

Supporting information for

## Role of Keto-Enol Tautomerisation in a Chiral Phosphoric Acid Catalyzed Asymmetric Thiocarboxylysis of meso-epoxide: A DFT Study

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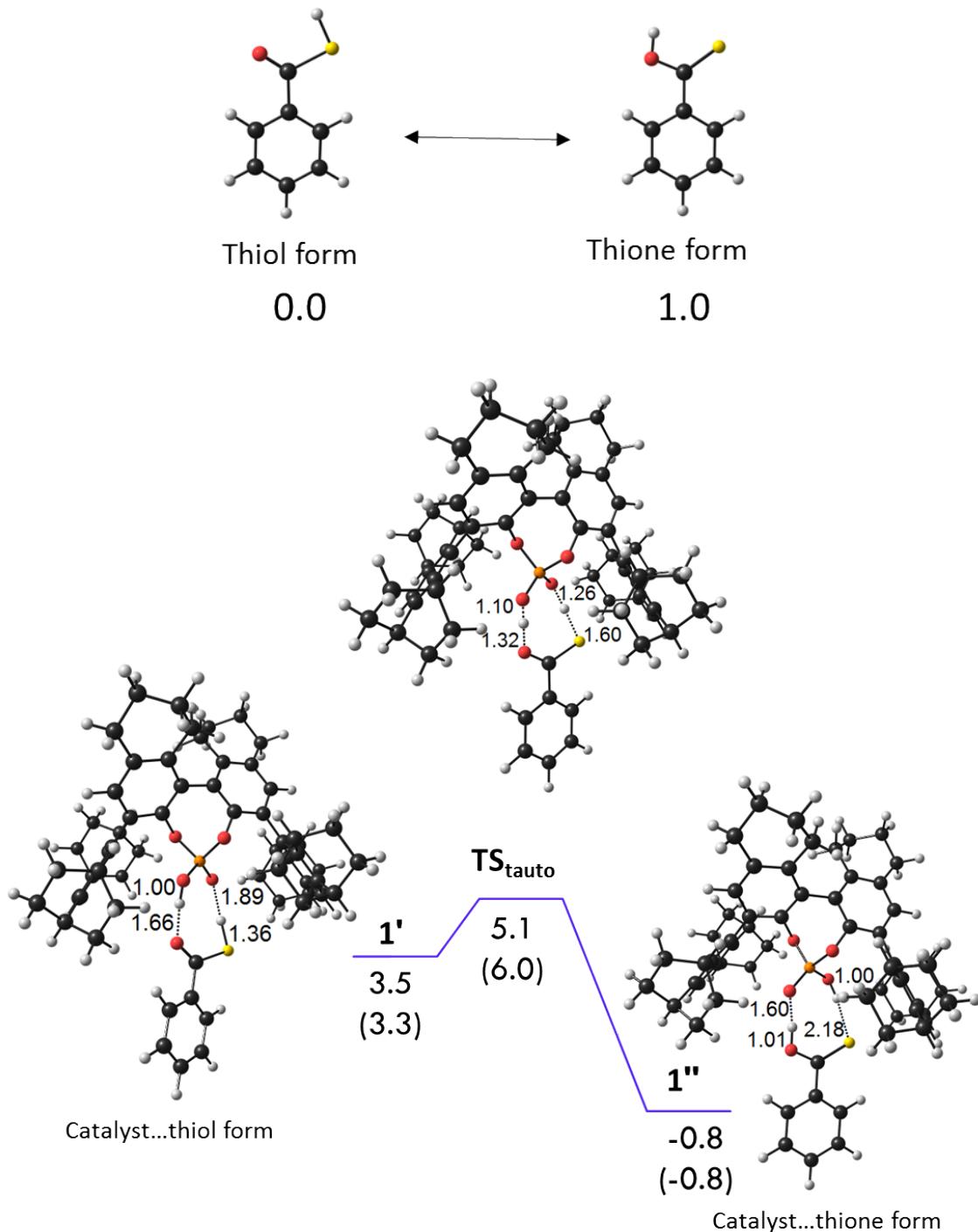
## Computational methods

All the calculations were carried out by using Gaussian 09 suite of computational programs.<sup>1</sup> Geometry optimization of all the key stationary points were carried out in the gas phase using Pople's 6-31G\* basis set at the M06-2X level of theory.<sup>2-4</sup> The stationary points were characterized using frequency calculations. The transition states were verified by single imaginary frequency pertaining to the desired reaction coordinate and by intrinsic reaction coordinate (IRC) calculations.<sup>5, 6</sup> Solvent effects were incorporated through the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM).<sup>7, 8</sup> Since the reaction was performed in toluene, a continuum solvent dielectric of  $\epsilon=2.374$  was employed in our calculations. Energies are further refined by doing a single point calculation using 6-311+G\*\* basis set. All calculations are performed at the standard temperature (298.15 K) and pressure (1 atm). Wave functions generated from the gas-phase-optimized geometries of the transition states were used to obtain corresponding electron density cube files as implemented in Gaussian suite of programs. The energetics of the reaction mechanisms are discussed on the basis of PCM-M06-2X/6-311+G\*\*//M06-2X/6-31G\* level relative Gibbs free energy ( $\Delta G_{\text{rel}}$ ) values with respect to the infinitely separated reactants. Activation free energy,  $\Delta G^\ddagger$  is the difference in Gibbs free energy between a transition state and the corresponding lower energy reactants. Electron densities at the bond critical points ( $\rho_{\text{bcp}}$ ) of the weak C-H···O interactions were calculated by using AIM2000 software.<sup>9</sup> AOMix software was used to calculate the Mayer bond order of weak C-H···O interactions.<sup>10, 11</sup>

## References:

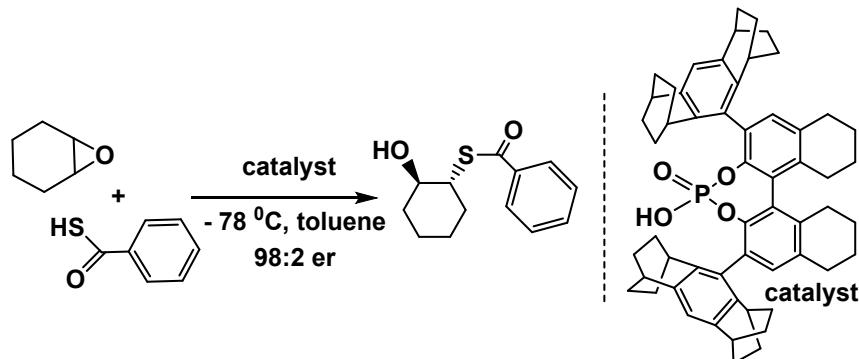
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**Figure S1.** Tautomerisation of thiobenzoic acid (Color code; orange-P, yellow-S, red-O, grey-C, white-H). Bond distances are given in Å and Gibbs energies are given in kcal/mol (BSSE corrected energies are given in parenthesis).

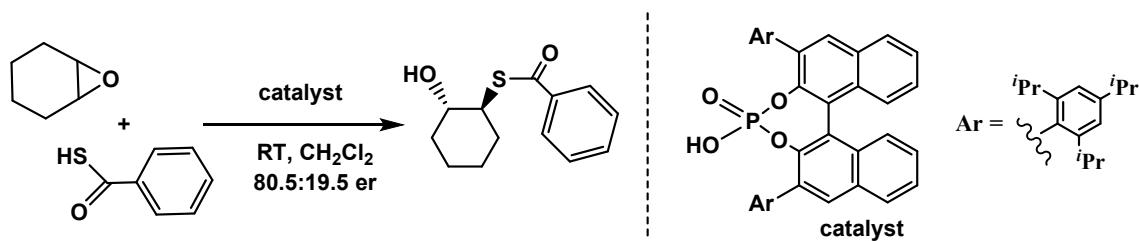


**Scheme S1.** Reactions under consideration.

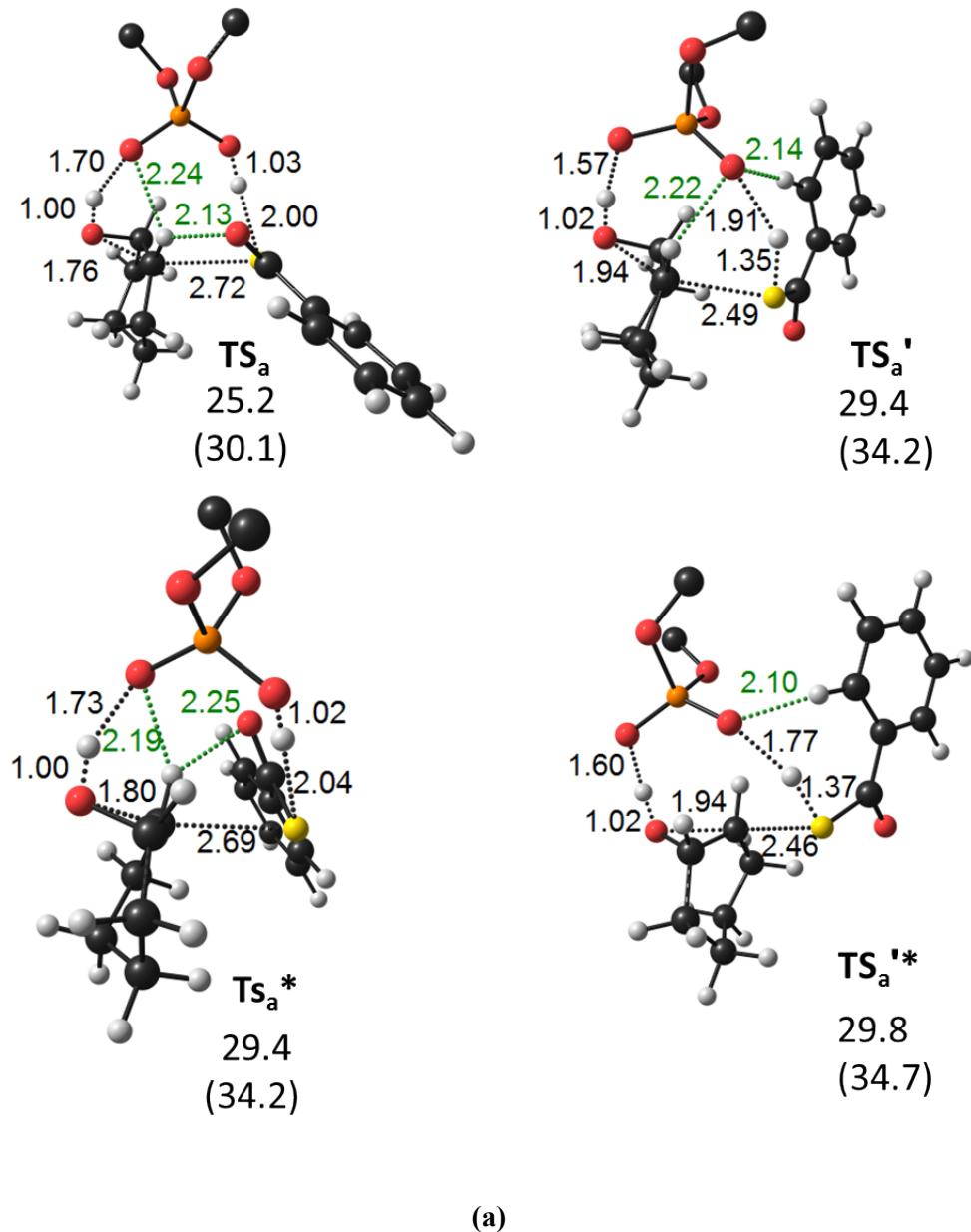
1) Hydrogenated BINOL catalyzed reaction.



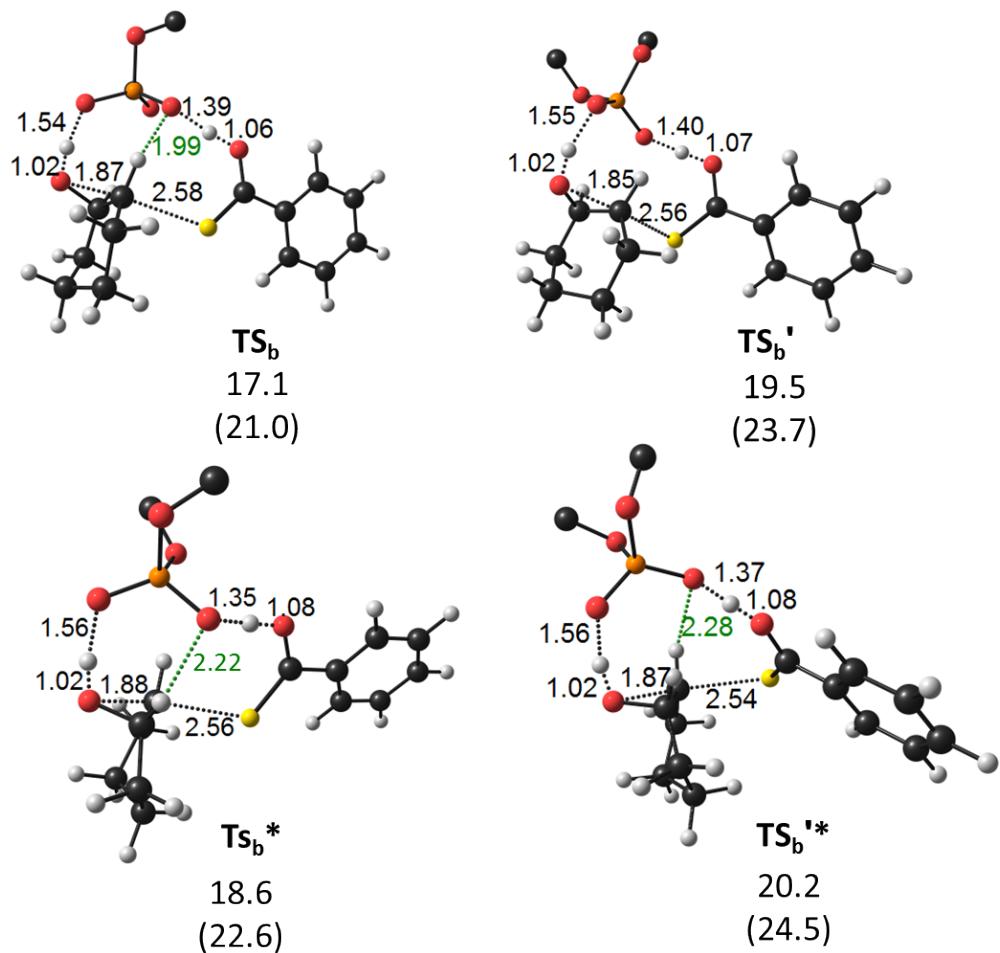
2) TRIP catalyzed reaction.



**Figure S2.** Stable geometries of diastereomeric transition states of hydrogenated BINOL catalyzed reaction.



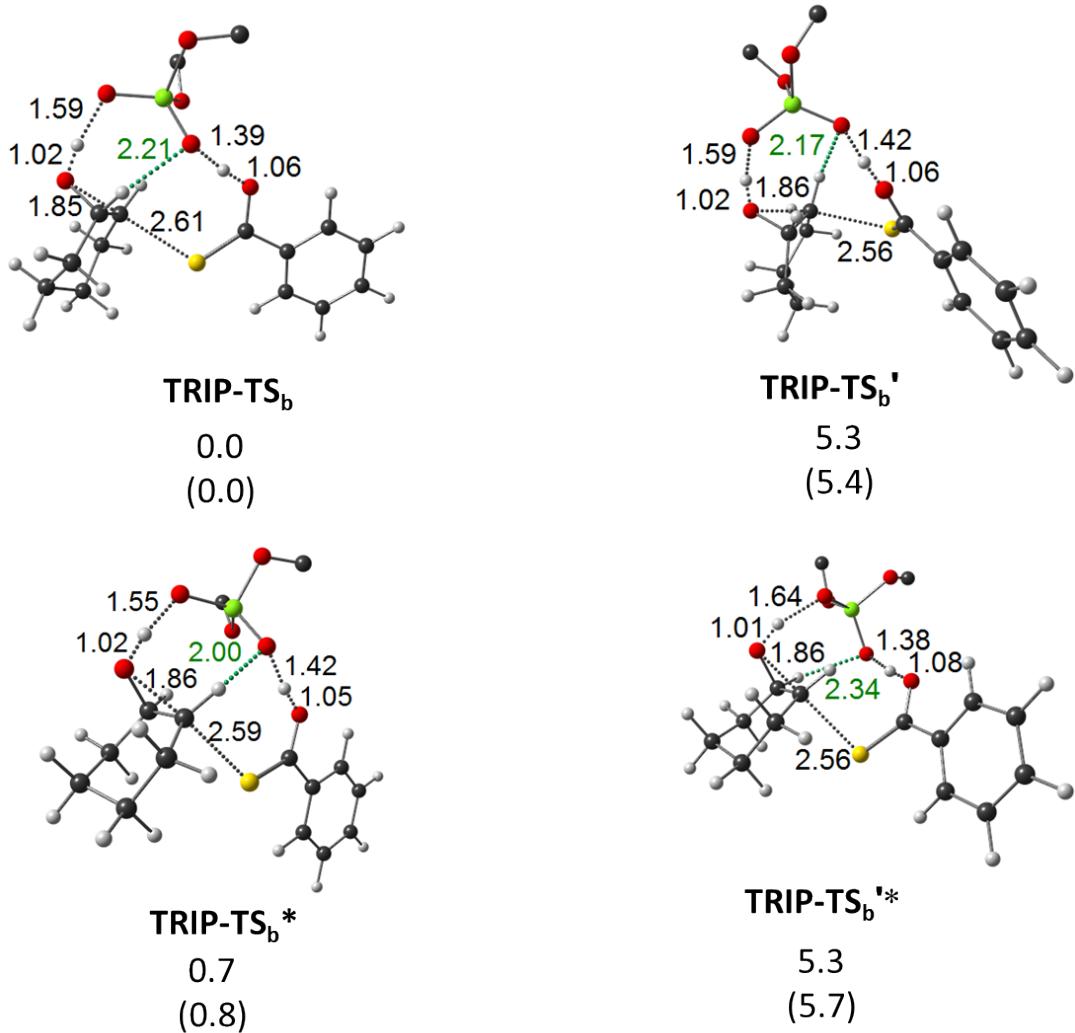
Mode a: Transition state involving thiol form of thiobenzoic acid (Color code; orange-P, yellow-S, red-O, grey-C, white-H). Catalyst back bone is not shown for clarity. Bond distances are given in Å (important C-H...O interactions are also shown in green color). \* denotes the diastereomeric TSs towards less favorable enantiomer.  $\Delta G_{\text{rel}}$  is given in kcal/mol with respect to catalyst.epoxide dimer reported in the main text (BSSE corrected energies are given in parenthesis).



**(b)**

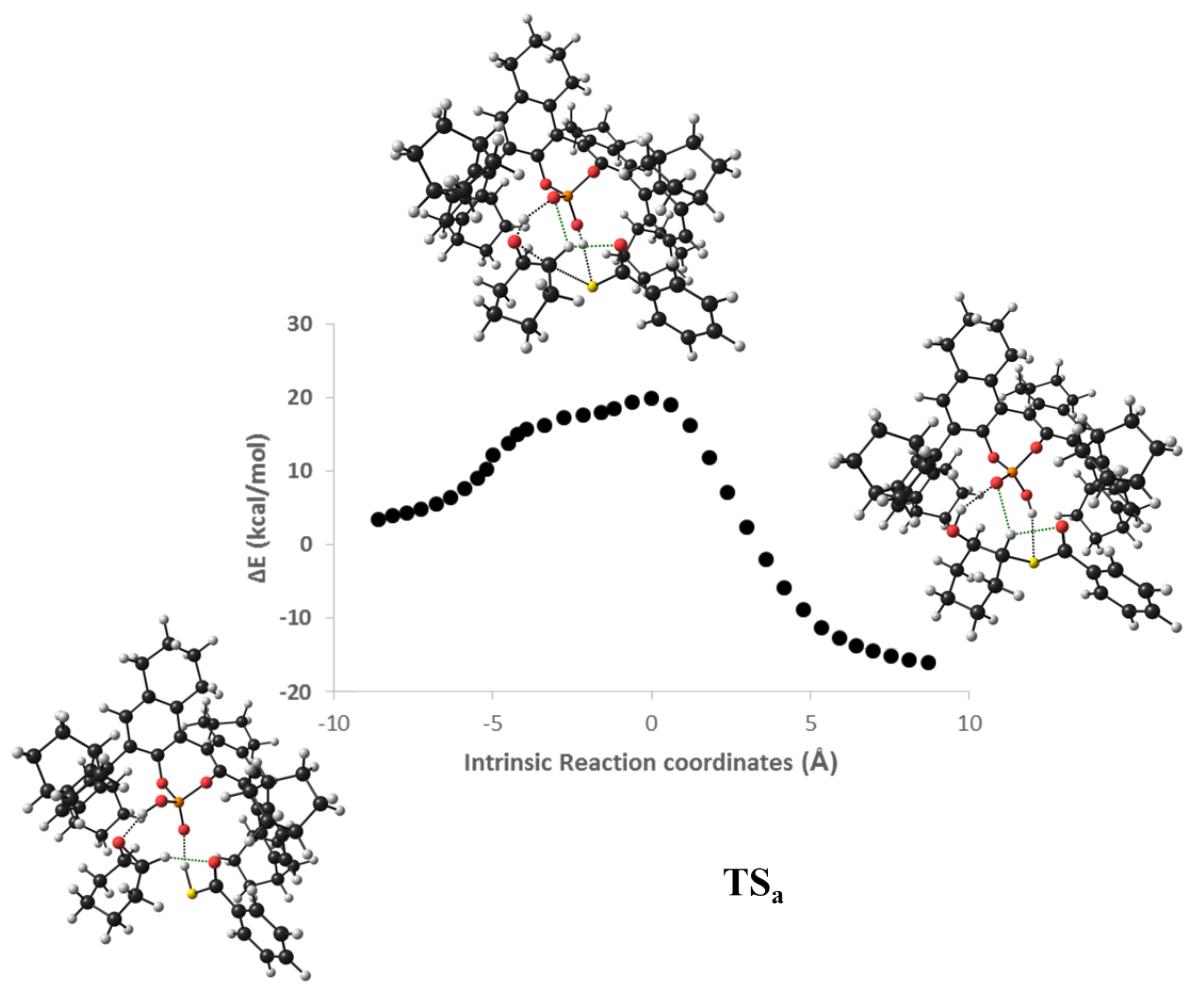
Mode b: Transition state involving thione form of thiobenzoic acid (Color code; orange-P, yellow-S, red-O, grey-C, white-H). Catalyst back bone is not shown for clarity. Bond distances are given in Å (important C-H...O interactions are also shown in green color). \* denotes the diastereomeric TSs towards less favorable enantiomer.  $\Delta G_{\text{rel}}$  is given in kcal/mol with respect to catalyst.epoxide dimer reported in the main text (BSSE corrected energies are given in parenthesis).

