	-0.965270
27	1	0	8.572067	1.140069	-0.917878
28	1	0	6.146883	1.073529	-0.608949
29	6	0	5.064164	1.118095	3.346427
30	6	0	4.532517	2.419225	3.479554
31	1	0	5.264443	-0.611329	2.114454
32	1	0	5.643078	0.690684	4.155901
33	1	0	4.707566	2.986415	4.385017
34	1	0	3.372984	3.949848	2.536107
35	6	0	-1.289952	3.952902	-0.269265
36	6	0	-2.418538	4.855617	-0.602999
37	6	0	-1.659440	2.773986	0.511560
38	6	0	-3.039718	2.633075	1.059673
39	8	0	-3.872297	3.757257	0.991494
40	8	0	-0.160824	4.154980	-0.695285
41	6	0	-0.845993	1.674881	0.479559
42	6	0	-1.221994	0.417202	1.007882
43	1	0	-2.979668	2.394520	2.124331
44	1	0	0.073256	1.756949	-0.093695
45	6	0	-0.649811	-0.787181	0.551522
46	8	0	-0.076219	-0.908448	-0.577661
47	1	0	-1.830140	0.335772	1.899036
48	8	0	-0.877222	-1.847349	1.313643
49	6	0	-0.377588	-3.122877	0.870205
50	1	0	0.710805	-3.113560	0.827356
51	1	0	-0.794834	-3.371327	-0.105495
52	1	0	-0.729935	-3.831167	1.612796
53	6	0	-3.661099	4.690353	0.009158
54	6	0	-2.252505	5.875742	-1.543279
55	6	0	-3.307238	6.714206	-1.865007
56	6	0	-4.542815	6.536837	-1.236967
57	6	0	-4.726910	5.529581	-0.299477
58	1	0	-5.673126	5.382150	0.203002
59	1	0	-5.370769	7.190512	-1.480270
60	1	0	-3.175870	7.502404	-2.593986
61	1	0	-1.275933	5.981104	-1.997554
62	30	0	1.797439	-1.195979	-1.000477
63	6	0	-3.684900	-0.792096	-0.301418
64	7	0	-3.812145	1.423238	0.530401
65	6	0	-3.251198	0.579082	-0.342745
66	6	0	-2.654914	1.060921	-1.637970
67	6	0	-4.807757	-1.226358	0.362478
68	6	0	-4.650123	0.856497	1.607318
69	6	0	-5.613027	-0.220677	1.119050
70	1	0	-1.676616	0.611556	-1.815999
71	1	0	-3.338231	0.728122	-2.423958
72	1	0	-2.577208	2.140237	-1.689129
73	6	0	-4.955842	-2.611430	0.059429
74	6	0	-3.875826	-2.951884	-0.789608
75	7	0	-3.135328	-1.818391	-1.034788
76	1	0	-2.219526	-1.790840	-1.457161
77	1	0	-3.992238	0.417745	2.368017

78	1	0	-5.184442	1.697921	2.047387
79	1	0	-6.104187	-0.661543	1.988100
80	1	0	-6.392191	0.214813	0.485776
81	6	0	-5.897921	-3.589917	0.438774
82	6	0	-5.714352	-4.878012	-0.024313
83	6	0	-4.615999	-5.206805	-0.859815
84	6	0	-3.694727	-4.263455	-1.249477
85	8	0	-6.532142	-5.926513	0.259162
86	6	0	-7.645832	-5.669757	1.092692
87	1	0	-8.165378	-6.617574	1.201419
88	1	0	-7.326048	-5.312448	2.075254
89	1	0	-8.315267	-4.934962	0.637358
90	1	0	-6.727061	-3.324434	1.078591
91	1	0	-4.532359	-6.234914	-1.185009
92	1	0	-2.867417	-4.527674	-1.895581

S6: Reference 24 details.

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