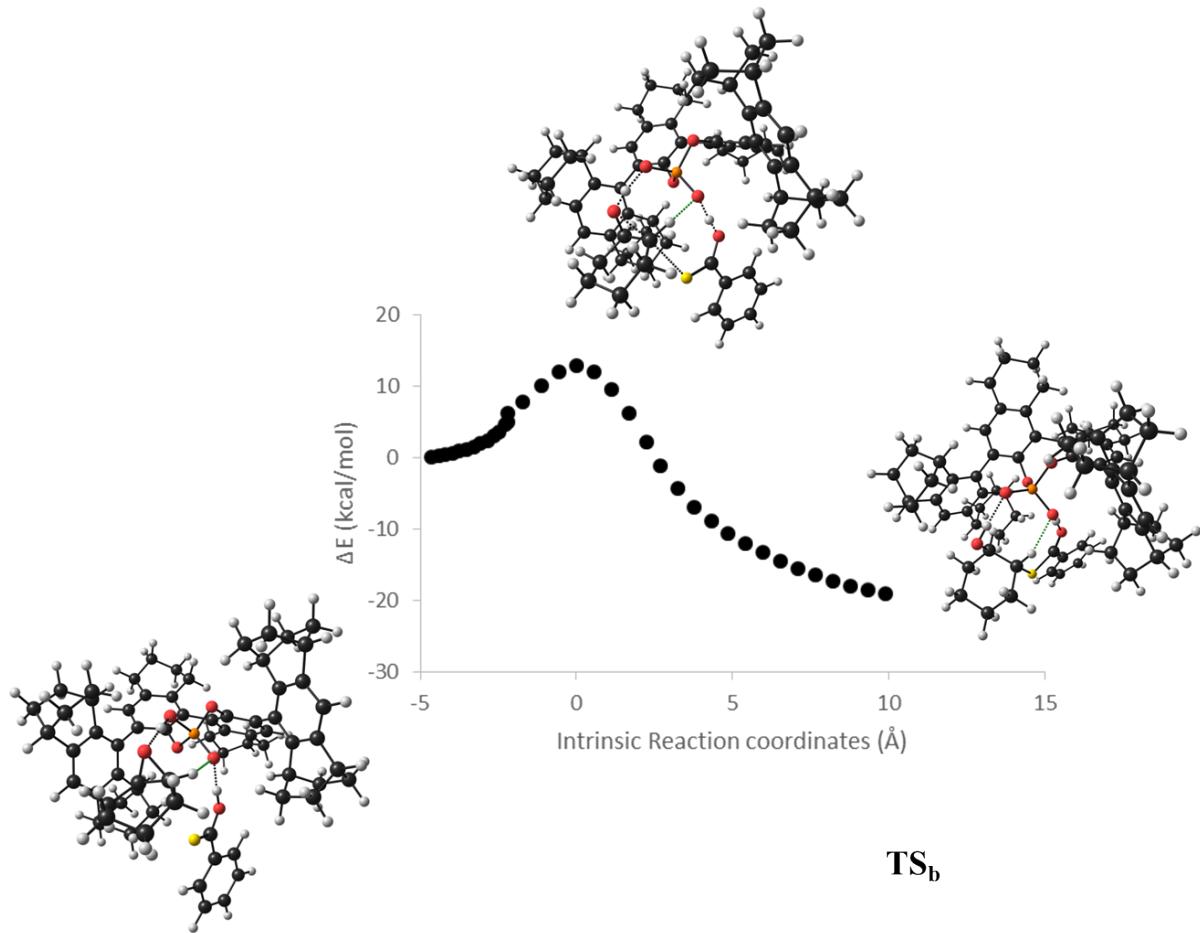
**Figure S3.** Stable geometries of diastereomeric transition states of mode b of TRIP-catalyzed reaction.

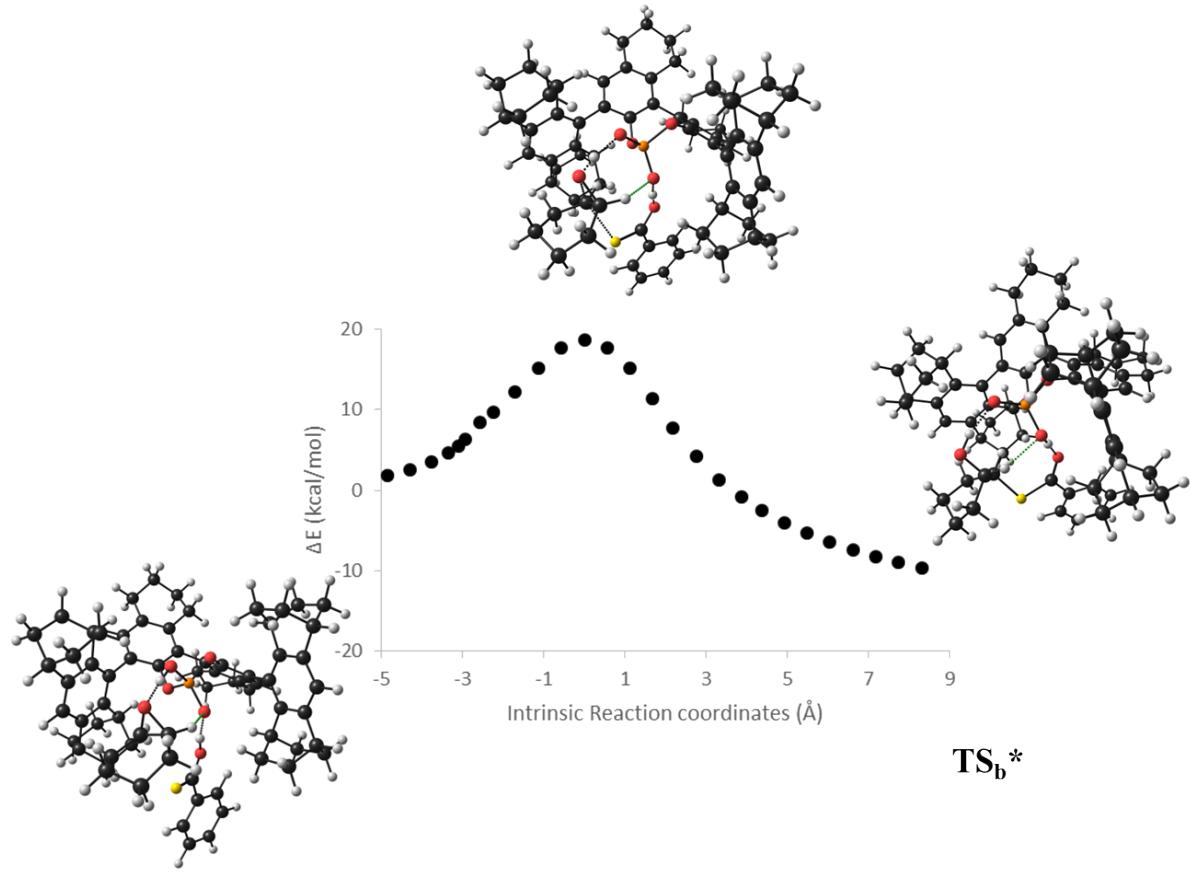


Transition state involving thione form of thiobenzoic acid (Color code; orange-P, yellow-S, red-O, grey-C, white-H). Catalyst back bone is not shown for clarity. Bond distances are given in Å (important C-H...O interactions are also shown in green color).  $\Delta G_{\text{rel}}$  is given in kcal/mol with respect to the most favorable diastereomeric TS (BSSE corrected energies are given in parenthesis). \* denotes the diastereomeric TSs towards less favorable enantiomer. 0.8 kcal/mol energy difference is in agreement with experimental enantiomeric ratio (see Scheme1)

**Figure S4.** Intrinsic Reaction Coordinates (IRC) of Key TSs.







**Table S1.** Computed energy parameters of important TSs and intermediates.

Geometries	Single point energy	G <sub>corr</sub>	Single point energy	ΔG <sub>rel</sub> (kcal/mol)
	(hartree)	(hartree)	(hartree)	PCM-M06-2X/6-
	M06-2X/6-31G*	M06-2X/6-31G*	M06-2X/6-311+G**	311+G**//
<b>1</b>	-3121.84638	1.13551	-3122.61003	0.0
<b>1'</b>	-3555.71674	1.08741	-3556.52079	3.5
<b>TS<sub>tauto</sub></b>	-3555.71038	1.08488	-3556.51576	5.1
<b>1''</b>	-3555.72539	1.09020	-3556.53053	-0.8
<b>2<sub>a</sub></b>	-3865.45503	1.24000	-3866.34680	7.4
<b>TS<sub>a</sub></b>	-3865.42405	1.24314	-3866.32161	25.2
<b>TS<sub>a</sub>'</b>	-3865.41145	1.24166	-3866.31345	29.4
<b>TS<sub>a</sub>*</b>	-3865.41423	1.24016	-3866.31192	29.4
<b>TS<sub>a</sub>'*</b>	-3865.40839	1.23996	-3866.31101	29.8
<b>3<sub>a</sub></b>	-3865.49026	1.24365	-3866.38882	-16.7
<b>2<sub>b</sub></b>	-3865.46082	1.23790	-3866.35686	-0.2
<b>TS<sub>b</sub></b>	-3865.43529	1.24295	-3866.33422	17.1
<b>TS<sub>b</sub>'</b>	-3865.43267	1.24354	-3866.33098	19.5
<b>TS<sub>b</sub>*</b>	-3865.42650	1.23815	-3866.32705	18.6
<b>TS<sub>b</sub>'*</b>	-3865.42922	1.24076	-3866.32710	20.2
<b>3<sub>b</sub></b>	-3865.49411	1.24412	-3866.39329	-19.2
Thiol form	-743.58686	0.07729	-743.72135	0.0
Thione form	-743.58540	0.08148	-743.72393	1.0
epoxide	-309.70993	0.12447	-309.80405	
<b>TRIP-TS<sub>b</sub></b>	-3634.41872	1.12911	-3635.30052	0.0
<b>TRIP-TS<sub>b</sub>'</b>	-3634.41360	1.13107	-3635.29400	5.3
<b>TRIP-TS<sub>b</sub>*</b>	-3634.41759	1.12767	-3635.29788	0.7
<b>TRIP-TS<sub>b</sub>'*</b>	-3634.41594	1.13245	-3635.29534	5.3

**Table S2.** Cartesian coordinates (Å) of optimized geometries of the stationary points and transition states.

Chiral phosphoric acid catalyst

Number of imaginary frequencies : 0

Electronic energy= -2812.10346949 (hartree/particle)

Zero-point correction= 1.069729

Thermal correction to Energy= 1.118682

Thermal correction to Enthalpy= 1.119626

Thermal correction to Gibbs Free Energy= 0.986835

Sum of electronic and zero-point Energies= -2811.033741

Sum of electronic and thermal Energies= -2810.984788

Sum of electronic and thermal Enthalpies= -2810.983844

Sum of electronic and thermal Free Energies= -2811.116634

Coordinates

6	2.836069000	0.787705000	-0.275831000
6	1.483535000	0.946628000	0.014705000
6	0.723630000	2.029992000	-0.435775000
6	1.319056000	2.953450000	-1.318964000
6	2.676518000	2.807775000	-1.643217000
6	3.411142000	1.756095000	-1.094622000
6	0.485124000	4.026632000	-1.992264000
6	1.099327000	4.489383000	-3.311695000
6	2.541072000	4.923938000	-3.065274000
6	3.376623000	3.720241000	-2.634732000
6	-0.712115000	2.099874000	-0.026875000
6	-1.522834000	1.005161000	-0.324336000
6	-2.864895000	0.917129000	0.040882000
6	-3.397436000	2.017212000	0.706431000
6	-2.619845000	3.119101000	1.068677000
6	-1.258770000	3.158671000	0.726209000
6	-3.278164000	4.203344000	1.903386000
6	-2.386929000	5.418779000	2.150283000
6	-0.968728000	4.958776000	2.475055000
6	-0.372149000	4.272904000	1.247684000
8	0.848338000	-0.042321000	0.773808000
8	-0.952095000	-0.077315000	-0.986011000
15	-0.037116000	-1.067051000	-0.097500000
8	0.643684000	-2.052795000	-0.939145000
8	-0.987224000	-1.592266000	1.074056000
6	5.055422000	-2.290986000	-0.137803000
6	4.243234000	-1.260763000	-0.634271000
6	3.625266000	-0.361585000	0.245890000
6	3.798629000	-0.542700000	1.625870000
6	4.605473000	-1.580974000	2.109371000
6	5.242227000	-2.450139000	1.230086000
6	4.699977000	-1.623354000	3.612765000

6	5.270024000	-0.272298000	4.096722000
6	3.214462000	0.302395000	2.732331000
6	4.381524000	0.881859000	3.563112000
6	2.382675000	-0.616998000	3.653222000
6	5.653188000	-3.159522000	-1.212980000
6	4.497192000	-3.798521000	-2.011587000
6	3.555996000	-2.683208000	-2.535886000
6	4.114143000	-1.296719000	-2.139133000
6	6.455155000	-2.254130000	-2.173022000
6	-4.934749000	-2.213958000	0.659418000
6	-4.201876000	-1.036808000	0.885517000
6	-3.639942000	-0.333288000	-0.198121000
6	-3.809123000	-0.849900000	-1.493688000
6	-4.541020000	-2.028183000	-1.701372000
6	-5.103118000	-2.710677000	-0.628331000
6	-4.654473000	-2.425416000	-3.149539000
6	-5.339258000	-1.268770000	-3.910035000
6	-3.315348000	-0.240376000	-2.784126000
6	-4.550373000	0.044752000	-3.669218000
6	-3.229764000	-2.593239000	-3.717622000
6	-5.501836000	-2.828470000	1.912683000
6	-4.330329000	-3.141528000	2.864769000
6	-3.559939000	-1.832161000	3.171372000
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6	-5.613130000	-0.468253000	2.821417000
1	4.467043000	1.659511000	-1.342844000
1	-0.534691000	3.655343000	-2.138804000
1	0.404473000	4.905723000	-1.341434000
1	0.506147000	5.310915000	-3.726105000
1	1.079476000	3.670948000	-4.043087000
1	2.979519000	5.378099000	-3.959537000
1	2.552130000	5.689467000	-2.278232000
1	4.333646000	4.046573000	-2.211200000
1	3.626302000	3.123034000	-3.522278000
1	-4.447356000	1.993369000	0.995349000
1	-4.217913000	4.504584000	1.425810000
1	-3.556937000	3.763329000	2.870797000
1	-2.359062000	6.051433000	1.253484000
1	-2.805248000	6.027047000	2.958445000
1	-0.991936000	4.260698000	3.321973000
1	-0.338090000	5.804279000	2.767448000
1	-0.233821000	5.038431000	0.474927000
1	0.623391000	3.869751000	1.462955000
1	-1.816754000	-1.974946000	0.731103000
1	5.875091000	-3.251198000	1.609229000
1	5.336541000	-2.451049000	3.943622000
1	5.300503000	-0.267200000	5.192351000

1	6.300081000	-0.163529000	3.744076000
1	2.590826000	1.112622000	2.344956000
1	4.967094000	1.566453000	2.941781000
1	3.968878000	1.469150000	4.391477000
1	1.524527000	-1.003552000	3.096923000
1	1.989790000	-0.020042000	4.484402000
1	6.301112000	-3.930219000	-0.781396000
1	4.917291000	-4.381913000	-2.839436000
1	3.949248000	-4.494267000	-1.369323000
1	2.550103000	-2.790347000	-2.124672000
1	3.475587000	-2.727112000	-3.628373000
1	3.448557000	-0.511664000	-2.507289000
1	7.293478000	-1.803582000	-1.632751000
1	6.879468000	-2.868597000	-2.975146000
1	-5.674220000	-3.622583000	-0.795163000
1	-5.227550000	-3.352389000	-3.258097000
1	-5.370985000	-1.515733000	-4.977112000
1	-6.374663000	-1.167844000	-3.570961000
1	-2.755888000	0.682226000	-2.611816000
1	-4.212064000	0.474762000	-4.618425000
1	-5.183266000	0.793441000	-3.182803000
1	-2.730146000	-3.425626000	-3.213099000
1	-3.297544000	-2.854216000	-4.779674000
1	-6.067367000	-3.737211000	1.681739000
1	-4.719482000	-3.590985000	3.784927000
1	-3.671967000	-3.882276000	2.399379000
1	-2.493387000	-1.937477000	2.956775000
1	-3.640683000	-1.577505000	4.234217000
1	-3.568102000	0.242858000	2.523493000
1	-6.070863000	0.361000000	2.271739000
1	-5.613252000	-0.192097000	3.881629000
6	-2.434416000	-1.276747000	-3.517643000
1	-1.518547000	-1.455181000	-2.948651000
1	-2.136480000	-0.854883000	-4.484191000
6	-6.410132000	-1.780556000	2.593582000
1	-6.770698000	-2.186699000	3.545269000
1	-7.288714000	-1.595930000	1.968464000
6	5.523231000	-1.157298000	-2.753500000
1	5.926486000	-0.159985000	-2.546738000
1	5.443582000	-1.252144000	-3.842489000
6	3.272775000	-1.772470000	4.180438000
1	2.863334000	-2.742038000	3.881921000
1	3.319631000	-1.763009000	5.275547000

Catalyst...epoxide hetero dimer (**1**)

Number of imaginary frequencies : 0

Electronic energy= -3121.84638242 (hartree/particle)

Zero-point correction= 1.226271  
 Thermal correction to Energy= 1.282127  
 Thermal correction to Enthalpy= 1.283071  
 Thermal correction to Gibbs Free Energy= 1.135507  
 Sum of electronic and zero-point Energies= -3120.620111  
 Sum of electronic and thermal Energies= -3120.564256  
 Sum of electronic and thermal Enthalpies= -3120.563311  
 Sum of electronic and thermal Free Energies= -3120.710875

Coordinates

6	-3.326309000	0.722348000	0.277710000
6	-2.032296000	1.134032000	-0.035265000
6	-1.476253000	2.327290000	0.427289000
6	-2.209084000	3.108989000	1.343374000
6	-3.514779000	2.718722000	1.676391000
6	-4.055431000	1.559061000	1.118002000
6	-1.558986000	4.289520000	2.041017000
6	-2.252193000	4.637797000	3.357026000
6	-3.747165000	4.815220000	3.106687000
6	-4.356246000	3.480773000	2.683818000
6	-0.089407000	2.668022000	-0.007790000
6	0.924785000	1.744700000	0.252590000
6	2.257903000	1.962869000	-0.088144000
6	2.547110000	3.165215000	-0.728064000
6	1.557557000	4.082390000	-1.083677000
6	0.220228000	3.830856000	-0.741799000
6	1.972177000	5.296093000	-1.895659000
6	0.850468000	6.313306000	-2.090437000
6	-0.443631000	5.584188000	-2.439962000
6	-0.885651000	4.739081000	-1.246491000
8	-1.246348000	0.304769000	-0.834205000
8	0.588659000	0.543114000	0.864998000
15	-0.145685000	-0.572264000	-0.049436000
8	-0.610281000	-1.683908000	0.795312000
8	0.816181000	-0.912280000	-1.245724000
6	-4.857752000	-2.751272000	0.185833000
6	-4.289152000	-1.561359000	0.664063000
6	-3.884881000	-0.560288000	-0.230433000
6	-4.034631000	-0.787165000	-1.606258000
6	-4.603891000	-1.980127000	-2.071530000
6	-5.019910000	-2.961513000	-1.178353000
6	-4.712713000	-2.052189000	-3.572475000
6	-5.570756000	-0.860055000	-4.048645000
6	-3.665214000	0.156159000	-2.725560000
6	-4.945073000	0.462949000	-3.534847000
6	-3.298250000	-1.890835000	-4.168467000
6	-5.227976000	-3.724363000	1.274523000

6	-3.944845000	-4.070264000	2.059394000
6	-3.293571000	-2.764385000	2.582847000
6	-4.152642000	-1.548178000	2.168760000
6	-5.557647000	-1.722336000	2.784178000
6	5.148642000	-0.437088000	-0.636941000
6	4.077348000	0.433375000	-0.886926000
6	3.320156000	0.953053000	0.175755000
6	3.620994000	0.533556000	1.480641000
6	4.691775000	-0.342156000	1.717914000
6	5.470364000	-0.808854000	0.664729000
6	4.879053000	-0.692571000	3.171404000
6	5.114625000	0.614208000	3.957024000
6	2.908679000	0.932661000	2.750532000
6	3.934857000	1.587341000	3.701214000
6	3.566444000	-1.326802000	3.683003000
6	5.874162000	-0.878610000	-1.882198000
6	4.867984000	-1.583540000	-2.816747000
6	3.674625000	-0.635997000	-3.091870000
6	3.885155000	0.707647000	-2.360892000
6	6.384974000	0.387637000	-2.606133000
1	-5.072334000	1.269490000	1.379024000
1	-0.497331000	4.072257000	2.201086000
1	-1.595837000	5.179800000	1.401976000
1	-1.811815000	5.548931000	3.774627000
1	-2.095064000	3.834793000	4.088926000
1	-4.259126000	5.192072000	3.997850000
1	-3.889896000	5.561239000	2.313798000
1	-5.362865000	3.626662000	2.275034000
1	-4.478235000	2.847597000	3.573496000
1	3.581835000	3.372241000	-0.997858000
1	2.842664000	5.765460000	-1.422518000
1	2.312389000	4.947794000	-2.880648000
1	0.699092000	6.886199000	-1.165966000
1	1.129014000	7.029389000	-2.870132000
1	-0.278142000	4.941865000	-3.314870000
1	-1.236722000	6.291647000	-2.702373000
1	-1.208359000	5.424823000	-0.454404000
1	-1.761073000	4.131174000	-1.499170000
1	1.285044000	-1.797864000	-1.154070000
1	-5.461996000	-3.887042000	-1.544447000
1	-5.160486000	-3.000057000	-3.890270000
1	-5.621257000	-0.868982000	-5.143452000
1	-6.593368000	-0.975350000	-3.676800000
1	-3.226240000	1.084096000	-2.349737000
1	-5.653878000	1.007625000	-2.903444000
1	-4.686241000	1.121275000	-4.372080000
1	-2.681741000	-2.747441000	-3.880231000

1	-3.368766000	-1.896319000	-5.262375000
1	-5.682691000	-4.628707000	0.855641000
1	-4.202122000	-4.742268000	2.886786000
1	-3.253945000	-4.610745000	1.405103000
1	-2.286666000	-2.636755000	2.179621000
1	-3.217333000	-2.781502000	3.676436000
1	-3.686897000	-0.626695000	2.526708000
1	-6.179114000	-0.852383000	2.546008000
1	-5.464145000	-1.761647000	3.875510000
1	6.312043000	-1.473722000	0.856181000
1	5.720268000	-1.381836000	3.304464000
1	5.204746000	0.379897000	5.023724000
1	6.062395000	1.061845000	3.642996000
1	2.083737000	1.622196000	2.559193000
1	3.431420000	1.843433000	4.640219000
1	4.293260000	2.523764000	3.262859000
1	3.400915000	-2.286983000	3.181415000
1	3.667231000	-1.540810000	4.753221000
1	6.709480000	-1.543872000	-1.635207000
1	5.379098000	-1.854726000	-3.747616000
1	4.513887000	-2.514819000	-2.362927000
1	2.735816000	-1.084320000	-2.760141000
1	3.574729000	-0.436964000	-4.164812000
1	3.031809000	1.364385000	-2.544616000
1	7.130301000	0.887783000	-1.980402000
1	6.886942000	0.092113000	-3.534329000
6	2.968719000	-6.025213000	0.371112000
6	4.069507000	-5.246578000	-0.347594000
6	4.201340000	-3.839675000	0.238726000
6	2.878184000	-3.116117000	0.285104000
6	1.613203000	-3.875228000	0.259217000
6	1.595697000	-5.385575000	0.143603000
8	2.098251000	-3.184452000	-0.920901000
1	2.949360000	-7.068353000	0.039948000
1	3.191249000	-6.037166000	1.446497000
1	5.028751000	-5.766613000	-0.261036000
1	3.834228000	-5.173738000	-1.416529000
1	4.920743000	-3.242472000	-0.329771000
1	4.582526000	-3.892171000	1.268513000
1	2.879295000	-2.120952000	0.737141000
1	0.729827000	-3.399594000	0.679705000
1	0.867252000	-5.782358000	0.857604000
1	1.223706000	-5.632816000	-0.857945000
6	-6.207188000	-3.022598000	2.240564000
1	-6.454127000	-3.706560000	3.060611000
1	-7.140303000	-2.799327000	1.714278000
6	-2.669936000	-0.566862000	-3.659607000

1	-1.738848000	-0.754638000	-3.118615000
1	-2.429690000	0.095664000	-4.499146000
6	2.383829000	-0.357713000	3.418995000
1	1.629817000	-0.817956000	2.772712000
1	1.883956000	-0.092973000	4.357398000
6	5.190435000	1.333919000	-2.902118000
1	5.083779000	1.499128000	-3.980170000
1	5.352489000	2.314075000	-2.441440000

Catalyst...thiol form (of thiobenzoic acid) hetero dimer (**1'**)

Number of imaginary frequencies : 0

Electronic energy= -3555.71673781 (hartree/particle)

Zero-point correction= 1.183224

Thermal correction to Energy= 1.241041

Thermal correction to Enthalpy= 1.241985

Thermal correction to Gibbs Free Energy= 1.087411

Sum of electronic and zero-point Energies= -3554.533514

Sum of electronic and thermal Energies= -3554.475697

Sum of electronic and thermal Enthalpies= -3554.474753

Sum of electronic and thermal Free Energies= -3554.629327

Coordinates

6	3.428846000	-0.407194000	-0.082998000
6	2.224444000	-1.028137000	-0.403813000
6	1.998434000	-2.399141000	-0.266008000
6	3.012894000	-3.192592000	0.308145000
6	4.242955000	-2.597364000	0.630239000
6	4.436264000	-1.233344000	0.406700000
6	2.750598000	-4.641266000	0.671195000
6	3.669781000	-5.129455000	1.789256000
6	5.119608000	-4.872504000	1.388923000
6	5.369171000	-3.368611000	1.295796000
6	0.651242000	-2.925789000	-0.645272000
6	-0.468713000	-2.351309000	-0.041169000
6	-1.778252000	-2.745353000	-0.309653000
6	-1.936173000	-3.762968000	-1.245747000
6	-0.856948000	-4.323810000	-1.931275000
6	0.450250000	-3.900913000	-1.644714000
6	-1.162335000	-5.333741000	-3.023540000
6	0.078656000	-5.996561000	-3.617003000
6	1.167379000	-4.948505000	-3.829653000
6	1.614627000	-4.412607000	-2.470866000
8	1.180697000	-0.227829000	-0.865362000
8	-0.276288000	-1.304628000	0.859660000
15	0.048664000	0.134430000	0.217524000
8	0.378633000	1.109444000	1.276196000
8	-1.122344000	0.525089000	-0.754950000

6	4.107363000	3.217666000	0.821534000
6	3.906872000	1.833897000	0.933733000
6	3.600289000	1.067398000	-0.200906000
6	3.463152000	1.719893000	-1.435468000
6	3.665201000	3.103136000	-1.533695000
6	3.992659000	3.853185000	-0.409196000
6	3.492335000	3.643433000	-2.929326000
6	4.490630000	2.919072000	-3.857605000
6	3.124654000	1.087641000	-2.764762000
6	4.281411000	1.386411000	-3.744446000
6	2.063948000	3.297515000	-3.400989000
6	4.424910000	3.892196000	2.130758000
6	3.243795000	3.645417000	3.092965000
6	2.990199000	2.120885000	3.215780000
6	4.019148000	1.347427000	2.360393000
6	5.679568000	3.220881000	2.729160000
6	-5.037861000	-0.858966000	0.224538000
6	-3.924568000	-1.434383000	-0.406995000
6	-2.938823000	-2.085321000	0.352242000
6	-3.078138000	-2.114849000	1.748739000
6	-4.191295000	-1.527399000	2.366279000
6	-5.173839000	-0.903134000	1.606740000
6	-4.200029000	-1.670783000	3.866293000
6	-4.175846000	-3.177617000	4.201586000
6	-2.146664000	-2.770180000	2.740939000
6	-2.951892000	-3.837562000	3.516208000
6	-1.676358000	-1.699434000	3.749929000
6	-6.005117000	-0.204825000	-0.726367000
6	-5.231634000	0.889283000	-1.490466000
6	-4.061359000	0.234568000	-2.264344000
6	-3.963583000	-1.267535000	-1.910254000
6	-5.261290000	-1.938369000	-2.414773000
1	5.393996000	-0.784107000	0.666033000
1	1.696260000	-4.761991000	0.942392000
1	2.922423000	-5.286207000	-0.198816000
1	3.494482000	-6.194533000	1.971420000
1	3.443545000	-4.596881000	2.722199000
1	5.817501000	-5.320116000	2.103552000
1	5.308269000	-5.345734000	0.416349000
1	6.307347000	-3.164746000	0.766537000
1	5.499622000	-2.965299000	2.309298000
1	-2.944818000	-4.103049000	-1.476461000
1	-1.854457000	-6.088591000	-2.632584000
1	-1.703934000	-4.811739000	-3.824218000
1	0.456542000	-6.766615000	-2.931777000
1	-0.181025000	-6.500165000	-4.553579000
1	0.776542000	-4.129722000	-4.447775000

1	2.026319000	-5.374490000	-4.358073000
1	2.119307000	-5.232692000	-1.946014000
1	2.357516000	-3.615860000	-2.584629000
1	-1.659238000	1.293505000	-0.420442000
1	4.149753000	4.927667000	-0.491284000
1	3.656949000	4.726003000	-2.955420000
1	4.332391000	3.259822000	-4.887321000
1	5.513362000	3.192406000	-3.580937000
1	2.972669000	0.008490000	-2.677901000
1	5.193904000	0.896001000	-3.391471000
1	4.039515000	0.953768000	-4.722005000
1	1.337834000	3.825906000	-2.775487000
1	1.928665000	3.655310000	-4.428209000
1	4.593207000	4.965308000	1.989349000
1	3.478427000	4.086036000	4.069080000
1	2.352774000	4.157815000	2.715531000
1	1.983488000	1.860069000	2.880906000
1	3.088404000	1.795596000	4.257996000
1	3.833714000	0.273778000	2.441919000
1	6.538775000	3.410800000	2.078687000
1	5.901489000	3.677565000	3.700421000
1	-6.039658000	-0.452083000	2.089049000
1	-5.084486000	-1.193226000	4.301618000
1	-4.127935000	-3.301123000	5.289590000
1	-5.107286000	-3.642078000	3.863853000
1	-1.285881000	-3.232548000	2.251377000
1	-2.295196000	-4.304444000	4.259049000
1	-3.271453000	-4.625562000	2.827218000
1	-1.064276000	-0.956046000	3.232765000
1	-1.038214000	-2.181071000	4.499834000
1	-6.854903000	0.226728000	-0.186592000
1	-5.913052000	1.410787000	-2.173670000
1	-4.850526000	1.624175000	-0.774073000
1	-3.116747000	0.733198000	-2.040830000
1	-4.218045000	0.317628000	-3.346423000
1	-3.086156000	-1.706218000	-2.391454000
1	-5.238291000	-3.008712000	-2.183824000
1	-5.314883000	-1.843907000	-3.505269000
6	-4.083230000	4.806011000	-1.001222000
6	-4.941980000	5.856810000	-1.295706000
6	-4.756500000	7.098039000	-0.688986000
6	-3.710419000	7.288574000	0.210935000
6	-2.843258000	6.241799000	0.503450000
6	-3.027591000	4.997042000	-0.104150000
6	-2.138019000	3.831385000	0.161614000
8	-2.495301000	2.700995000	-0.137372000
16	-0.560520000	4.193310000	0.876295000

1	-4.209268000	3.832224000	-1.463404000
1	-5.755283000	5.709546000	-1.998969000
1	-5.429660000	7.918863000	-0.917005000
1	-3.571555000	8.252922000	0.688681000
1	-2.039306000	6.390088000	1.217992000
1	-0.187539000	2.898109000	1.042713000
6	-2.907217000	-1.036872000	4.421694000
1	-2.881483000	-1.172520000	5.509071000
1	-2.917817000	0.040254000	4.230484000
6	-6.486929000	-1.262029000	-1.743680000
1	-7.108199000	-2.004706000	-1.234200000
1	-7.119443000	-0.772658000	-2.493513000
6	5.430475000	1.696653000	2.880785000
1	6.184023000	1.126613000	2.326732000
1	5.505970000	1.393176000	3.931238000
6	1.848748000	1.763902000	-3.314126000
1	1.631170000	1.346538000	-4.304110000
1	1.001159000	1.520560000	-2.668431000

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#### Tautomerisation transition state (**TS<sub>tauto</sub>**)

Number of imaginary frequencies : 1

Electronic energy= -3555.71037761 (hartree/particle)

Zero-point correction= 1.178655

Thermal correction to Energy= 1.235370

Thermal correction to Enthalpy= 1.236314

Thermal correction to Gibbs Free Energy= 1.084883

Sum of electronic and zero-point Energies= -3554.531723

Sum of electronic and thermal Energies= -3554.475007

Sum of electronic and thermal Enthalpies= -3554.474063

Sum of electronic and thermal Free Energies= -3554.625495

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#### Coordinates

6	2.020062000	-2.541124000	-0.146152000
6	0.726159000	-2.165706000	-0.495717000
6	-0.386621000	-3.001946000	-0.385388000
6	-0.205987000	-4.291279000	0.155857000
6	1.091897000	-4.712781000	0.487823000
6	2.172110000	-3.847453000	0.313023000
6	-1.396956000	-5.174848000	0.472726000
6	-1.084959000	-6.197738000	1.563698000
6	0.155376000	-6.990429000	1.162419000
6	1.368431000	-6.064120000	1.123345000
6	-1.725376000	-2.432740000	-0.735936000
6	-2.131317000	-1.264632000	-0.086226000
6	-3.350844000	-0.632940000	-0.315894000
6	-4.182651000	-1.229369000	-1.258944000

6	-3.800150000	-2.354854000	-1.990067000
6	-2.558341000	-2.961159000	-1.743514000
6	-4.733337000	-2.831955000	-3.088120000
6	-4.299424000	-4.140816000	-3.744838000
6	-2.790346000	-4.127169000	-3.972752000
6	-2.081050000	-4.102716000	-2.620031000
8	0.519132000	-0.853625000	-0.931572000
8	-1.254118000	-0.664750000	0.827566000
15	-0.038613000	0.147378000	0.185876000
8	0.938572000	0.446916000	1.303287000
8	-0.502300000	1.372199000	-0.610629000
6	5.008313000	-0.481949000	0.970258000
6	3.877156000	-1.311997000	1.001557000
6	3.162891000	-1.584228000	-0.177705000
6	3.569051000	-0.960020000	-1.366493000
6	4.694620000	-0.122908000	-1.380602000
6	5.422560000	0.106174000	-0.219312000
6	5.007228000	0.451872000	-2.737019000
6	5.229632000	-0.723121000	-3.714012000
6	2.924223000	-1.083425000	-2.725906000
6	3.974970000	-1.634013000	-3.715907000
6	3.777551000	1.249362000	-3.219110000
6	5.677817000	-0.316185000	2.309534000
6	4.655242000	0.304591000	3.283161000
6	3.387090000	-0.584529000	3.324935000
6	3.566245000	-1.808152000	2.395511000
6	6.055190000	-1.718184000	2.836584000
6	-4.375444000	2.976264000	0.278360000
6	-3.983297000	1.795560000	-0.369816000
6	-3.720387000	0.634505000	0.374133000
6	-3.828020000	0.691651000	1.771823000
6	-4.221905000	1.878066000	2.405634000
6	-4.498854000	3.019581000	1.661839000
6	-4.318425000	1.761533000	3.904541000
6	-5.336985000	0.648984000	4.233445000
6	-3.596373000	-0.437251000	2.747826000
6	-4.908298000	-0.666151000	3.531835000
6	-2.511133000	0.003063000	3.755249000
6	-4.608963000	4.133324000	-0.657209000
6	-3.293297000	4.386738000	-1.422516000
6	-2.898127000	3.102717000	-2.194104000
6	-3.891118000	1.963397000	-1.869672000
6	-5.281808000	2.402345000	-2.377487000
1	3.169448000	-4.183142000	0.593036000
1	-2.251848000	-4.548335000	0.748471000
1	-1.697602000	-5.733076000	-0.421821000
1	-1.945953000	-6.858886000	1.704924000

1	-0.905082000	-5.687433000	2.518855000
1	0.342832000	-7.816372000	1.855801000
1	-0.010682000	-7.434000000	0.172023000
1	2.203869000	-6.543894000	0.600441000
1	1.715554000	-5.886905000	2.150621000
1	-5.148440000	-0.768244000	-1.460185000
1	-5.748420000	-2.920719000	-2.683903000
1	-4.780042000	-2.046378000	-3.854723000
1	-4.553008000	-4.988898000	-3.095444000
1	-4.843519000	-4.282968000	-4.683898000
1	-2.512944000	-3.241690000	-4.559175000
1	-2.470600000	-5.006896000	-4.540233000
1	-2.277721000	-5.063088000	-2.128887000
1	-0.994705000	-4.035316000	-2.742659000
1	-0.044508000	2.324629000	-0.307640000
1	6.299572000	0.751091000	-0.237933000
1	5.893882000	1.093464000	-2.696908000
1	5.424037000	-0.324431000	-4.716219000
1	6.117695000	-1.286872000	-3.412362000
1	2.048835000	-1.737195000	-2.707744000
1	4.238615000	-2.658629000	-3.435831000
1	3.527623000	-1.678879000	-4.715523000
1	3.633618000	2.120884000	-2.573521000
1	3.968134000	1.619466000	-4.233267000
1	6.568312000	0.316134000	2.227326000
1	5.110537000	0.388471000	4.276870000
1	4.406825000	1.318500000	2.953589000
1	2.502212000	-0.023198000	3.016360000
1	3.203036000	-0.948324000	4.342552000
1	2.662895000	-2.422321000	2.417904000
1	6.806274000	-2.164119000	2.177480000
1	6.512452000	-1.617280000	3.827297000
1	-4.804944000	3.939089000	2.158512000
1	-4.627403000	2.711743000	4.353325000
1	-5.382222000	0.514749000	5.320233000
1	-6.333895000	0.957233000	3.904214000
1	-3.293363000	-1.358738000	2.243463000
1	-4.747326000	-1.463147000	4.266550000
1	-5.687877000	-1.011926000	2.846034000
1	-1.557273000	0.125614000	3.235810000
1	-2.376228000	-0.793755000	4.495598000
1	-4.915564000	5.028330000	-0.105336000
1	-3.427953000	5.231630000	-2.107804000
1	-2.508616000	4.662979000	-0.710753000
1	-1.884796000	2.788437000	-1.938570000
1	-2.921553000	3.278547000	-3.276074000
1	-3.571659000	1.042847000	-2.364169000

1	-6.016363000	1.615808000	-2.173483000
1	-5.241388000	2.532238000	-3.464836000
6	1.385553000	6.010490000	-0.635693000
6	1.823987000	7.311042000	-0.847337000
6	3.136433000	7.662453000	-0.537246000
6	4.008157000	6.709683000	-0.014169000
6	3.573198000	5.406885000	0.198913000
6	2.258116000	5.048939000	-0.113234000
6	1.733779000	3.664841000	0.084459000
8	0.502592000	3.506392000	-0.070283000
16	2.851232000	2.403296000	0.474269000
1	0.368398000	5.719250000	-0.873264000
1	1.142798000	8.051081000	-1.255326000
1	3.480287000	8.679267000	-0.701922000
1	5.029246000	6.982806000	0.232391000
1	4.248668000	4.667003000	0.615103000
1	1.802519000	1.294897000	0.947653000
6	-2.941383000	1.324404000	4.445332000
1	-3.007889000	1.195635000	5.531766000
1	-2.208249000	2.114358000	4.257819000
6	-5.692590000	3.727264000	-1.680114000
1	-6.654410000	3.614825000	-1.170948000
1	-5.808765000	4.532070000	-2.414980000
6	4.785644000	-2.607825000	2.903618000
1	4.916999000	-3.512878000	2.300518000
1	4.592677000	-2.932604000	3.932454000
6	2.524990000	0.336484000	-3.188239000
1	2.065724000	0.269441000	-4.181108000
1	1.768261000	0.738547000	-2.507703000

Catalyst...thione form (of thiobenzoic acid) hetero dimer (**1''**)

Number of imaginary frequencies : 0

Electronic energy= -3555.72538926 (hartree/particle)

Zero-point correction= 1.185927

Thermal correction to Energy= 1.243467

Thermal correction to Enthalpy= 1.244411

Thermal correction to Gibbs Free Energy= 1.090195

Sum of electronic and zero-point Energies= -3554.539462

Sum of electronic and thermal Energies= -3554.481922

Sum of electronic and thermal Enthalpies= -3554.480978

Sum of electronic and thermal Free Energies= -3554.635194

#### Coordinates

6	1.581857000	-2.778506000	-0.070161000
6	0.342234000	-2.242716000	-0.409837000
6	-0.868356000	-2.917930000	-0.243887000

6	-0.850936000	-4.192843000	0.357020000
6	0.383921000	-4.769370000	0.692262000
6	1.566921000	-4.069390000	0.452086000
6	-2.142445000	-4.894361000	0.727920000
6	-1.950941000	-5.883824000	1.875255000
6	-0.836204000	-6.860448000	1.510086000
6	0.490390000	-6.111635000	1.394464000
6	-2.124272000	-2.197462000	-0.618667000
6	-2.370710000	-0.955370000	-0.029461000
6	-3.498100000	-0.182737000	-0.298204000
6	-4.400367000	-0.708420000	-1.219021000
6	-4.169799000	-1.909848000	-1.891252000
6	-3.020370000	-2.662174000	-1.602782000
6	-5.151543000	-2.311066000	-2.977568000
6	-4.897669000	-3.699047000	-3.561391000
6	-3.399911000	-3.903304000	-3.770764000
6	-2.701848000	-3.904441000	-2.412083000
8	0.305831000	-0.935155000	-0.898390000
8	-1.418093000	-0.435389000	0.855049000
15	-0.112864000	0.186232000	0.169512000
8	0.881099000	0.136968000	1.388270000
8	-0.250848000	1.492567000	-0.516798000
6	4.906217000	-1.162473000	0.807285000
6	3.663082000	-1.801827000	0.935505000
6	2.847205000	-2.000178000	-0.192160000
6	3.274322000	-1.485552000	-1.426345000
6	4.509384000	-0.829114000	-1.534201000
6	5.333419000	-0.682727000	-0.425148000
6	4.825420000	-0.349739000	-2.926579000
6	4.827157000	-1.574133000	-3.865795000
6	2.551200000	-1.569763000	-2.748994000
6	3.464576000	-2.305748000	-3.754682000
6	3.695149000	0.598602000	-3.380100000
6	5.680711000	-1.070133000	2.095747000
6	4.836688000	-0.269953000	3.107182000
6	3.454674000	-0.951655000	3.264863000
6	3.371269000	-2.206091000	2.363849000
6	5.868517000	-2.499739000	2.648941000
6	-3.910268000	3.570564000	0.118843000
6	-3.736617000	2.309638000	-0.472207000
6	-3.680700000	1.157116000	0.326010000
6	-3.784188000	1.295876000	1.717920000
6	-3.962568000	2.560655000	2.294537000
6	-4.026291000	3.698496000	1.497566000
6	-4.075697000	2.530797000	3.796576000
6	-5.274422000	1.631745000	4.169601000
6	-3.757927000	0.187906000	2.744224000

6	-5.091246000	0.233050000	3.523813000
6	-2.614613000	0.469793000	3.743557000
6	-3.923000000	4.706592000	-0.870484000
6	-2.581167000	4.677582000	-1.632230000
6	-2.419064000	3.304417000	-2.332218000
6	-3.612076000	2.388296000	-1.976565000
6	-4.895754000	3.053781000	-2.519881000
1	2.516613000	-4.527312000	0.724820000
1	-2.905935000	-4.147449000	0.970666000
1	-2.522911000	-5.458760000	-0.132149000
1	-2.890051000	-6.412939000	2.065941000
1	-1.686135000	-5.346282000	2.795031000
1	-0.745824000	-7.659729000	2.252383000
1	-1.082277000	-7.338017000	0.552564000
1	1.237835000	-6.728350000	0.881785000
1	0.887336000	-5.931405000	2.402962000
1	-5.294431000	-0.132651000	-1.453410000
1	-6.172565000	-2.237254000	-2.585510000
1	-5.081719000	-1.567486000	-3.783276000
1	-5.268599000	-4.469393000	-2.872708000
1	-5.451137000	-3.813690000	-4.498732000
1	-3.000426000	-3.096435000	-4.398916000
1	-3.200290000	-4.847527000	-4.287413000
1	-3.035599000	-4.799162000	-1.873158000
1	-1.616222000	-3.997300000	-2.523320000
1	0.712734000	2.746324000	-0.267434000
1	6.296792000	-0.183890000	-0.517939000
1	5.793938000	0.160925000	-2.954926000
1	5.007570000	-1.237346000	-4.893042000
1	5.650354000	-2.242462000	-3.595244000
1	1.595790000	-2.092494000	-2.663414000
1	3.605706000	-3.340907000	-3.428329000
1	2.961096000	-2.340396000	-4.727553000
1	3.706415000	1.500354000	-2.760810000
1	3.885578000	0.908539000	-4.414244000
1	6.651569000	-0.589588000	1.935040000
1	5.365439000	-0.229502000	4.066508000
1	4.724660000	0.759853000	2.753565000
1	2.644109000	-0.264227000	3.011315000
1	3.291201000	-1.261869000	4.303394000
1	2.385858000	-2.666665000	2.465641000
1	6.497971000	-3.075810000	1.963975000
1	6.397575000	-2.446830000	3.607256000
1	-4.160163000	4.680003000	1.949812000
1	-4.209026000	3.539324000	4.202305000
1	-5.336710000	1.552298000	5.260931000
1	-6.202729000	2.098072000	3.826146000

1	-3.624566000	-0.794121000	2.282105000
1	-5.080649000	-0.550377000	4.290261000
1	-5.919148000	0.008361000	2.844275000
1	-1.652743000	0.386904000	3.231258000
1	-2.633958000	-0.300899000	4.522923000
1	-4.060986000	5.667771000	-0.363729000
1	-2.561941000	5.495876000	-2.361427000
1	-1.760627000	4.848026000	-0.927715000
1	-1.489286000	2.819168000	-2.030019000
1	-2.391458000	3.426257000	-3.421429000
1	-3.469080000	1.402976000	-2.426554000
1	-5.763272000	2.425351000	-2.291265000
1	-4.826963000	3.125195000	-3.611237000
6	2.608762000	5.881522000	-0.437006000
6	3.305608000	7.081361000	-0.506995000
6	4.665296000	7.117640000	-0.206691000
6	5.327979000	5.949123000	0.165223000
6	4.636065000	4.747407000	0.237140000
6	3.270417000	4.703874000	-0.064832000
6	2.507834000	3.431905000	0.003331000
8	1.232844000	3.605125000	-0.212082000
16	3.228831000	1.954075000	0.302242000
1	1.551255000	5.845178000	-0.671165000
1	2.786536000	7.989377000	-0.797048000
1	5.208864000	8.056152000	-0.261045000
1	6.386768000	5.975326000	0.402314000
1	5.142215000	3.833473000	0.529280000
1	1.706448000	0.646929000	1.158876000
6	-2.795860000	1.879836000	4.362900000
1	-2.876161000	1.820993000	5.454440000
1	-1.934434000	2.514719000	4.135453000
6	-5.059183000	4.460714000	-1.886408000
1	-6.026917000	4.549783000	-1.383660000
1	-5.022483000	5.240239000	-2.656154000
6	4.482573000	-3.177231000	2.822084000
1	4.431871000	-4.103888000	2.240448000
1	4.308916000	-3.445528000	3.870352000
6	2.330615000	-0.128533000	-3.260978000
1	1.826914000	-0.173376000	-4.233475000
1	1.664422000	0.403135000	-2.574807000

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### Pre-reacting complex (**2a**)

Number of imaginary frequencies : 0

Electronic energy= -3865.45503490 (hartree/particle)

Zero-point correction= 1.339741

Thermal correction to Energy= 1.404388

Thermal correction to Enthalpy= 1.405332

Thermal correction to Gibbs Free Energy= 1.239995  
 Sum of electronic and zero-point Energies= -3864.115294  
 Sum of electronic and thermal Energies= -3864.050647  
 Sum of electronic and thermal Enthalpies= -3864.049702  
 Sum of electronic and thermal Free Energies= -3864.215039

Coordinates

6	3.625622000	0.988031000	-0.237432000
6	2.384723000	1.513339000	0.117787000
6	1.917920000	2.752115000	-0.320262000
6	2.711691000	3.496406000	-1.212281000
6	4.001680000	3.036251000	-1.520531000
6	4.436222000	1.805806000	-1.023561000
6	2.134855000	4.688058000	-1.954078000
6	3.207972000	5.646720000	-2.462181000
6	4.248964000	4.874263000	-3.268495000
6	4.952801000	3.852768000	-2.376846000
6	0.565832000	3.197639000	0.128851000
6	-0.534357000	2.374424000	-0.113045000
6	-1.842378000	2.735728000	0.212718000
6	-2.006344000	3.973297000	0.828504000
6	-0.928130000	4.790475000	1.176555000
6	0.376238000	4.395215000	0.849366000
6	-1.213632000	6.071283000	1.937533000
6	-0.004480000	6.997941000	2.024125000
6	1.222584000	6.187534000	2.431006000
6	1.577509000	5.197291000	1.322604000
8	1.539625000	0.744271000	0.909910000
8	-0.326569000	1.142514000	-0.730640000
1	5.428012000	1.446653000	-1.293480000
1	1.582333000	4.290022000	-2.818324000
1	1.390353000	5.211220000	-1.352101000
1	3.696392000	6.143591000	-1.612192000
1	2.746283000	6.430202000	-3.071962000
1	3.747076000	4.359045000	-4.097684000
1	4.987086000	5.551649000	-3.710221000
1	5.643212000	4.385501000	-1.707346000
1	5.572010000	3.178329000	-2.978594000
1	-3.016313000	4.295490000	1.077501000
1	-2.063472000	6.582683000	1.471016000
1	-1.535336000	5.808834000	2.955006000
1	0.179267000	7.465615000	1.047518000
1	-0.201844000	7.805218000	2.736584000
1	1.005696000	5.645674000	3.360998000
1	2.080170000	6.838247000	2.629697000
1	2.019149000	5.758890000	0.488247000

1	2.356069000	4.503479000	1.658688000
6	4.435646000	-2.100307000	1.842628000
6	4.055472000	-0.796037000	1.495470000
6	4.016212000	-0.397854000	0.148421000
6	4.355621000	-1.340499000	-0.838243000
6	4.760984000	-2.634029000	-0.474528000
6	5.151747000	-3.503185000	-1.640980000
6	3.940483000	-3.635099000	-2.586132000
6	4.352208000	-1.143185000	-2.337728000
6	3.452221000	-2.220620000	-2.984860000
6	6.281486000	-2.781987000	-2.409001000
6	5.501079000	-1.353066000	3.930844000
6	5.083975000	0.093720000	3.558956000
6	3.794266000	0.069551000	2.705975000
6	3.100286000	-2.025398000	3.939704000
1	4.238513000	-4.211667000	-3.469476000
1	3.996517000	-0.149516000	-2.618351000
1	2.415579000	-2.063289000	-2.677621000
1	3.485060000	-2.089324000	-4.072549000
1	7.164929000	-2.703085000	-1.768128000
1	6.565252000	-3.383942000	-3.279575000
1	6.500510000	-1.580066000	3.547699000
1	5.880878000	0.595623000	3.001923000
1	4.897231000	0.687468000	4.461012000
1	3.512504000	1.087829000	2.428394000
1	2.361513000	-2.755267000	3.592887000
1	3.162543000	-2.132948000	5.028765000
1	5.532348000	-1.484148000	5.018419000
1	4.773580000	-3.379190000	3.548571000
6	4.481670000	-2.345630000	3.329305000
6	4.798758000	-3.016460000	0.860261000
1	5.120135000	-4.020920000	1.134939000
1	5.487088000	-4.488591000	-1.299125000
1	3.141766000	-4.184722000	-2.081011000
6	-4.930003000	0.578268000	0.715756000
6	-3.826912000	1.405192000	0.979803000
6	-2.992549000	1.831530000	-0.063663000
6	-3.281695000	1.408837000	-1.369772000
6	-4.378820000	0.574347000	-1.621283000
6	-4.575924000	0.260734000	-3.082352000
6	-4.790952000	1.600335000	-3.820435000
6	-2.561265000	1.819663000	-2.631677000
6	-3.583060000	2.534696000	-3.545570000
6	-2.078037000	0.548176000	-3.358669000
6	-4.898053000	-0.412639000	3.009251000
6	-3.592168000	0.391842000	3.214035000
6	-3.686033000	1.728410000	2.448735000

6	-6.218814000	1.634311000	2.519243000
1	-4.897723000	1.406358000	-4.893940000
1	-1.718087000	2.483569000	-2.423678000
1	-3.912409000	3.463049000	-3.068419000
1	-3.085465000	2.812033000	-4.481978000
1	-1.335326000	0.036796000	-2.741015000
1	-1.583248000	0.841694000	-4.291896000
1	-4.663595000	-1.437115000	2.713392000
1	-2.727649000	-0.168298000	2.841451000
1	-3.421177000	0.594128000	4.277475000
1	-2.800196000	2.334541000	2.651355000
1	-6.816503000	2.169536000	1.775021000
1	-6.860300000	1.460610000	3.390685000
1	-5.475014000	-0.466989000	3.940648000
1	-6.630918000	-0.342424000	1.672614000
6	-5.765810000	0.277599000	1.934990000
6	-5.210266000	0.165273000	-0.582506000
1	-6.074140000	-0.468174000	-0.785666000
1	-5.435396000	-0.404816000	-3.225542000
1	-5.723303000	2.061069000	-3.479728000
6	-3.286359000	-0.379482000	-3.640914000
1	-3.412861000	-0.546300000	-4.717405000
1	-3.117939000	-1.347915000	-3.166964000
6	-4.965420000	2.460560000	2.914789000
1	-4.916349000	2.595369000	4.001719000
1	-5.008123000	3.460714000	2.470348000
6	2.677931000	-0.586632000	3.546396000
1	1.746418000	-0.589786000	2.973493000
1	2.503451000	0.022249000	4.440763000
6	5.793187000	-1.375306000	-2.847884000
1	5.801342000	-1.284094000	-3.940011000
1	6.457405000	-0.597777000	-2.455658000
15	0.360579000	-0.030343000	0.125254000
8	-0.458838000	-0.771915000	1.103930000
8	1.023311000	-0.837884000	-1.046297000
1	1.403456000	-1.726167000	-0.758707000
6	0.517049000	-6.263650000	0.086739000
6	1.891590000	-5.964166000	0.687152000
6	1.806019000	-4.767090000	1.635291000
6	1.157674000	-3.575301000	0.978949000
6	0.286215000	-3.749666000	-0.196962000
6	0.021786000	-5.113002000	-0.796204000
8	1.644621000	-3.265623000	-0.339846000
1	0.539781000	-7.191262000	-0.493987000
1	-0.196769000	-6.417761000	0.906765000
1	2.268832000	-6.835218000	1.232520000
1	2.611671000	-5.743793000	-0.111502000

1	2.798033000	-4.479735000	2.000732000
1	1.198926000	-5.029002000	2.512531000
1	1.001934000	-2.690783000	1.597463000
1	-0.448667000	-2.974177000	-0.408565000
1	-1.054715000	-5.205608000	-0.975034000
1	0.511482000	-5.144740000	-1.777655000
6	-5.089444000	-3.085549000	-1.801358000
6	-6.419505000	-3.286125000	-2.147113000
6	-7.383975000	-3.430948000	-1.149705000
6	-7.011041000	-3.391838000	0.191493000
6	-5.677465000	-3.197648000	0.540446000
6	-4.713757000	-3.032497000	-0.456123000
6	-3.286834000	-2.705674000	-0.153300000
8	-2.541451000	-2.240555000	-0.984391000
16	-2.726568000	-3.070807000	1.514837000
1	-4.328157000	-2.956778000	-2.563047000
1	-6.706914000	-3.323471000	-3.193395000
1	-8.425842000	-3.576977000	-1.418448000
1	-7.759826000	-3.505583000	0.968963000
1	-5.395712000	-3.146177000	1.587268000
1	-1.659872000	-2.246151000	1.411352000

Epoxide ring opening transition state (**TS<sub>a</sub>**)

Number of imaginary frequencies :1

Electronic energy= -3865.42404599 (hartree/particle)

Zero-point correction= 1.340358

Thermal correction to Energy= 1.404077

Thermal correction to Enthalpy= 1.405021

Thermal correction to Gibbs Free Energy= 1.243144

Sum of electronic and zero-point Energies= -3864.083688

Sum of electronic and thermal Energies= -3864.019969

Sum of electronic and thermal Enthalpies= -3864.019025

Sum of electronic and thermal Free Energies= -3864.180902

Coordinates

6	3.682936000	0.730365000	-0.189601000
6	2.479450000	1.354154000	0.129850000
6	2.144428000	2.644438000	-0.282605000
6	3.045515000	3.342436000	-1.106916000
6	4.305342000	2.778060000	-1.368715000
6	4.602949000	1.496582000	-0.902913000
6	2.618515000	4.607719000	-1.826770000
6	3.799632000	5.484547000	-2.233132000
6	4.810442000	4.652799000	-3.019202000
6	5.370456000	3.536068000	-2.139920000
6	0.820032000	3.190975000	0.136880000
6	-0.332421000	2.461461000	-0.156235000

6	-1.615260000	2.881206000	0.193741000
6	-1.701794000	4.097698000	0.865269000
6	-0.575025000	4.830170000	1.246651000
6	0.703839000	4.366795000	0.907387000
6	-0.784409000	6.087518000	2.070301000
6	0.486449000	6.914415000	2.243740000
6	1.645497000	5.990847000	2.607249000
6	1.948294000	5.062412000	1.432702000
8	1.540434000	0.641695000	0.870120000
8	-0.198029000	1.245589000	-0.830592000
1	5.571871000	1.059150000	-1.138458000
1	2.084617000	4.294377000	-2.736246000
1	1.888118000	5.169562000	-1.242729000
1	4.281388000	5.898727000	-1.336329000
1	3.445641000	6.331537000	-2.829627000
1	4.310576000	4.219057000	-3.894979000
1	5.629279000	5.276517000	-3.392253000
1	6.069642000	3.974757000	-1.413873000
1	5.957232000	2.831285000	-2.739508000
1	-2.689420000	4.467457000	1.136682000
1	-1.579090000	6.687543000	1.612038000
1	-1.157486000	5.793381000	3.061102000
1	0.723757000	7.437929000	1.307866000
1	0.331956000	7.680349000	3.010271000
1	1.374270000	5.398817000	3.491063000
1	2.542701000	6.562963000	2.864039000
1	2.423407000	5.656763000	0.640326000
1	2.684888000	4.303544000	1.719247000
6	4.090546000	-2.494356000	1.796712000
6	3.865802000	-1.144144000	1.487646000
6	3.922748000	-0.698113000	0.158059000
6	4.207280000	-1.633526000	-0.851836000
6	4.461676000	-2.975383000	-0.527123000
6	4.835126000	-3.826863000	-1.713699000
6	3.681362000	-3.807132000	-2.738600000
6	4.283955000	-1.377896000	-2.340117000
6	3.304924000	-2.336957000	-3.053657000
6	6.066632000	-3.174377000	-2.381142000
6	5.165843000	-1.936233000	3.937643000
6	4.928296000	-0.440927000	3.599731000
6	3.664948000	-0.293885000	2.719480000
6	2.707136000	-2.336491000	3.860146000
1	4.009674000	-4.327185000	-3.646044000
1	4.033454000	-0.344587000	-2.588827000
1	2.282608000	-2.103202000	-2.740438000
1	3.352159000	-2.148443000	-4.131982000
1	6.904295000	-3.175197000	-1.677159000

1	6.368364000	-3.775280000	-3.246130000
1	6.145381000	-2.265787000	3.578684000
1	5.790762000	-0.020594000	3.073585000
1	4.790169000	0.146075000	4.514706000
1	3.503212000	0.756548000	2.467273000
1	1.899907000	-2.961557000	3.464876000
1	2.721266000	-2.492830000	4.944625000
1	5.144653000	-2.101051000	5.020795000
1	4.231405000	-3.855360000	3.466878000
6	4.061196000	-2.789724000	3.274886000
6	4.396693000	-3.408846000	0.792882000
1	4.602458000	-4.450124000	1.039417000
1	5.062855000	-4.852651000	-1.404653000
1	2.823248000	-4.356219000	-2.342265000
6	-4.802070000	0.864500000	0.647382000
6	-3.656098000	1.621697000	0.934697000
6	-2.812767000	2.048211000	-0.102835000
6	-3.132185000	1.688208000	-1.420697000
6	-4.272757000	0.921576000	-1.693293000
6	-4.503157000	0.682998000	-3.163621000
6	-4.653509000	2.067644000	-3.832549000
6	-2.396194000	2.100651000	-2.672882000
6	-3.376416000	2.905357000	-3.558515000
6	-1.993467000	0.824896000	-3.440349000
6	-4.769818000	-0.245268000	2.869474000
6	-3.470563000	0.543514000	3.158466000
6	-3.500828000	1.894464000	2.413091000
6	-6.033367000	1.874785000	2.523912000
1	-4.809140000	1.934482000	-4.909409000
1	-1.513621000	2.705413000	-2.448501000
1	-3.629980000	3.846670000	-3.061021000
1	-2.871868000	3.161827000	-4.497332000
1	-1.311882000	0.231237000	-2.825713000
1	-1.455300000	1.112245000	-4.351348000
1	-4.525108000	-1.230469000	2.465623000
1	-2.595620000	-0.027551000	2.835556000
1	-3.358329000	0.734854000	4.232177000
1	-2.590954000	2.458161000	2.632321000
1	-6.661884000	2.450662000	1.837647000
1	-6.631908000	1.669623000	3.418847000
1	-5.349020000	-0.400157000	3.787864000
1	-6.521905000	-0.040432000	1.581322000
6	-5.634210000	0.538061000	1.860825000
6	-5.115949000	0.519348000	-0.662436000
1	-6.012066000	-0.061972000	-0.876478000
1	-5.402159000	0.076329000	-3.324805000
1	-5.540536000	2.571002000	-3.435669000

6	-3.261494000	0.004021000	-3.781720000
1	-3.406477000	-0.066419000	-4.866599000
1	-3.151211000	-1.008211000	-3.389958000
6	-4.750381000	2.669334000	2.891194000
1	-4.681101000	2.815382000	3.975505000
1	-4.769945000	3.664788000	2.434078000
6	2.464640000	-0.843971000	3.517985000
1	1.546683000	-0.711624000	2.938287000
1	2.350275000	-0.252441000	4.433193000
6	5.713033000	-1.726276000	-2.812777000
1	5.758910000	-1.623251000	-3.902944000
1	6.429754000	-1.012773000	-2.392996000
15	0.351220000	-0.010442000	0.000121000
8	-0.622423000	-0.381338000	1.156876000
8	0.793710000	-1.069556000	-0.943563000
1	1.475163000	-2.620644000	-0.797567000
6	-0.705617000	-6.074837000	0.306509000
6	0.723510000	-6.080127000	0.852285000
6	1.020390000	-4.773171000	1.591232000
6	0.701731000	-3.558184000	0.759121000
6	-0.363210000	-3.636456000	-0.235702000
6	-0.891964000	-4.954650000	-0.716695000
8	1.371063000	-3.583855000	-0.541735000
1	-0.948126000	-7.035961000	-0.156453000
1	-1.412757000	-5.918644000	1.130491000
1	0.870062000	-6.921151000	1.536548000
1	1.439015000	-6.204809000	0.029557000
1	2.068636000	-4.714467000	1.903167000
1	0.399084000	-4.704583000	2.493541000
1	0.841257000	-2.600947000	1.263594000
1	-0.693159000	-2.723526000	-0.720229000
1	-1.944453000	-4.810636000	-0.976388000
1	-0.365087000	-5.188688000	-1.650427000
6	-5.112399000	-2.621013000	-1.774003000
6	-6.445154000	-2.903762000	-2.046682000
6	-7.305074000	-3.268613000	-1.011080000
6	-6.819477000	-3.368957000	0.290400000
6	-5.479297000	-3.103311000	0.560544000
6	-4.620682000	-2.711166000	-0.468100000
6	-3.183707000	-2.334442000	-0.227200000
8	-2.556769000	-1.757499000	-1.109683000
16	-2.437937000	-2.787974000	1.306418000
1	-4.436694000	-2.315439000	-2.564945000
1	-6.817069000	-2.832503000	-3.064638000
1	-8.349953000	-3.479082000	-1.219704000
1	-7.483924000	-3.658871000	1.098684000
1	-5.090494000	-3.194093000	1.569458000

1 -1.254660000 -1.190906000 1.099293000

**TS<sub>a</sub>'**

Number of imaginary frequencies :1

Electronic energy= -3865.42404599 (hartree/particle)

Zero-point correction= 1.339028

Thermal correction to Energy= 1.402818

Thermal correction to Enthalpy= 1.403763

Thermal correction to Gibbs Free Energy= 1.241374

Sum of electronic and zero-point Energies= -3864.072544

Sum of electronic and thermal Energies= -3864.008754

Sum of electronic and thermal Enthalpies= -3864.007810

Sum of electronic and thermal Free Energies= -3864.170198

Coordinates

6	2.137835000	2.117280000	-0.001517000
6	0.896680000	1.641950000	0.416397000
6	-0.086329000	2.490767000	0.935988000
6	0.132398000	3.878810000	0.960850000
6	1.385486000	4.375648000	0.572966000
6	2.361318000	3.488640000	0.119159000
6	-1.010868000	4.833149000	1.253871000
6	-0.537491000	6.224238000	1.667162000
6	0.479826000	6.749438000	0.657165000
6	1.717202000	5.854062000	0.651087000
6	-1.378669000	1.882678000	1.362593000
6	-2.109082000	1.180126000	0.405696000
6	-3.368619000	0.641166000	0.667287000
6	-3.843160000	0.771455000	1.969954000
6	-3.096343000	1.370318000	2.988215000
6	-1.849637000	1.936780000	2.689804000
6	-3.653656000	1.349547000	4.399158000
6	-2.888304000	2.250871000	5.365160000
6	-1.387550000	2.047467000	5.173579000
6	-0.976848000	2.528596000	3.783089000
8	0.605454000	0.292094000	0.329891000
8	-1.536307000	0.996992000	-0.844326000
1	3.332687000	3.878138000	-0.181552000
1	-1.603384000	4.919716000	0.330712000
1	-1.694967000	4.417706000	1.995985000
1	-0.073659000	6.177876000	2.662530000
1	-1.396266000	6.899255000	1.742972000
1	0.022450000	6.756612000	-0.340882000
1	0.766944000	7.780742000	0.887145000
1	2.287796000	6.034610000	1.573326000
1	2.382571000	6.121278000	-0.177316000

1	-4.825855000	0.364152000	2.203826000
1	-4.714712000	1.623288000	4.373096000
1	-3.614674000	0.315841000	4.770418000
1	-3.134285000	3.303260000	5.170453000
1	-3.189490000	2.035385000	6.395346000
1	-1.153469000	0.978620000	5.282700000
1	-0.814623000	2.584893000	5.936292000
1	-1.030268000	3.626361000	3.764672000
1	0.072650000	2.283372000	3.579158000
6	5.270655000	-0.010574000	-0.055584000
6	4.072947000	0.576257000	0.377682000
6	3.237563000	1.251045000	-0.523745000
6	3.586824000	1.262786000	-1.881663000
6	4.771113000	0.642188000	-2.311865000
6	5.042842000	0.822778000	-3.782279000
6	3.833184000	0.273006000	-4.563587000
6	2.885833000	2.018707000	-2.986462000
6	2.570311000	1.078187000	-4.171782000
6	5.149317000	2.340218000	-4.065795000
6	6.395496000	0.677751000	2.013929000
6	5.044051000	1.209831000	2.561663000
6	3.876749000	0.470785000	1.869212000
6	5.359947000	-1.578775000	1.889671000
1	4.028893000	0.349921000	-5.639313000
1	1.970111000	2.494589000	-2.626024000
1	1.735017000	0.426543000	-3.915917000
1	2.236477000	1.700194000	-5.010918000
1	6.063587000	2.737297000	-3.614398000
1	5.233676000	2.490170000	-5.148476000
1	6.924637000	1.460108000	1.461584000
1	4.950383000	2.286390000	2.388103000
1	4.972678000	1.049429000	3.643879000
1	2.913384000	0.885189000	2.182315000
1	5.280799000	-2.515135000	1.329631000
1	5.931332000	-1.803279000	2.798078000
1	7.048911000	0.358728000	2.833773000
1	7.076554000	-0.929070000	0.696750000
6	6.132275000	-0.521974000	1.073752000
6	5.620597000	0.020383000	-1.403036000
1	6.562712000	-0.411430000	-1.738734000
1	5.965137000	0.310595000	-4.077519000
1	3.701187000	-0.787159000	-4.325887000
6	-5.483519000	-1.919739000	-1.178541000
6	-4.614894000	-1.342915000	-0.240010000
6	-4.179891000	-0.019707000	-0.390851000
6	-4.580793000	0.690686000	-1.532488000
6	-5.424076000	0.093871000	-2.479959000

6	-5.752817000	0.988451000	-3.646791000
6	-6.439479000	2.259133000	-3.103127000
6	-4.216765000	2.110701000	-1.895287000
6	-5.523238000	2.922200000	-2.042193000
6	-3.506423000	2.084413000	-3.266326000
6	-4.612097000	-4.206136000	-0.804033000
6	-3.561476000	-3.530385000	0.111767000
6	-4.190713000	-2.316361000	0.833396000
6	-6.493578000	-3.329852000	0.576976000
1	-6.635565000	2.945547000	-3.934844000
1	-3.571889000	2.575151000	-1.145439000
1	-6.028718000	2.977159000	-1.072946000
1	-5.271296000	3.948344000	-2.333122000
1	-2.557607000	1.550272000	-3.168563000
1	-3.272002000	3.113830000	-3.561074000
1	-4.218089000	-4.333525000	-1.816718000
1	-2.714559000	-3.165556000	-0.475941000
1	-3.179232000	-4.239541000	0.856348000
1	-3.461076000	-1.871733000	1.515693000
1	-7.386914000	-2.697917000	0.583742000
1	-6.812333000	-4.345459000	0.837576000
1	-4.876395000	-5.202926000	-0.431502000
1	-6.603708000	-3.723885000	-1.568800000
6	-5.883854000	-3.333316000	-0.841653000
6	-5.891635000	-1.203302000	-2.297226000
1	-6.563148000	-1.653930000	-3.026639000
1	-6.403226000	0.475992000	-4.364093000
1	-7.408226000	1.994062000	-2.668495000
6	-4.426701000	1.408950000	-4.316561000
1	-4.645184000	2.092594000	-5.145124000
1	-3.940976000	0.527177000	-4.745114000
6	-5.442802000	-2.805698000	1.592100000
1	-5.146462000	-3.598600000	2.288842000
1	-5.859973000	-1.991247000	2.193627000
6	3.959959000	-1.022609000	2.246393000
1	3.175412000	-1.564706000	1.707320000
1	3.750424000	-1.144624000	3.314359000
6	3.897150000	3.067999000	-3.505691000
1	3.420297000	3.673789000	-4.284138000
1	4.175687000	3.746063000	-2.692091000
15	-0.412176000	-0.184067000	-0.885808000
8	-0.971318000	-1.499113000	-0.433524000
8	0.308031000	-0.077344000	-2.199362000
1	1.540842000	-1.026806000	-2.428963000
6	2.755883000	-5.140464000	-2.032326000
6	3.897209000	-4.135888000	-1.862228000
6	3.523324000	-3.063011000	-0.837613000

6	2.207332000	-2.391077000	-1.159281000
6	1.144470000	-3.237454000	-1.738314000
6	1.503162000	-4.438753000	-2.557317000
8	2.216887000	-1.790739000	-2.460635000
1	3.037873000	-5.943469000	-2.719726000
1	2.531908000	-5.604065000	-1.061363000
1	4.807640000	-4.647110000	-1.535693000
1	4.119092000	-3.658575000	-2.824670000
1	4.284518000	-2.278851000	-0.781866000
1	3.437170000	-3.516971000	0.158616000
1	1.880139000	-1.688925000	-0.384299000
1	0.172799000	-2.761717000	-1.855803000
1	0.639462000	-5.106870000	-2.610130000
1	1.673075000	-4.065817000	-3.575779000
6	1.759341000	-3.422141000	3.869104000
6	1.729825000	-2.444958000	4.853316000
6	1.097855000	-1.223651000	4.605657000
6	0.484037000	-0.989655000	3.378826000
6	0.477907000	-1.979187000	2.399518000
6	1.121486000	-3.194472000	2.641384000
6	1.242713000	-4.279497000	1.629896000
8	2.055729000	-5.165450000	1.690895000
16	0.086193000	-4.353559000	0.216509000
1	2.265790000	-4.368222000	4.030027000
1	2.209573000	-2.625948000	5.810072000
1	1.091701000	-0.452239000	5.371141000
1	0.000645000	-0.040440000	3.162163000
1	-0.001937000	-1.753587000	1.452716000
1	-0.599472000	-3.195038000	0.354607000

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**TS<sub>a</sub>\***

Number of imaginary frequencies :1

Electronic energy= -3865.41422798 (hartree/particle)

Zero-point correction= 1.340145

Thermal correction to Energy= 1.404369

Thermal correction to Enthalpy= 1.405313

Thermal correction to Gibbs Free Energy= 1.240156

Sum of electronic and zero-point Energies= -3864.074083

Sum of electronic and thermal Energies= -3864.009859

Sum of electronic and thermal Enthalpies= -3864.008915

Sum of electronic and thermal Free Energies= -3864.174072

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Coordinates

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6	1.982313000	2.790671000	-0.442866000
6	0.717472000	2.412802000	0.000671000
6	-0.396781000	3.254990000	-0.052718000

6	-0.271202000	4.493446000	-0.712396000
6	0.992875000	4.904809000	-1.162634000
6	2.093556000	4.062029000	-0.999789000
6	-1.503386000	5.307448000	-1.065210000
6	-1.190438000	6.780626000	-1.311463000
6	-0.066686000	6.902771000	-2.337628000
6	1.211130000	6.268838000	-1.792206000
6	-1.684223000	2.795924000	0.551351000
6	-2.222474000	1.590305000	0.117229000
6	-3.418147000	1.053755000	0.594228000
6	-4.085983000	1.808881000	1.552816000
6	-3.556411000	2.994458000	2.074524000
6	-2.331645000	3.485154000	1.598445000
6	-4.316483000	3.684905000	3.191379000
6	-3.780528000	5.077388000	3.512488000
6	-2.258462000	5.023469000	3.611244000
6	-1.664882000	4.687050000	2.244178000
8	0.576181000	1.136383000	0.547174000
8	-1.510264000	0.867504000	-0.830544000
1	3.073425000	4.393184000	-1.339692000
1	-1.920891000	4.878687000	-1.988451000
1	-2.285167000	5.190607000	-0.313299000
1	-0.881479000	7.257507000	-0.370670000
1	-2.091492000	7.298675000	-1.655739000
1	-0.369919000	6.391697000	-3.260577000
1	0.120138000	7.950083000	-2.596230000
1	1.637756000	6.933850000	-1.028030000
1	1.967535000	6.186835000	-2.580490000
1	-5.035015000	1.439799000	1.938871000
1	-5.379428000	3.729575000	2.927113000
1	-4.252416000	3.060784000	4.093542000
1	-4.065135000	5.779702000	2.717481000
1	-4.226673000	5.444642000	4.442131000
1	-1.969936000	4.256379000	4.341777000
1	-1.850282000	5.975459000	3.965044000
1	-1.758237000	5.571157000	1.598559000
1	-0.589675000	4.491654000	2.326486000
6	4.733028000	0.710820000	1.140370000
6	3.609074000	1.531854000	0.987954000
6	3.151621000	1.881063000	-0.290341000
6	3.821309000	1.370615000	-1.408658000
6	4.947189000	0.551265000	-1.245884000
6	5.529866000	0.063825000	-2.546340000
6	4.424474000	-0.722434000	-3.284398000
6	3.455784000	1.579939000	-2.858332000
6	3.193596000	0.197120000	-3.497916000
6	5.907656000	1.286556000	-3.409503000

6	5.379086000	1.812248000	3.248313000
6	4.136603000	2.727166000	3.085437000
6	3.030297000	1.977141000	2.308439000
6	3.886876000	-0.188906000	3.289083000
1	4.816072000	-1.085259000	-4.241864000
1	2.573195000	2.216605000	-2.964992000
1	2.296636000	-0.237757000	-3.050417000
1	2.997167000	0.338935000	-4.567329000
1	6.735436000	1.824803000	-2.938178000
1	6.263133000	0.938143000	-4.385968000
1	6.261709000	2.272274000	2.793117000
1	4.399654000	3.645851000	2.551610000
1	3.741799000	3.023938000	4.063845000
1	2.159652000	2.625913000	2.175120000
1	3.693573000	-1.178307000	2.868081000
1	4.132241000	-0.325129000	4.348877000
1	5.607800000	1.649909000	4.307749000
1	5.976252000	-0.206110000	2.646945000
6	5.100247000	0.449029000	2.577741000
6	5.411903000	0.231265000	0.024387000
1	6.293111000	-0.399362000	0.145453000
1	6.405721000	-0.571068000	-2.372722000
1	4.151523000	-1.600590000	-2.689694000
6	-4.486027000	-2.596610000	0.584782000
6	-4.066046000	-1.334580000	1.035175000
6	-3.884797000	-0.281219000	0.123915000
6	-4.109713000	-0.528956000	-1.241133000
6	-4.525616000	-1.795182000	-1.677828000
6	-4.772125000	-1.880430000	-3.162000000
6	-5.857088000	-0.839820000	-3.515344000
6	-4.001076000	0.461940000	-2.377285000
6	-5.387490000	0.564932000	-3.053987000
6	-3.004313000	-0.094879000	-3.417153000
6	-3.246243000	-3.743799000	2.371134000
6	-2.850765000	-2.369353000	2.961571000
6	-3.876159000	-1.294787000	2.535025000
6	-5.638998000	-3.098151000	2.719172000
1	-6.035017000	-0.857387000	-4.596484000
1	-3.678115000	1.446754000	-2.031547000
1	-6.104264000	1.001331000	-2.351989000
1	-5.313557000	1.249000000	-3.906841000
1	-2.010132000	-0.155407000	-2.965168000
1	-2.933353000	0.609550000	-4.253540000
1	-2.497466000	-4.075875000	1.641876000
1	-1.847320000	-2.082615000	2.642288000
1	-2.838540000	-2.410659000	4.056946000
1	-3.546579000	-0.312688000	2.880109000

1	-6.641981000	-3.093923000	2.281844000
1	-5.661451000	-3.787514000	3.570966000
1	-3.294323000	-4.510101000	3.152745000
1	-4.943458000	-4.586806000	1.277175000
6	-4.620907000	-3.620511000	1.680959000
6	-4.721863000	-2.827213000	-0.765994000
1	-5.061784000	-3.804791000	-1.106977000
1	-5.094562000	-2.887482000	-3.449626000
1	-6.797266000	-1.114004000	-3.027495000
6	-3.480205000	-1.485392000	-3.907813000
1	-3.683047000	-1.473180000	-4.984885000
1	-2.702548000	-2.238067000	-3.740841000
6	-5.231547000	-1.672433000	3.175315000
1	-5.137960000	-1.625710000	4.265894000
1	-5.994209000	-0.942071000	2.883953000
6	2.644029000	0.719939000	3.116563000
1	1.848120000	0.184686000	2.593146000
1	2.251662000	1.034966000	4.090615000
6	4.671538000	2.211389000	-3.570789000
1	4.431125000	2.357699000	-4.629967000
1	4.872402000	3.200820000	-3.146376000
15	-0.228075000	0.047514000	-0.312542000
8	-0.801538000	-0.926326000	0.764511000
8	0.437273000	-0.516577000	-1.516721000
1	-0.150837000	-1.777695000	-2.538161000
6	-1.039211000	-5.784312000	-1.748419000
6	0.278313000	-5.616471000	-2.503989000
6	1.184747000	-4.641138000	-1.749878000
6	0.456835000	-3.422112000	-1.271657000
6	-0.979191000	-3.252286000	-1.496119000
6	-1.840009000	-4.477423000	-1.735882000
8	-0.360862000	-2.737751000	-2.724944000
1	-1.645731000	-6.580289000	-2.190045000
1	-0.818265000	-6.079069000	-0.714576000
1	0.792256000	-6.576043000	-2.609754000
1	0.084758000	-5.235790000	-3.513776000
1	2.035271000	-4.314308000	-2.357426000
1	1.601428000	-5.117170000	-0.854875000
1	1.020508000	-2.553278000	-0.949885000
1	-1.482595000	-2.457234000	-0.944342000
1	-2.604875000	-4.502542000	-0.954467000
1	-2.365901000	-4.326544000	-2.686767000
6	4.467311000	-3.046040000	1.092631000
6	5.663921000	-3.716151000	1.315798000
6	5.661590000	-4.944871000	1.975190000
6	4.459867000	-5.502213000	2.406445000
6	3.258548000	-4.836997000	2.178563000

6	3.258468000	-3.603986000	1.523677000
6	2.000963000	-2.831695000	1.239396000
8	2.086724000	-1.679443000	0.823475000
16	0.442718000	-3.640100000	1.406000000
1	4.441125000	-2.084306000	0.587173000
1	6.599709000	-3.281648000	0.975429000
1	6.596844000	-5.467703000	2.153200000
1	4.458330000	-6.456477000	2.924417000
1	2.316528000	-5.260983000	2.511733000
1	-0.304979000	-1.784799000	1.005156000

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**TS<sub>a</sub>'\***

Number of imaginary frequencies :1

Electronic energy= -3865.40839103 (hartree/particle)

Zero-point correction= 1.338444

Thermal correction to Energy= 1.402530

Thermal correction to Enthalpy= 1.403475

Thermal correction to Gibbs Free Energy= 1.239964

Sum of electronic and zero-point Energies= -3864.069947

Sum of electronic and thermal Energies= -3864.005861

Sum of electronic and thermal Enthalpies= -3864.004916

Sum of electronic and thermal Free Energies= -3864.168427

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Coordinates

6	2.256957000	2.280311000	0.214774000
6	0.960468000	1.854022000	0.504863000
6	-0.061900000	2.739815000	0.841860000
6	0.179660000	4.126500000	0.786118000
6	1.471538000	4.578110000	0.479525000
6	2.486983000	3.651846000	0.229192000
6	-0.960374000	5.111408000	0.965970000
6	-0.652025000	6.477707000	0.355784000
6	0.696445000	6.970138000	0.873210000
6	1.804748000	6.053963000	0.361163000
6	-1.393977000	2.150493000	1.163049000
6	-2.006989000	1.365946000	0.182296000
6	-3.273983000	0.806375000	0.356276000
6	-3.881039000	1.003902000	1.595277000
6	-3.256383000	1.685970000	2.640921000
6	-1.997634000	2.269873000	2.429724000
6	-3.942272000	1.705282000	3.994912000
6	-3.271639000	2.631341000	5.006597000
6	-1.757462000	2.455271000	4.937429000
6	-1.253082000	2.928560000	3.575692000
8	0.657945000	0.502284000	0.449426000
8	-1.319767000	1.138417000	-0.999273000

15	-0.121820000	0.029743000	-0.923036000
8	-0.662489000	-1.338659000	-0.627111000
8	0.765370000	0.245801000	-2.115039000
6	4.742703000	-0.519326000	0.789381000
6	3.715701000	0.412537000	0.985162000
6	3.338245000	1.291530000	-0.040812000
6	4.027191000	1.238605000	-1.259466000
6	5.073767000	0.319487000	-1.440353000
6	5.427487000	-0.562631000	-0.424902000
6	5.769962000	0.457497000	-2.770160000
6	4.739235000	0.270982000	-3.902434000
6	3.826135000	2.140277000	-2.453826000
6	3.580255000	1.282739000	-3.714383000
6	6.314757000	1.901696000	-2.860858000
6	5.059876000	-1.331708000	2.022528000
6	5.478040000	-0.325890000	3.119116000
6	4.305460000	0.654605000	3.380527000
6	3.153811000	0.379377000	2.386326000
6	2.622245000	-1.042835000	2.635253000
6	-5.106805000	-1.983832000	-1.456205000
6	-4.389134000	-1.280482000	-0.477789000
6	-3.956975000	0.031777000	-0.714466000
6	-4.234983000	0.613600000	-1.960480000
6	-4.944701000	-0.102185000	-2.934785000
6	-5.389243000	-1.395738000	-2.683439000
6	-5.170695000	0.669928000	-4.208592000
6	-5.958259000	1.951011000	-3.858877000
6	-3.879647000	2.010491000	-2.411275000
6	-5.191368000	2.744546000	-2.769784000
6	-3.024825000	1.903528000	-3.692680000
6	-5.502869000	-3.375430000	-1.032357000
6	-4.221968000	-4.182626000	-0.727699000
6	-3.326093000	-3.365021000	0.235184000
6	-4.094329000	-2.124423000	0.739898000
6	-6.306621000	-3.259919000	0.280978000
1	3.492457000	4.012903000	0.016212000
1	-1.874253000	4.686360000	0.536523000
1	-1.165390000	5.260026000	2.033554000
1	-1.452236000	7.181809000	0.605792000
1	-0.617618000	6.399618000	-0.738739000
1	0.891176000	8.001272000	0.561087000
1	0.682222000	6.962927000	1.971254000
1	2.746190000	6.254930000	0.885892000
1	1.992570000	6.280107000	-0.697558000
1	-4.869228000	0.575181000	1.757179000
1	-4.997450000	1.972090000	3.864299000
1	-3.937397000	0.680491000	4.395150000

1	-3.519035000	3.676625000	4.779575000
1	-3.652650000	2.423137000	6.011656000
1	-1.503834000	1.394953000	5.078082000
1	-1.256865000	3.015204000	5.733832000
1	-1.375715000	4.018119000	3.532353000
1	-0.180338000	2.735762000	3.466108000
1	2.011387000	-0.733215000	-2.299887000
1	6.247276000	-1.266391000	-0.570157000
1	6.585950000	-0.267698000	-2.864077000
1	5.240823000	0.426156000	-4.864809000
1	4.358117000	-0.753358000	-3.889838000
1	2.991479000	2.828838000	-2.300161000
1	2.615276000	0.778637000	-3.627566000
1	3.510160000	1.954767000	-4.577501000
1	7.084850000	2.050747000	-2.097927000
1	6.793874000	2.041104000	-3.836542000
1	5.865513000	-2.048901000	1.828938000
1	5.741963000	-0.872418000	4.031443000
1	6.371664000	0.214825000	2.793045000
1	4.637854000	1.692097000	3.279317000
1	3.921546000	0.537140000	4.400446000
1	2.354864000	1.111654000	2.523682000
1	1.847263000	-1.246726000	1.890722000
1	2.135533000	-1.099817000	3.616519000
1	-5.947710000	-1.942422000	-3.441896000
1	-5.719359000	0.068563000	-4.941706000
1	-6.083000000	2.552909000	-4.766516000
1	-6.959740000	1.680821000	-3.510338000
1	-3.337736000	2.564147000	-1.641014000
1	-4.947316000	3.752859000	-3.123136000
1	-5.803403000	2.857778000	-1.869432000
1	-2.067984000	1.433796000	-3.450741000
1	-2.807908000	2.915400000	-4.054076000
1	-6.099378000	-3.869098000	-1.806957000
1	-4.506583000	-5.142320000	-0.280175000
1	-3.688702000	-4.404949000	-1.656749000
1	-2.435994000	-3.006141000	-0.286747000
1	-2.999905000	-3.973568000	1.088200000
1	-3.487806000	-1.584826000	1.472646000
1	-7.208352000	-2.666880000	0.100269000
1	-6.631001000	-4.257363000	0.598405000
6	2.981962000	-4.764860000	-2.875292000
6	4.052239000	-4.058766000	-2.044708000
6	3.437035000	-3.476281000	-0.769638000
6	2.141339000	-2.768355000	-1.025528000
6	1.619905000	-2.650033000	-2.401794000
6	1.927855000	-3.771717000	-3.383718000

8	2.562186000	-1.569447000	-2.485498000
1	3.430927000	-5.288719000	-3.724114000
1	2.499528000	-5.528814000	-2.251759000
1	4.849794000	-4.753974000	-1.767307000
1	4.508177000	-3.247523000	-2.624594000
1	4.111423000	-2.759187000	-0.293306000
1	3.246088000	-4.266488000	-0.031293000
1	1.802849000	-2.013319000	-0.318063000
1	0.596007000	-2.277485000	-2.460780000
1	0.998865000	-4.296102000	-3.627732000
1	2.271129000	-3.281574000	-4.301584000
6	0.559265000	-3.601049000	4.004601000
6	0.028830000	-2.825858000	5.025881000
6	-0.825647000	-1.764845000	4.722111000
6	-1.154044000	-1.486794000	3.397712000
6	-0.647696000	-2.277110000	2.368957000
6	0.217090000	-3.334131000	2.671746000
6	0.889517000	-4.190661000	1.655792000
8	1.791321000	-4.949811000	1.913226000
16	0.364618000	-4.187885000	-0.088925000
1	1.243449000	-4.416330000	4.215501000
1	0.286034000	-3.041585000	6.058101000
1	-1.231824000	-1.152060000	5.522070000
1	-1.796133000	-0.644181000	3.149232000
1	-0.902003000	-2.007044000	1.347995000
1	-0.328647000	-3.015767000	-0.184587000
6	-3.794798000	1.091857000	-4.767368000
1	-3.946262000	1.686970000	-5.675479000
1	-3.230501000	0.199984000	-5.055533000
6	-5.421706000	-2.597021000	1.369263000
1	-5.942807000	-1.750422000	1.828740000
1	-5.196503000	-3.307471000	2.173277000
6	5.149363000	2.910956000	-2.670573000
1	5.045476000	3.554249000	-3.551689000
1	5.343706000	3.565912000	-1.814595000
6	3.790216000	-2.054645000	2.534002000
1	4.012972000	-2.487056000	3.516826000
1	3.528323000	-2.896428000	1.886361000

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### Product complex (**3a**)

Number of imaginary frequencies : 0

Electronic energy=-3865.49025910 (hartree/particle)

Zero-point correction= 1.342872

Thermal correction to Energy= 1.407281

Thermal correction to Enthalpy= 1.408225

Thermal correction to Gibbs Free Energy= 1.243648

Sum of electronic and zero-point Energies= -3864.147387

Sum of electronic and thermal Energies= -3864.082978

Sum of electronic and thermal Enthalpies= -3864.082034  
 Sum of electronic and thermal Free Energies= -3864.246611

Coordinates

6	3.707204000	0.588129000	-0.274343000
6	2.528065000	1.274166000	0.001401000
6	2.260712000	2.566250000	-0.455655000
6	3.192362000	3.186693000	-1.307282000
6	4.418524000	2.547718000	-1.553394000
6	4.657753000	1.279715000	-1.023833000
6	2.825801000	4.447496000	-2.067442000
6	4.047333000	5.236438000	-2.532645000
6	4.997158000	4.313550000	-3.293009000
6	5.511765000	3.212943000	-2.368345000
6	0.982205000	3.207035000	-0.029007000
6	-0.215488000	2.536547000	-0.271291000
6	-1.456107000	3.006614000	0.155550000
6	-1.457939000	4.233395000	0.813700000
6	-0.283219000	4.925217000	1.117431000
6	0.956193000	4.397150000	0.728360000
6	-0.396571000	6.203191000	1.928072000
6	0.918682000	6.970107000	2.036404000
6	2.046924000	5.995942000	2.362885000
6	2.253050000	5.038589000	1.190936000
8	1.542058000	0.621808000	0.750736000
8	-0.167379000	1.317810000	-0.951363000
1	5.605375000	0.786459000	-1.233297000
1	2.253012000	4.134115000	-2.952728000
1	2.144784000	5.074803000	-1.489964000
1	4.567259000	5.664062000	-1.663845000
1	3.729901000	6.073650000	-3.162654000
1	4.458637000	3.865283000	-4.138045000
1	5.840816000	4.873083000	-3.709886000
1	6.241322000	3.648082000	-1.670698000
1	6.053461000	2.450892000	-2.939257000
1	-2.412144000	4.642287000	1.142941000
1	-1.179321000	6.835164000	1.492574000
1	-0.742418000	5.942080000	2.937816000
1	1.139826000	7.470683000	1.084295000
1	0.832260000	7.751123000	2.798334000
1	1.787499000	5.429484000	3.266808000
1	2.981127000	6.526903000	2.571212000
1	2.720651000	5.598210000	0.369558000
1	2.964437000	4.248726000	1.456490000
6	4.166450000	-2.484059000	1.922671000
6	3.900142000	-1.166029000	1.525212000

6	3.928555000	-0.815994000	0.167254000
6	4.210769000	-1.815168000	-0.779583000
6	4.506196000	-3.121612000	-0.364213000
6	4.812413000	-4.063339000	-1.499098000
6	3.577635000	-4.126504000	-2.423312000
6	4.209548000	-1.673410000	-2.285017000
6	3.198714000	-2.690002000	-2.865376000
6	5.988326000	-3.472537000	-2.307743000
6	5.168289000	-1.762617000	4.061187000
6	4.922116000	-0.302358000	3.600455000
6	3.668691000	-0.241409000	2.697731000
6	2.723235000	-2.244744000	3.917330000
1	3.815524000	-4.752013000	-3.291654000
1	3.939772000	-0.662481000	-2.599988000
1	2.189631000	-2.425052000	-2.535065000
1	3.207508000	-2.603871000	-3.958139000
1	6.882573000	-3.436537000	-1.677953000
1	6.213290000	-4.134296000	-3.151742000
1	6.171018000	-2.095345000	3.776609000
1	5.785948000	0.080809000	3.048315000
1	4.770669000	0.357289000	4.462604000
1	3.488219000	0.788346000	2.378617000
1	1.956548000	-2.895541000	3.486240000
1	2.677556000	-2.368362000	5.005464000
1	5.097372000	-1.845539000	5.151885000
1	4.304830000	-3.733146000	3.676416000
6	4.113496000	-2.686760000	3.415023000
6	4.483466000	-3.457950000	0.983741000
1	4.697377000	-4.478071000	1.298452000
1	5.065720000	-5.060381000	-1.123347000
1	2.747922000	-4.594834000	-1.887834000
6	-4.595637000	1.026992000	0.950547000
6	-3.417363000	1.770640000	1.108783000
6	-2.694313000	2.198087000	-0.017610000
6	-3.160858000	1.842046000	-1.291352000
6	-4.344451000	1.103756000	-1.433871000
6	-4.738106000	0.862291000	-2.867494000
6	-4.906946000	2.237823000	-3.548884000
6	-2.548852000	2.220789000	-2.618371000
6	-3.593302000	3.050921000	-3.400037000
6	-2.273663000	0.928782000	-3.418856000
6	-4.229739000	-0.171717000	3.066121000
6	-2.970688000	0.695367000	3.319781000
6	-3.093482000	2.036504000	2.562240000
6	-5.574157000	1.935613000	3.038947000
1	-5.154172000	2.086064000	-4.605711000
1	-1.626676000	2.794479000	-2.493617000

1	-3.778245000	3.993651000	-2.875904000
1	-3.179083000	3.303077000	-4.382841000
1	-1.508465000	0.336663000	-2.909352000
1	-1.867145000	1.203968000	-4.398774000
1	-3.963756000	-1.074286000	2.505178000
1	-2.063097000	0.175036000	3.006592000
1	-2.862794000	0.914558000	4.388452000
1	-2.171494000	2.610815000	2.677188000
1	-6.365746000	2.490720000	2.527137000
1	-5.960146000	1.661633000	4.027743000
1	-4.682101000	-0.495653000	4.010556000
1	-6.163378000	0.064288000	2.071203000
6	-5.252757000	0.646019000	2.250989000
6	-5.064526000	0.696236000	-0.315850000
1	-5.987849000	0.129278000	-0.429370000
1	-5.669543000	0.287830000	-2.924512000
1	-5.746446000	2.771241000	-3.092535000
6	-3.586673000	0.118418000	-3.575862000
1	-3.843363000	-0.008628000	-4.634191000
1	-3.467691000	-0.881387000	-3.148972000
6	-4.291826000	2.799896000	3.169122000
1	-4.079837000	3.025274000	4.220298000
1	-4.418554000	3.757241000	2.652525000
6	2.470368000	-0.768587000	3.515445000
1	1.553899000	-0.672370000	2.926584000
1	2.349468000	-0.139398000	4.405076000
6	5.611933000	-2.052767000	-2.808172000
1	5.602916000	-2.015596000	-3.903541000
1	6.348612000	-1.316509000	-2.468490000
15	0.340150000	0.033189000	-0.131710000
8	-0.701181000	-0.239396000	1.035845000
8	0.637733000	-1.089298000	-1.038676000
1	1.578591000	-2.794302000	-0.491626000
6	-1.030132000	-6.192924000	0.170464000
6	0.215297000	-6.088498000	1.050492000
6	0.287445000	-4.713509000	1.714447000
6	0.272235000	-3.581332000	0.690076000
6	-0.910141000	-3.688156000	-0.297104000
6	-1.025886000	-5.094110000	-0.891093000
8	1.469010000	-3.656914000	-0.050231000
1	-1.078409000	-7.173208000	-0.316208000
1	-1.930431000	-6.104236000	0.794791000
1	0.215809000	-6.872902000	1.815269000
1	1.111942000	-6.232696000	0.434971000
1	1.207366000	-4.617685000	2.300887000
1	-0.561191000	-4.587493000	2.401436000
1	0.220245000	-2.621791000	1.227047000

1	-0.757038000	-2.958984000	-1.095625000
1	-1.902649000	-5.153023000	-1.541451000
1	-0.142664000	-5.219239000	-1.531136000
6	-5.727205000	-2.414053000	-1.803238000
6	-7.087214000	-2.168926000	-1.658887000
6	-7.663797000	-2.169660000	-0.389047000
6	-6.879022000	-2.423979000	0.734015000
6	-5.516689000	-2.671033000	0.592638000
6	-4.935962000	-2.656994000	-0.676440000
6	-3.482689000	-2.908650000	-0.914144000
8	-3.011500000	-2.974614000	-2.023321000
16	-2.449687000	-3.139668000	0.551639000
1	-5.257448000	-2.422449000	-2.781954000
1	-7.698481000	-1.976946000	-2.535387000
1	-8.726610000	-1.978976000	-0.274871000
1	-7.328089000	-2.437382000	1.722354000
1	-4.915981000	-2.889170000	1.470417000
1	-1.387293000	-0.901961000	0.802033000

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### Pre-reacting complex (**2b**)

Number of imaginary frequencies : 0

Electronic energy= -3865.46082474 (hartree/particle)

Zero-point correction= 1.341728

Thermal correction to Energy= 1.406569

Thermal correction to Enthalpy= 1.407513

Thermal correction to Gibbs Free Energy= 1.237904

Sum of electronic and zero-point Energies= -3864.119097

Sum of electronic and thermal Energies= -3864.054256

Sum of electronic and thermal Enthalpies= -3864.053312

Sum of electronic and thermal Free Energies= -3864.222921

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### Coordinates

6	2.215773000	2.301452000	0.872555000
6	0.906176000	1.837735000	0.962108000
6	-0.143070000	2.597908000	1.477983000
6	0.098745000	3.940464000	1.820897000
6	1.411277000	4.433926000	1.755693000
6	2.441678000	3.605793000	1.305818000
6	-1.056797000	4.875052000	2.126337000
6	-0.628776000	6.110875000	2.913907000
6	0.550588000	6.784463000	2.216624000
6	1.754247000	5.844651000	2.198202000
6	-1.477349000	1.943979000	1.618260000
6	-2.069310000	1.393579000	0.484182000
6	-3.306314000	0.752963000	0.496958000
6	-3.933706000	0.656046000	1.736085000

6	-3.347173000	1.121331000	2.915738000
6	-2.099624000	1.759256000	2.870285000
6	-4.074764000	0.872816000	4.223757000
6	-3.475904000	1.637078000	5.401210000
6	-1.957842000	1.483375000	5.385339000
6	-1.381454000	2.164975000	4.145488000
8	0.635204000	0.541959000	0.530465000
8	-1.359496000	1.458555000	-0.720014000
1	3.458114000	3.994606000	1.268744000
1	-1.476048000	5.199067000	1.162222000
1	-1.867819000	4.347234000	2.631756000
1	-0.334987000	5.819634000	3.932035000
1	-1.473164000	6.801483000	3.006844000
1	0.261264000	7.036276000	1.188118000
1	0.818961000	7.722022000	2.714103000
1	2.179676000	5.793277000	3.210538000
1	2.545617000	6.244494000	1.554659000
1	-4.907675000	0.171669000	1.784075000
1	-5.134797000	1.121511000	4.097507000
1	-4.038116000	-0.203784000	4.440916000
1	-3.731064000	2.702526000	5.325059000
1	-3.902448000	1.270124000	6.340133000
1	-1.701756000	0.415700000	5.375316000
1	-1.506511000	1.914669000	6.284510000
1	-1.440460000	3.252795000	4.288280000
1	-0.314945000	1.935948000	4.041048000
6	4.721648000	-0.543269000	0.615424000
6	3.648341000	0.249299000	1.048035000
6	3.311252000	1.429059000	0.365741000
6	4.045085000	1.777574000	-0.777524000
6	5.117098000	0.978107000	-1.201198000
6	5.798057000	1.490848000	-2.443419000
6	4.745856000	1.575739000	-3.570413000
6	3.823126000	2.976120000	-1.670152000
6	3.575544000	2.481533000	-3.112323000
6	6.307094000	2.921134000	-2.156968000
6	5.212737000	-1.304315000	2.910521000
6	4.010161000	-0.456064000	3.398865000
6	2.966712000	-0.321478000	2.268053000
6	3.662732000	-2.615362000	1.454938000
1	5.220659000	1.975294000	-4.473781000
1	2.978244000	3.581973000	-1.332892000
1	2.626250000	1.943415000	-3.156927000
1	3.480538000	3.355093000	-3.767426000
1	7.094772000	2.883039000	-1.398528000
1	6.755784000	3.329914000	-3.069407000
1	6.139018000	-0.722798000	2.947805000

1	4.339393000	0.538851000	3.714172000
1	3.529403000	-0.926452000	4.263949000
1	2.131279000	0.298769000	2.601758000
1	3.488583000	-3.028917000	0.455511000
1	3.786647000	-3.468210000	2.132826000
1	5.355100000	-2.183628000	3.548639000
1	5.803387000	-2.350392000	1.085379000
6	4.954546000	-1.768811000	1.461442000
6	5.467898000	-0.169469000	-0.497091000
1	6.310311000	-0.778782000	-0.822648000
1	6.628486000	0.837975000	-2.735280000
1	4.374570000	0.574940000	-3.815348000
6	-4.960955000	-1.624224000	-1.963060000
6	-4.255095000	-1.148446000	-0.847485000
6	-3.935625000	0.212658000	-0.739991000
6	-4.277014000	1.069443000	-1.796979000
6	-4.953296000	0.575684000	-2.920367000
6	-5.252216000	1.627672000	-3.956790000
6	-6.117138000	2.722160000	-3.295602000
6	-4.024820000	2.556116000	-1.878364000
6	-5.387148000	3.266096000	-2.039973000
6	-3.185362000	2.834607000	-3.144306000
6	-3.970660000	-3.891551000	-1.811558000
6	-3.097278000	-3.321242000	-0.666912000
6	-3.890527000	-2.250848000	0.119200000
6	-6.066257000	-3.337192000	-0.578847000
1	-6.296537000	3.523525000	-4.021436000
1	-3.508642000	2.934272000	-0.992183000
1	-5.989658000	3.105006000	-1.140564000
1	-5.217166000	4.345348000	-2.126182000
1	-2.196375000	2.383188000	-3.028415000
1	-3.039417000	3.916924000	-3.238581000
1	-3.440846000	-3.831723000	-2.766728000
1	-2.189444000	-2.868525000	-1.073144000
1	-2.786394000	-4.114315000	0.023067000
1	-3.286366000	-1.880760000	0.952679000
1	-7.000641000	-2.767941000	-0.601486000
1	-6.333461000	-4.397583000	-0.508283000
1	-4.206368000	-4.948014000	-1.638103000
1	-5.884049000	-3.405953000	-2.755258000
6	-5.288052000	-3.093557000	-1.891041000
6	-5.310601000	-0.766112000	-2.998766000
1	-5.856876000	-1.140220000	-3.863482000
1	-5.770737000	1.194471000	-4.818895000
1	-7.092295000	2.304665000	-3.027128000
6	-3.916547000	2.269222000	-4.390025000
1	-4.119773000	3.062624000	-5.118446000

1	-3.299588000	1.518857000	-4.893322000
6	-5.191614000	-2.908701000	0.629348000
1	-4.928206000	-3.775767000	1.245811000
1	-5.738705000	-2.211793000	1.273304000
6	2.466982000	-1.732727000	1.892270000
1	1.735309000	-1.640996000	1.085180000
1	1.945480000	-2.175556000	2.749042000
6	5.125639000	3.807408000	-1.679620000
1	4.992644000	4.668211000	-2.344446000
1	5.319971000	4.202063000	-0.676750000
15	-0.192911000	0.362739000	-0.840595000
8	-0.620547000	-1.053785000	-0.942048000
8	0.636524000	0.952864000	-2.021416000
1	1.206829000	0.287798000	-2.549305000
6	2.877330000	-3.706284000	-4.420675000
6	4.026847000	-2.716584000	-4.239158000
6	4.045988000	-2.175968000	-2.807795000
6	2.699419000	-1.655154000	-2.373710000
6	1.477213000	-2.069184000	-3.080276000
6	1.522511000	-3.010699000	-4.263769000
8	2.063369000	-0.753191000	-3.305793000
1	2.932660000	-4.193989000	-5.399179000
1	2.967576000	-4.495759000	-3.662777000
1	4.987232000	-3.194371000	-4.457413000
1	3.911653000	-1.883736000	-4.944210000
1	4.792524000	-1.384177000	-2.695480000
1	4.322383000	-2.976185000	-2.106979000
1	2.612063000	-1.333213000	-1.331571000
1	0.543386000	-2.016593000	-2.528337000
1	0.726360000	-3.751344000	-4.139649000
1	1.284849000	-2.429791000	-5.163190000
6	-0.263091000	-4.165304000	3.358515000
6	-0.087590000	-4.869122000	4.544227000
6	0.703581000	-6.015489000	4.566365000
6	1.319884000	-6.457569000	3.397055000
6	1.145461000	-5.758972000	2.209302000
6	0.352011000	-4.607075000	2.179748000
6	0.167703000	-3.839021000	0.920017000
8	-0.560419000	-2.758322000	1.106737000
16	0.803258000	-4.275215000	-0.543383000
1	-0.874169000	-3.270381000	3.334089000
1	-0.568307000	-4.522125000	5.453687000
1	0.840789000	-6.562962000	5.494145000
1	1.937800000	-7.349849000	3.410780000
1	1.618025000	-6.092551000	1.291318000
1	-0.609146000	-2.202824000	0.279759000

Epoxide ring opening transition state involving thione form (**TS<sub>b</sub>**)

Number of imaginary frequencies : 1

Electronic energy= -3865.43528936 (hartree/particle)

Zero-point correction= 1.340811

Thermal correction to Energy= 1.404308

Thermal correction to Enthalpy= 1.405253

Thermal correction to Gibbs Free Energy= 1.242946

Sum of electronic and zero-point Energies= -3864.094478

Sum of electronic and thermal Energies= -3864.030981

Sum of electronic and thermal Enthalpies= -3864.030037

Sum of electronic and thermal Free Energies= -3864.192343

Coordinates

6	2.320316000	-2.280561000	-0.753107000
6	0.993181000	-1.873635000	-0.866557000
6	-0.016335000	-2.710284000	-1.348492000
6	0.287201000	-4.056163000	-1.622655000
6	1.619732000	-4.486861000	-1.533744000
6	2.608989000	-3.591839000	-1.123539000
6	-0.824366000	-5.057652000	-1.874732000
6	-0.342141000	-6.310441000	-2.601948000
6	0.868146000	-6.894209000	-1.877255000
6	2.026783000	-5.899771000	-1.909190000
6	-1.375812000	-2.121834000	-1.529321000
6	-1.993144000	-1.533946000	-0.426424000
6	-3.244517000	-0.922605000	-0.492777000
6	-3.863237000	-0.913103000	-1.740200000
6	-3.256676000	-1.431730000	-2.886566000
6	-1.990609000	-2.027037000	-2.794376000
6	-3.981380000	-1.284455000	-4.211561000
6	-3.350466000	-2.101229000	-5.335725000
6	-1.838161000	-1.898192000	-5.321262000
6	-1.250794000	-2.485497000	-4.039180000
8	0.659441000	-0.580245000	-0.494357000
8	-1.305982000	-1.536755000	0.782049000
1	3.641558000	-3.932363000	-1.062725000
1	-1.223806000	-5.352034000	-0.892880000
1	-1.661185000	-4.593122000	-2.399751000
1	-0.062954000	-6.056469000	-3.634113000
1	-1.154276000	-7.042603000	-2.658330000
1	0.592279000	-7.108530000	-0.836560000
1	1.179268000	-7.841848000	-2.329067000
1	2.446821000	-5.878812000	-2.925008000
1	2.837606000	-6.231602000	-1.251123000
1	-4.849319000	-0.458570000	-1.823529000
1	-5.034704000	-1.556998000	-4.077512000

1	-3.975150000	-0.222812000	-4.495790000
1	-3.571641000	-3.167324000	-5.192425000
1	-3.782115000	-1.808638000	-6.298346000
1	-1.616017000	-0.824199000	-5.374848000
1	-1.366895000	-2.368694000	-6.190200000
1	-1.277005000	-3.581184000	-4.117625000
1	-0.192128000	-2.219827000	-3.941718000
6	4.759718000	0.630793000	-0.591473000
6	3.719378000	-0.210391000	-1.011314000
6	3.378174000	-1.351077000	-0.269292000
6	4.078130000	-1.613300000	0.916352000
6	5.121119000	-0.769415000	1.327041000
6	5.774106000	-1.201890000	2.613722000
6	4.689940000	-1.244087000	3.711961000
6	3.849607000	-2.764551000	1.866506000
6	3.547857000	-2.193459000	3.269146000
6	6.315944000	-2.635860000	2.419134000
6	5.332602000	1.211065000	-2.916567000
6	4.140381000	0.342224000	-3.395434000
6	3.067814000	0.263743000	-2.286949000
6	3.716564000	2.621713000	-1.645897000
1	5.143474000	-1.585129000	4.649747000
1	3.024136000	-3.400492000	1.537490000
1	2.587532000	-1.674795000	3.240671000
1	3.444951000	-3.029548000	3.970273000
1	7.124431000	-2.623078000	1.681877000
1	6.745737000	-2.985926000	3.364496000
1	6.249317000	0.616063000	-2.861246000
1	4.475005000	-0.666441000	-3.655913000
1	3.683609000	0.772431000	-4.294064000
1	2.249156000	-0.391230000	-2.595502000
1	3.508234000	3.146762000	-0.707182000
1	3.859783000	3.390692000	-2.414768000
1	5.521168000	2.033824000	-3.615272000
1	5.841406000	2.411025000	-1.162085000
6	5.012906000	1.790653000	-1.521464000
6	5.473464000	0.342519000	0.568149000
1	6.295411000	0.985204000	0.882430000
1	6.584780000	-0.519159000	2.892779000
1	4.297981000	-0.236752000	3.889723000
6	-5.014749000	1.577674000	1.752377000
6	-4.262723000	1.042678000	0.696513000
6	-3.901363000	-0.312923000	0.696814000
6	-4.237219000	-1.094575000	1.811792000
6	-4.951602000	-0.537395000	2.881761000
6	-5.223888000	-1.511025000	3.999073000
6	-6.034082000	-2.692605000	3.424175000

6	-3.931341000	-2.558911000	2.018145000
6	-5.266928000	-3.306636000	2.224440000
6	-3.098635000	-2.695583000	3.311148000
6	-4.103646000	3.864460000	1.456444000
6	-3.168217000	3.235325000	0.394869000
6	-3.897040000	2.083036000	-0.337592000
6	-6.131979000	3.136293000	0.203566000
1	-6.188143000	-3.438636000	4.212260000
1	-3.388893000	-2.988259000	1.172572000
1	-5.864045000	-3.245228000	1.309281000
1	-5.055016000	-4.367250000	2.401302000
1	-2.126783000	-2.216411000	3.166003000
1	-2.911217000	-3.759127000	3.498730000
1	-3.608847000	3.903965000	2.431627000
1	-2.268263000	2.836919000	0.868644000
1	-2.849570000	3.983676000	-0.341734000
1	-3.248536000	1.670418000	-1.116081000
1	-7.040906000	2.527896000	0.238092000
1	-6.441993000	4.175270000	0.043929000
1	-4.370247000	4.893439000	1.187730000
1	-6.029470000	3.378808000	2.372614000
6	-5.392343000	3.023744000	1.555365000
6	-5.360673000	0.791125000	2.845250000
1	-5.940849000	1.211934000	3.665337000
1	-5.771144000	-1.028996000	4.816444000
1	-7.022977000	-2.341472000	3.113916000
6	-3.868056000	-2.057030000	4.497232000
1	-4.046878000	-2.792768000	5.289862000
1	-3.288586000	-1.240936000	4.939279000
6	-5.196862000	2.659563000	-0.940069000
1	-4.938600000	3.494037000	-1.603072000
1	-5.694909000	1.903439000	-1.556042000
6	2.537731000	1.686580000	-2.013607000
1	1.817921000	1.624798000	-1.193476000
1	1.995245000	2.058626000	-2.891032000
6	5.164862000	-3.569446000	1.958080000
1	5.027755000	-4.394418000	2.666005000
1	5.395634000	-4.014882000	0.984602000
15	-0.155267000	-0.403014000	0.909363000
8	-0.750883000	0.986218000	0.822149000
8	0.682272000	-0.753909000	2.100189000
1	1.492678000	0.244383000	2.946118000
6	2.450322000	4.355344000	3.643551000
6	3.657750000	3.421170000	3.722671000
6	3.751286000	2.542239000	2.473335000
6	2.464925000	1.799509000	2.192173000
6	1.199469000	2.474434000	2.516237000

6	1.150874000	3.553186000	3.559386000
8	2.037270000	1.020654000	3.330736000
1	2.411691000	5.017052000	4.514097000
1	2.539975000	4.996047000	2.756568000
1	4.580999000	3.999078000	3.828646000
1	3.572801000	2.782355000	4.610566000
1	4.553619000	1.804723000	2.564695000
1	3.976073000	3.156399000	1.591121000
1	2.482842000	1.206917000	1.270123000
1	0.281982000	1.999972000	2.186735000
1	0.286603000	4.190423000	3.354027000
1	0.951474000	3.049251000	4.513330000
6	-0.780161000	4.283202000	-3.096904000
6	-0.781327000	5.081308000	-4.234496000
6	0.186283000	6.071200000	-4.393810000
6	1.154316000	6.265498000	-3.410131000
6	1.150514000	5.481550000	-2.262934000
6	0.181662000	4.486137000	-2.099103000
6	0.152687000	3.617599000	-0.891986000
8	-0.515253000	2.534268000	-1.065382000
16	0.926788000	4.096332000	0.527506000
1	-1.524250000	3.505390000	-2.963555000
1	-1.536874000	4.930132000	-4.998875000
1	0.187554000	6.690202000	-5.285870000
1	1.913549000	7.030495000	-3.537111000
1	1.898409000	5.626507000	-1.490619000
1	-0.576366000	1.873914000	-0.234955000

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### TS<sub>b</sub>'

Number of imaginary frequencies : 1

Electronic energy= -3865.43267349 (hartree/particle)

Zero-point correction= 1.340339

Thermal correction to Energy= 1.403566

Thermal correction to Enthalpy= 1.404511

Thermal correction to Gibbs Free Energy= 1.243536

Sum of electronic and zero-point Energies= -3864.092334

Sum of electronic and thermal Energies= -3864.029107

Sum of electronic and thermal Enthalpies= -3864.028163

Sum of electronic and thermal Free Energies= -3864.189137

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### Coordinates

6	3.663081000	0.608250000	-0.218807000
6	2.463981000	1.261546000	0.059763000
6	2.223486000	2.591828000	-0.290518000
6	3.197109000	3.287846000	-1.029238000
6	4.434156000	2.671278000	-1.276426000

6	4.649243000	1.358475000	-0.855542000
6	2.871355000	4.623242000	-1.670861000
6	4.116735000	5.448535000	-1.983317000
6	5.102367000	4.607279000	-2.791407000
6	5.566875000	3.406757000	-1.969142000
6	0.924257000	3.190148000	0.134178000
6	-0.256727000	2.545915000	-0.239066000
6	-1.515714000	2.979522000	0.174455000
6	-1.550167000	4.127097000	0.963451000
6	-0.395040000	4.777847000	1.399102000
6	0.861871000	4.289915000	1.013783000
6	-0.548601000	5.961751000	2.335973000
6	0.758719000	6.710715000	2.578771000
6	1.872425000	5.705587000	2.857067000
6	2.135301000	4.870840000	1.605106000
8	1.454005000	0.555278000	0.697747000
8	-0.162184000	1.409016000	-1.032297000
1	5.609951000	0.887438000	-1.058114000
1	2.345923000	4.409631000	-2.613349000
1	2.161156000	5.189964000	-1.065907000
1	4.592168000	5.772885000	-1.047023000
1	3.835327000	6.352634000	-2.533076000
1	4.6064444000	4.260341000	-3.707292000
1	5.967889000	5.202585000	-3.100267000
1	6.270239000	3.756420000	-1.200000000
1	6.127123000	2.704439000	-2.596499000
1	-2.520696000	4.501771000	1.285416000
1	-1.314269000	6.637839000	1.937949000
1	-0.934561000	5.596088000	3.297612000
1	1.022077000	7.301608000	1.691350000
1	0.638523000	7.413716000	3.409323000
1	1.571248000	5.051778000	3.686089000
1	2.794751000	6.210282000	3.162251000
1	2.646826000	5.506941000	0.869782000
1	2.829596000	4.051983000	1.824552000
6	3.958783000	-2.604399000	1.792392000
6	3.745486000	-1.258720000	1.462808000
6	3.856254000	-0.824919000	0.131981000
6	4.176848000	-1.767326000	-0.857219000
6	4.414887000	-3.106839000	-0.511928000
6	4.801671000	-3.974017000	-1.681406000
6	3.661707000	-3.940349000	-2.721167000
6	4.314242000	-1.519682000	-2.341671000
6	3.353841000	-2.467908000	-3.093948000
6	6.057531000	-3.354213000	-2.334193000
6	4.930968000	-2.032450000	3.978430000
6	4.712272000	-0.539876000	3.617422000

6	3.492513000	-0.396912000	2.677530000
6	2.477736000	-2.426347000	3.787767000
1	3.971201000	-4.511401000	-3.604359000
1	4.087611000	-0.483399000	-2.601807000
1	2.321696000	-2.199774000	-2.852637000
1	3.480921000	-2.306316000	-4.170688000
1	6.891716000	-3.391531000	-1.627015000
1	6.343156000	-3.955988000	-3.204316000
1	5.925916000	-2.366155000	3.668680000
1	5.599320000	-0.125547000	3.128677000
1	4.533085000	0.055055000	4.520182000
1	3.347125000	0.652270000	2.411224000
1	1.686945000	-3.054115000	3.365097000
1	2.443790000	-2.570333000	4.873749000
1	4.858446000	-2.188398000	5.060817000
1	4.014563000	-3.953004000	3.478765000
6	3.857342000	-2.888366000	3.270105000
6	4.305978000	-3.526763000	0.808005000
1	4.500792000	-4.566479000	1.070998000
1	5.003148000	-5.001650000	-1.359092000
1	2.773831000	-4.425648000	-2.307261000
6	-4.830291000	1.184189000	0.602616000
6	-3.590025000	1.772184000	0.888092000
6	-2.766252000	2.238648000	-0.149056000
6	-3.178108000	2.033355000	-1.472982000
6	-4.408128000	1.418986000	-1.746605000
6	-4.689449000	1.263426000	-3.218886000
6	-4.699694000	2.665864000	-3.864884000
6	-2.447516000	2.456658000	-2.724589000
6	-3.376671000	3.397969000	-3.523263000
6	-2.187753000	1.201069000	-3.584631000
6	-4.783940000	-0.232669000	2.640855000
6	-3.360883000	0.329702000	2.878854000
6	-3.285225000	1.786784000	2.368120000
6	-5.781256000	2.050831000	2.702080000
1	-4.818349000	2.557969000	-4.949386000
1	-1.506207000	2.962069000	-2.497940000
1	-3.574096000	4.298903000	-2.934115000
1	-2.861641000	3.715372000	-4.436981000
1	-1.468085000	0.552892000	-3.077109000
1	-1.730168000	1.512636000	-4.530789000
1	-4.749000000	-1.190639000	2.113048000
1	-2.601752000	-0.269670000	2.367395000
1	-3.114252000	0.315607000	3.946555000
1	-2.294806000	2.199667000	2.573279000
1	-6.348992000	2.801760000	2.143946000
1	-6.364283000	1.799686000	3.595243000

1	-5.294962000	-0.419808000	3.592931000
1	-6.585487000	0.369109000	1.556479000
6	-5.610437000	0.787622000	1.829274000
6	-5.250212000	1.024593000	-0.712401000
1	-6.219334000	0.575871000	-0.928054000
1	-5.646690000	0.754775000	-3.385829000
1	-5.562713000	3.231148000	-3.500306000
6	-3.526206000	0.460364000	-3.842425000
1	-3.707643000	0.337812000	-4.916489000
1	-3.495711000	-0.543269000	-3.404657000
6	-4.382543000	2.598255000	3.092681000
1	-4.222400000	2.516790000	4.174091000
1	-4.298129000	3.659722000	2.836382000
6	2.252672000	-0.937175000	3.419449000
1	1.367215000	-0.808133000	2.789703000
1	2.091076000	-0.337246000	4.322262000
6	5.756261000	-1.889544000	-2.752400000
1	5.859372000	-1.765993000	-3.836533000
1	6.465977000	-1.200805000	-2.281902000
15	0.260567000	0.035486000	-0.276618000
8	-0.819835000	-0.450805000	0.663638000
8	0.771557000	-0.902513000	-1.333527000
1	1.244870000	-2.327817000	-0.952466000
6	-0.599576000	-6.030236000	-0.102943000
6	0.828943000	-5.944590000	0.438284000
6	1.002829000	-4.703887000	1.315801000
6	0.611541000	-3.437246000	0.591209000
6	-0.542705000	-3.514791000	-0.306895000
6	-0.941738000	-4.808836000	-0.957809000
8	1.256851000	-3.319567000	-0.695718000
1	-0.735877000	-6.937395000	-0.699602000
1	-1.304577000	-6.085192000	0.736368000
1	1.065799000	-6.838846000	1.022674000
1	1.544623000	-5.902120000	-0.392497000
1	2.035323000	-4.604263000	1.661187000
1	0.359877000	-4.775453000	2.203497000
1	0.686604000	-2.522620000	1.184131000
1	-0.903233000	-2.576722000	-0.713795000
1	-2.009243000	-4.766993000	-1.191252000
1	-0.409510000	-4.850072000	-1.916259000
6	-5.307753000	-2.202654000	-1.220815000
6	-6.560999000	-2.598481000	-1.673354000
6	-7.232409000	-3.645085000	-1.044201000
6	-6.645027000	-4.302548000	0.035794000
6	-5.386697000	-3.921470000	0.482131000
6	-4.711503000	-2.864806000	-0.140288000
6	-3.368370000	-2.434511000	0.323905000

8	-2.963572000	-1.327346000	-0.191164000
16	-2.447742000	-3.360267000	1.397429000
1	-4.780686000	-1.381084000	-1.692397000
1	-7.014927000	-2.087467000	-2.517152000
1	-8.213421000	-3.950263000	-1.395834000
1	-7.168028000	-5.115544000	0.529030000
1	-4.915554000	-4.430193000	1.316315000
1	-2.035070000	-0.954179000	0.196282000

**TS<sub>b</sub>\***

Number of imaginary frequencies : 1

Electronic energy= -3865.42649539 (hartree/particle)

Zero-point correction= 1.339050

Thermal correction to Energy= 1.403046

Thermal correction to Enthalpy= 1.403990

Thermal correction to Gibbs Free Energy= 1.238150

Sum of electronic and zero-point Energies= -3864.087445

Sum of electronic and thermal Energies= -3864.023449

Sum of electronic and thermal Enthalpies= -3864.022505

Sum of electronic and thermal Free Energies= -3864.188873

Coordinates

6	2.625617000	2.070431000	0.658304000
6	1.264506000	1.793240000	0.765023000
6	0.341277000	2.718426000	1.254217000
6	0.767583000	4.031781000	1.519986000
6	2.131492000	4.342615000	1.408508000
6	3.034384000	3.355216000	1.007387000
6	-0.247403000	5.123816000	1.800662000
6	0.358766000	6.320861000	2.526743000
6	1.596079000	6.806062000	1.774503000
6	2.666834000	5.716906000	1.766650000
6	-1.059823000	2.250354000	1.465042000
6	-1.753011000	1.725565000	0.376652000
6	-3.052903000	1.229593000	0.472014000
6	-3.638580000	1.266506000	1.734698000
6	-2.959437000	1.720842000	2.867738000
6	-1.648040000	2.201833000	2.744813000
6	-3.659680000	1.630162000	4.210484000
6	-2.929422000	2.380992000	5.320701000
6	-1.442308000	2.043401000	5.266315000
6	-0.837502000	2.583538000	3.971573000
8	0.806385000	0.537498000	0.395519000
8	-1.094352000	1.671089000	-0.847150000
1	4.094961000	3.595939000	0.950054000
1	-0.641579000	5.461274000	0.830725000

1	-1.109421000	4.728203000	2.341606000
1	0.641566000	6.031485000	3.548585000
1	-0.384846000	7.119946000	2.611944000
1	1.311752000	7.053281000	0.743459000
1	1.999138000	7.719380000	2.224149000
1	3.120337000	5.658530000	2.766409000
1	3.478656000	5.981297000	1.079818000
1	-4.659237000	0.901602000	1.840193000
1	-4.687531000	1.996316000	4.105526000
1	-3.740014000	0.570411000	4.490548000
1	-3.058193000	3.463462000	5.187398000
1	-3.360750000	2.122643000	6.293220000
1	-1.316402000	0.953513000	5.310352000
1	-0.909043000	2.464879000	6.124556000
1	-0.760761000	3.676584000	4.055272000
1	0.189374000	2.222434000	3.844872000
6	4.735862000	-1.082224000	0.756723000
6	3.785068000	-0.106003000	1.083751000
6	3.590041000	1.009803000	0.253778000
6	4.342217000	1.109685000	-0.922681000
6	5.288209000	0.123399000	-1.245717000
6	5.986509000	0.368788000	-2.557179000
6	4.900290000	0.442403000	-3.652101000
6	4.272429000	2.212853000	-1.950707000
6	3.918157000	1.595978000	-3.322222000
6	6.697465000	1.738340000	-2.489626000
6	5.218361000	-1.526954000	3.129516000
6	4.126621000	-0.492461000	3.509146000
6	3.073065000	-0.402460000	2.382146000
6	3.473873000	-2.860246000	1.949170000
1	5.377072000	0.599745000	-4.626288000
1	3.534050000	2.971159000	-1.677467000
1	2.882930000	1.249117000	-3.303051000
1	3.979912000	2.384744000	-4.080975000
1	7.530211000	1.686135000	-1.781786000
1	7.124560000	1.963436000	-3.473634000
1	6.197150000	-1.045279000	3.044117000
1	4.568750000	0.494264000	3.676589000
1	3.622675000	-0.782417000	4.438180000
1	2.326311000	0.358419000	2.622442000
1	3.216748000	-3.429207000	1.049924000
1	3.533267000	-3.581359000	2.772957000
1	5.304797000	-2.304212000	3.897143000
1	5.612239000	-2.915260000	1.487906000
6	4.851372000	-2.183183000	1.780295000
6	5.498451000	-0.962025000	-0.402287000
1	6.246259000	-1.715369000	-0.649757000

1	6.705912000	-0.428163000	-2.775775000
1	4.364881000	-0.511976000	-3.701015000
6	-5.087251000	-1.065706000	-1.771818000
6	-4.268984000	-0.618802000	-0.723976000
6	-3.792962000	0.700387000	-0.707168000
6	-4.092728000	1.534171000	-1.794434000
6	-4.877342000	1.063208000	-2.856214000
6	-5.099083000	2.083079000	-3.942592000
6	-5.798568000	3.308378000	-3.317310000
6	-3.675312000	2.974338000	-1.975115000
6	-4.952528000	3.830825000	-2.127134000
6	-2.868200000	3.077081000	-3.287595000
6	-4.346088000	-3.419562000	-1.556869000
6	-3.343887000	-2.896565000	-0.498851000
6	-3.963083000	-1.709041000	0.277046000
6	-6.283180000	-2.576876000	-0.232511000
1	-5.917077000	4.083564000	-4.083066000
1	-3.078138000	3.337005000	-1.134897000
1	-5.527860000	3.795341000	-1.196793000
1	-4.661157000	4.875259000	-2.286917000
1	-1.935104000	2.517232000	-3.181699000
1	-2.600075000	4.126666000	-3.455024000
1	-3.876723000	-3.463066000	-2.544378000
1	-2.420535000	-2.562004000	-0.977187000
1	-3.081079000	-3.689667000	0.213175000
1	-3.266843000	-1.363675000	1.047578000
1	-7.145806000	-1.903489000	-0.228682000
1	-6.665200000	-3.594225000	-0.091355000
1	-4.682086000	-4.434546000	-1.313967000
1	-6.251769000	-2.768025000	-2.408593000
6	-5.570275000	-2.483229000	-1.599715000
6	-5.392764000	-0.228186000	-2.838322000
1	-6.024627000	-0.580101000	-3.652563000
1	-5.704474000	1.667150000	-4.755356000
1	-6.802618000	3.026371000	-2.985812000
6	-3.718360000	2.534393000	-4.465994000
1	-3.860481000	3.303365000	-5.234054000
1	-3.217792000	1.688062000	-4.945749000
6	-5.289125000	-2.200416000	0.898593000
1	-5.078110000	-3.069046000	1.534789000
1	-5.714312000	-1.425325000	1.544905000
6	2.398706000	-1.782379000	2.233297000
1	1.672672000	-1.724713000	1.417995000
1	1.834938000	-2.019195000	3.143064000
6	5.682547000	2.832873000	-2.065483000
1	5.657368000	3.645512000	-2.800011000
1	5.970160000	3.273765000	-1.105131000

15	-0.046830000	0.445093000	-0.997454000
8	-0.744643000	-0.894989000	-0.890915000
8	0.796028000	0.714606000	-2.204029000
1	1.521701000	-0.448599000	-2.950808000
6	2.023450000	-4.530051000	-3.705304000
6	3.324235000	-3.844461000	-3.289624000
6	3.153285000	-3.168712000	-1.925103000
6	1.850133000	-2.430936000	-1.802351000
6	0.940280000	-2.348623000	-2.950013000
6	0.910200000	-3.501026000	-3.939064000
8	1.896713000	-1.322190000	-3.317319000
1	2.168993000	-5.126537000	-4.610853000
1	1.718659000	-5.226527000	-2.912645000
1	4.143086000	-4.567352000	-3.228755000
1	3.603009000	-3.093174000	-4.037154000
1	3.955607000	-2.453271000	-1.716197000
1	3.190483000	-3.916620000	-1.124772000
1	1.731951000	-1.701655000	-1.005186000
1	-0.034690000	-1.920340000	-2.725035000
1	-0.070592000	-3.982043000	-3.880958000
1	0.998180000	-3.056590000	-4.936858000
6	-1.771621000	-4.036175000	2.892156000
6	-2.161469000	-4.847895000	3.950180000
6	-1.469995000	-6.028294000	4.214791000
6	-0.390508000	-6.399917000	3.415287000
6	-0.005816000	-5.599748000	2.346441000
6	-0.694944000	-4.412985000	2.078932000
6	-0.320539000	-3.526335000	0.945579000
8	-0.757127000	-2.327988000	1.069214000
16	0.573019000	-4.120813000	-0.358797000
1	-2.296995000	-3.110955000	2.678069000
1	-3.004802000	-4.559365000	4.569524000
1	-1.771384000	-6.658824000	5.045814000
1	0.152685000	-7.315588000	3.625883000
1	0.832540000	-5.880178000	1.717460000
1	-0.675172000	-1.691019000	0.201460000

### TS<sub>b</sub>'\*

Number of imaginary frequencies : 1

Electronic energy= -3865.42922347 (hartree/particle)

Zero-point correction= 1.339618

Thermal correction to Energy= 1.403106

Thermal correction to Enthalpy= 1.404050

Thermal correction to Gibbs Free Energy= 1.240759

Sum of electronic and zero-point Energies= -3864.089606

Sum of electronic and thermal Energies= -3864.026117

Sum of electronic and thermal Enthalpies= -3864.025173

Sum of electronic and thermal Free Energies= -3864.188464

Coordinates

6	-3.735566000	0.264061000	0.077289000
6	-2.615208000	1.060015000	-0.152566000
6	-2.536702000	2.404172000	0.215984000
6	-3.617950000	2.976152000	0.910016000
6	-4.788833000	2.222371000	1.089759000
6	-4.832075000	0.892932000	0.663209000
6	-3.474739000	4.329146000	1.581198000
6	-4.817145000	5.013511000	1.824335000
6	-5.748902000	4.061500000	2.570863000
6	-6.031582000	2.824620000	1.719916000
6	-1.287625000	3.144015000	-0.137142000
6	-0.060452000	2.620144000	0.276983000
6	1.163474000	3.190729000	-0.069873000
6	1.112354000	4.356961000	-0.829749000
6	-0.085555000	4.894009000	-1.304169000
6	-1.300234000	4.266307000	-0.991220000
6	-0.015544000	6.110748000	-2.208345000
6	-1.382127000	6.723062000	-2.502134000
6	-2.366239000	5.612517000	-2.855926000
6	-2.598486000	4.725159000	-1.634293000
8	-1.505623000	0.480050000	-0.746545000
8	-0.059312000	1.467355000	1.048990000
1	-5.739014000	0.313170000	0.828564000
1	-2.988108000	4.157974000	2.552718000
1	-2.792753000	4.975513000	1.026140000
1	-5.271390000	5.293953000	0.863588000
1	-4.666695000	5.937303000	2.392583000
1	-5.270714000	3.761578000	3.512433000
1	-6.690746000	4.555179000	2.831906000
1	-6.724366000	3.102038000	0.912517000
1	-6.546482000	2.060152000	2.312499000
1	2.050752000	4.839660000	-1.099402000
1	0.654521000	6.853374000	-1.759723000
1	0.452479000	5.811909000	-3.156768000
1	-1.749577000	7.260608000	-1.617699000
1	-1.297359000	7.454977000	-3.311768000
1	-1.957030000	5.014062000	-3.680632000
1	-3.321558000	6.023031000	-3.198342000
1	-3.208429000	5.287659000	-0.914471000
1	-3.191222000	3.843710000	-1.902240000
6	-3.385332000	-3.003148000	-1.845056000
6	-3.433168000	-1.632820000	-1.552427000
6	-3.703246000	-1.189811000	-0.247208000

6	-3.922296000	-2.150397000	0.753884000
6	-3.903129000	-3.519337000	0.443095000
6	-4.240951000	-4.411294000	1.610201000
6	-3.219059000	-4.172958000	2.741030000
6	-4.203051000	-1.896142000	2.217359000
6	-3.160189000	-2.658958000	3.064295000
6	-5.631322000	-3.985187000	2.132541000
6	-4.315076000	-2.660733000	-4.095319000
6	-4.366064000	-1.141462000	-3.784065000
6	-3.249224000	-0.771190000	-2.779732000
6	-1.846906000	-2.621766000	-3.775098000
1	-3.526553000	-4.750253000	3.620952000
1	-4.166216000	-0.831818000	2.459084000
1	-2.167443000	-2.246618000	2.866288000
1	-3.376306000	-2.480217000	4.123876000
1	-6.379826000	-4.152983000	1.352158000
1	-5.904765000	-4.615686000	2.986030000
1	-5.255117000	-3.146716000	-3.817262000
1	-5.339119000	-0.864188000	-3.367299000
1	-4.226559000	-0.554065000	-4.698727000
1	-3.296772000	0.293631000	-2.539851000
1	-0.977728000	-3.095415000	-3.307612000
1	-1.740829000	-2.776431000	-4.855000000
1	-4.162469000	-2.835936000	-5.166301000
1	-3.114631000	-4.382840000	-3.485566000
6	-3.151796000	-3.301960000	-3.305506000
6	-3.628179000	-3.947774000	-0.850740000
1	-3.620256000	-5.011894000	-1.087049000
1	-4.249496000	-5.464644000	1.308817000
1	-2.235862000	-4.537685000	2.432595000
6	4.631582000	1.694734000	-0.436196000
6	3.359243000	2.197468000	-0.744103000
6	2.464907000	2.554377000	0.278930000
6	2.845358000	2.322097000	1.608478000
6	4.108664000	1.788707000	1.902087000
6	4.345932000	1.568148000	3.373078000
6	4.224361000	2.922123000	4.103792000
6	2.042625000	2.625849000	2.851526000
6	2.875473000	3.588041000	3.728223000
6	1.847043000	1.313635000	3.643423000
6	4.768773000	0.354546000	-2.516155000
6	3.312892000	0.809911000	-2.783223000
6	3.103488000	2.240142000	-2.232929000
6	5.578847000	2.712273000	-2.470954000
1	4.287834000	2.750646000	5.184731000
1	1.075257000	3.074104000	2.613547000
1	3.043734000	4.521690000	3.182517000

1	2.302665000	3.838202000	4.628184000
1	1.173094000	0.649432000	3.096175000
1	1.360172000	1.552194000	4.596213000
1	4.793767000	-0.617204000	-2.014289000
1	2.591647000	0.137116000	-2.309213000
1	3.097893000	0.807591000	-3.857781000
1	2.090681000	2.579330000	-2.461823000
1	6.067287000	3.486242000	-1.870816000
1	6.207921000	2.538356000	-3.351333000
1	5.322134000	0.238490000	-3.455681000
1	6.479022000	1.061825000	-1.352316000
6	5.482826000	1.410271000	-1.646283000
6	5.013867000	1.503915000	0.885934000
1	6.006182000	1.119521000	1.121189000
1	5.330701000	1.119167000	3.549057000
1	5.065729000	3.565545000	3.829595000
6	3.223100000	0.641106000	3.887667000
1	3.378183000	0.437685000	4.953435000
1	3.278550000	-0.318211000	3.361508000
6	4.154252000	3.160637000	-2.891924000
1	4.036158000	3.105269000	-3.980372000
1	3.975637000	4.202080000	-2.603831000
6	-1.893574000	-1.111165000	-3.432313000
1	-1.081910000	-0.830921000	-2.755286000
1	-1.777403000	-0.506703000	-4.339076000
6	-5.593339000	-2.488120000	2.543295000
1	-5.781964000	-2.375176000	3.617034000
1	-6.373192000	-1.925553000	2.019075000
15	-0.327177000	0.061687000	0.287833000
8	0.817497000	-0.337868000	-0.619489000
8	-0.796312000	-0.900648000	1.338881000
1	-0.972010000	-2.421318000	1.048645000
6	1.313536000	-5.854474000	0.456277000
6	0.006170000	-5.889162000	-0.335274000
6	-0.076298000	-4.687897000	-1.282500000
6	0.337047000	-3.399665000	-0.624268000
6	0.713274000	-3.398753000	0.793425000
6	1.369238000	-4.633549000	1.384132000
8	-0.726832000	-3.402662000	0.912522000
1	1.435943000	-6.768867000	1.044317000
1	2.152585000	-5.810533000	-0.249582000
1	-0.066335000	-6.810242000	-0.921114000
1	-0.850318000	-5.865360000	0.348719000
1	-1.095074000	-4.550645000	-1.659257000
1	0.566800000	-4.843336000	-2.156034000
1	0.068877000	-2.445837000	-1.068391000
1	1.120508000	-2.459920000	1.166954000

1	2.408690000	-4.390862000	1.629182000
1	0.852748000	-4.836315000	2.329472000
6	5.432883000	-1.869945000	1.003494000
6	6.717367000	-2.193978000	1.423817000
6	7.417257000	-3.225615000	0.800826000
6	6.827645000	-3.939456000	-0.241201000
6	5.541449000	-3.625886000	-0.660175000
6	4.837060000	-2.585414000	-0.043571000
6	3.464132000	-2.215310000	-0.477712000
8	2.984803000	-1.191115000	0.132965000
16	2.634792000	-3.094642000	-1.659054000
1	4.880932000	-1.063274000	1.473140000
1	7.173623000	-1.639200000	2.238215000
1	8.422339000	-3.474973000	1.127715000
1	7.371233000	-4.742937000	-0.727778000
1	5.071984000	-4.176971000	-1.467917000
1	2.028822000	-0.834840000	-0.211078000

Product complex (**3b**)

Number of imaginary frequencies : 0

Electronic energy= -3865.49410501 (hartree/particle)

Zero-point correction= 1.343016

Thermal correction to Energy= 1.406543

Thermal correction to Enthalpy= 1.407487

Thermal correction to Gibbs Free Energy= 1.244122

Sum of electronic and zero-point Energies= -3864.151089

Sum of electronic and thermal Energies= -3864.087562

Sum of electronic and thermal Enthalpies= -3864.086618

Sum of electronic and thermal Free Energies= -3864.249983

Coordinates

6	1.178427000	3.043275000	0.556964000
6	0.009811000	2.297341000	0.688790000
6	-1.260966000	2.874911000	0.757703000
6	-1.385907000	4.265241000	0.583522000
6	-0.223665000	5.048231000	0.501277000
6	1.025470000	4.428689000	0.509853000
6	-2.745021000	4.895642000	0.339460000
6	-2.772329000	6.389814000	0.651149000
6	-1.628283000	7.090298000	-0.078496000
6	-0.285332000	6.562203000	0.421979000
6	-2.439507000	1.985728000	0.975511000
6	-2.658850000	0.932593000	0.091199000
6	-3.739329000	0.057240000	0.194720000
6	-4.612227000	0.279942000	1.255082000
6	-4.394735000	1.272763000	2.213841000

6	-3.288273000	2.124160000	2.094915000
6	-5.354337000	1.359181000	3.385440000
6	-5.167748000	2.620829000	4.223734000
6	-3.681035000	2.829597000	4.497283000
6	-2.952578000	3.125225000	3.187319000
8	0.109605000	0.912424000	0.769846000
8	-1.732911000	0.721986000	-0.933347000
1	1.922259000	5.041400000	0.433531000
1	-2.976358000	4.756250000	-0.727124000
1	-3.533419000	4.366300000	0.877015000
1	-2.667527000	6.546589000	1.733964000
1	-3.738604000	6.811506000	0.355757000
1	-1.723144000	6.899802000	-1.155399000
1	-1.676806000	8.175031000	0.061810000
1	-0.097817000	6.967143000	1.426541000
1	0.531813000	6.926148000	-0.210715000
1	-5.479142000	-0.371643000	1.354390000
1	-6.382572000	1.288878000	3.012260000
1	-5.201482000	0.479364000	4.026130000
1	-5.559497000	3.491855000	3.681352000
1	-5.736499000	2.538806000	5.155424000
1	-3.266900000	1.922883000	4.957633000
1	-3.518756000	3.651838000	5.201404000
1	-3.214042000	4.143670000	2.869219000
1	-1.867699000	3.131253000	3.340516000
6	4.354976000	1.059029000	1.259697000
6	3.056082000	1.570210000	1.395174000
6	2.519625000	2.413159000	0.410311000
6	3.290186000	2.688192000	-0.730898000
6	4.586329000	2.167084000	-0.856916000
6	5.278428000	2.561865000	-2.136187000
6	4.442194000	2.056808000	-3.332832000
6	2.864803000	3.472959000	-1.950301000
6	2.978464000	2.530707000	-3.168565000
6	5.305462000	4.104735000	-2.196269000
6	4.702967000	0.993764000	3.708961000
6	3.274241000	1.575649000	3.862021000
6	2.392106000	1.125136000	2.676438000
6	3.777527000	-0.988793000	2.497681000
1	4.882536000	2.451648000	-4.256344000
1	1.841396000	3.843775000	-1.861330000
1	2.317719000	1.672633000	-3.016849000
1	2.634222000	3.061773000	-4.063416000
1	5.885793000	4.492265000	-1.353018000
1	5.813324000	4.422041000	-3.113875000
1	5.447931000	1.794967000	3.686101000
1	3.302824000	2.669027000	3.897314000

1	2.813957000	1.234588000	4.796417000
1	1.385536000	1.536086000	2.782142000
1	3.851218000	-1.588608000	1.583010000
1	4.046051000	-1.644728000	3.334960000
1	4.953311000	0.343748000	4.555185000
1	5.799816000	-0.203470000	2.245844000
6	4.784681000	0.176950000	2.403111000
6	5.126963000	1.370470000	0.146186000
1	6.138479000	0.977399000	0.052313000
1	6.296229000	2.156656000	-2.172517000
1	4.469085000	0.965614000	-3.390772000
6	-4.345818000	-3.432328000	-1.176150000
6	-4.034889000	-2.387759000	-0.293802000
6	-3.952871000	-1.065955000	-0.758993000
6	-4.134579000	-0.824494000	-2.128688000
6	-4.421285000	-1.881457000	-3.004536000
6	-4.605293000	-1.448909000	-4.435649000
6	-5.765175000	-0.430863000	-4.482902000
6	-4.095270000	0.513114000	-2.828877000
6	-5.462792000	0.738681000	-3.511540000
6	-3.014233000	0.449248000	-3.929573000
6	-3.096740000	-5.110547000	0.148663000
6	-2.687108000	-3.945361000	1.084515000
6	-3.801827000	-2.874588000	1.118344000
6	-5.509535000	-4.672493000	0.612120000
1	-5.879307000	-0.065816000	-5.509961000
1	-3.883184000	1.332421000	-2.137525000
1	-6.242541000	0.821653000	-2.748066000
1	-5.435368000	1.693273000	-4.049215000
1	-2.030645000	0.335163000	-3.466451000
1	-3.009209000	1.400865000	-4.473241000
1	-2.340588000	-5.268501000	-0.625722000
1	-1.758602000	-3.485212000	0.739267000
1	-2.513871000	-4.308266000	2.104830000
1	-3.511795000	-2.058950000	1.785464000
1	-6.484954000	-4.449227000	0.169431000
1	-5.597702000	-5.640260000	1.118777000
1	-3.190283000	-6.049211000	0.706990000
1	-4.733549000	-5.554421000	-1.228966000
6	-4.452186000	-4.779104000	-0.508266000
6	-4.539481000	-3.182744000	-2.530051000
1	-4.781085000	-3.997365000	-3.211132000
1	-4.819970000	-2.307268000	-5.081370000
1	-6.700566000	-0.929633000	-4.211415000
6	-3.317483000	-0.730265000	-4.891347000
1	-3.451827000	-0.373473000	-5.918893000
1	-2.487057000	-1.442243000	-4.901969000

6	-5.093492000	-3.562315000	1.614102000
1	-4.911224000	-3.985579000	2.608736000
1	-5.892290000	-2.821269000	1.723474000
6	2.345061000	-0.419817000	2.676696000
1	1.683848000	-0.764632000	1.874231000
1	1.910019000	-0.763111000	3.622786000
6	3.851055000	4.644276000	-2.157197000
1	3.600197000	5.151050000	-3.096232000
1	3.733761000	5.381199000	-1.355192000
15	-0.353275000	0.028573000	-0.498088000
8	-0.796613000	-1.310045000	0.206405000
8	0.603905000	-0.063960000	-1.612699000
1	2.088885000	-0.632817000	-2.572566000
6	5.260290000	-3.595252000	-3.144064000
6	5.638863000	-2.115141000	-3.069243000
6	5.060526000	-1.464074000	-1.811859000
6	3.542182000	-1.612743000	-1.745147000
6	3.119802000	-3.095724000	-1.860310000
6	3.739670000	-3.760025000	-3.091954000
8	2.983091000	-0.917826000	-2.838745000
1	5.648310000	-4.047462000	-4.063168000
1	5.725078000	-4.136975000	-2.306861000
1	6.727841000	-1.997338000	-3.086099000
1	5.242080000	-1.596082000	-3.950705000
1	5.292418000	-0.396208000	-1.789418000
1	5.506312000	-1.913326000	-0.913450000
1	3.168057000	-1.196132000	-0.796055000
1	2.029359000	-3.146433000	-1.908954000
1	3.449437000	-4.814998000	-3.137888000
1	3.296421000	-3.255771000	-3.958631000
6	1.173656000	-3.622146000	2.915271000
6	1.167807000	-3.951927000	4.264779000
6	2.242138000	-4.648305000	4.814898000
6	3.322499000	-5.016760000	4.014743000
6	3.333933000	-4.686186000	2.664951000
6	2.257955000	-3.987239000	2.111045000
6	2.226069000	-3.563424000	0.683516000
8	1.302798000	-2.904556000	0.232229000
16	3.584246000	-4.031297000	-0.346796000
1	0.349698000	-3.070091000	2.473561000
1	0.326929000	-3.663501000	4.887251000
1	2.239355000	-4.903739000	5.870202000
1	4.159744000	-5.556422000	4.445290000
1	4.185619000	-4.961195000	2.050117000
1	-0.069208000	-1.976408000	0.236280000

.....  
Thiol form of thiobenzoic acid

Number of imaginary frequencies : 0  
 Electronic energy= -743.586857777 (hartree/particle)  
 Zero-point correction= 0.111206  
 Thermal correction to Energy= 0.119039  
 Thermal correction to Enthalpy= 0.119984  
 Thermal correction to Gibbs Free Energy= 0.077293  
 Sum of electronic and zero-point Energies= -743.475652  
 Sum of electronic and thermal Energies= -743.467818  
 Sum of electronic and thermal Enthalpies= -743.466874  
 Sum of electronic and thermal Free Energies= -743.509565

Coordinates

6	-0.589678000	-1.131529000	-0.000053000
6	-1.953387000	-1.403999000	-0.000025000
6	-2.873303000	-0.358096000	0.000062000
6	-2.431274000	0.963858000	0.000120000
6	-1.069956000	1.239707000	0.000090000
6	-0.145488000	0.191722000	0.000004000
6	1.300057000	0.563366000	-0.000021000
8	1.689897000	1.702327000	0.000007000
16	2.468531000	-0.818210000	-0.000077000
1	0.119361000	-1.954643000	-0.000124000
1	-2.297808000	-2.433015000	-0.000070000
1	-3.937377000	-0.573961000	0.000085000
1	-3.148570000	1.778439000	0.000189000
1	-0.698714000	2.259234000	0.000134000
1	3.525609000	0.006517000	-0.000101000

Thione form of thiobenzoic acid

Number of imaginary frequencies : 0  
 Electronic energy= -743.585397778 (hartree/particle)  
 Zero-point correction= 0.114708  
 Thermal correction to Energy= 0.122086  
 Thermal correction to Enthalpy= 0.123030  
 Thermal correction to Gibbs Free Energy= 0.081476  
 Sum of electronic and zero-point Energies= -743.470690  
 Sum of electronic and thermal Energies= -743.463312  
 Sum of electronic and thermal Enthalpies= -743.462368  
 Sum of electronic and thermal Free Energies= -743.503921

Coordinates

6	-0.986992000	1.219984000	0.000230000
6	-2.362279000	1.020336000	0.000339000
6	-2.880887000	-0.272196000	0.000064000
6	-2.019980000	-1.368843000	-0.000205000
6	-0.645507000	-1.175522000	-0.000294000

6	-0.117680000	0.120970000	-0.000231000
6	1.345548000	0.334037000	-0.000263000
8	1.659622000	1.632983000	-0.000548000
16	2.503221000	-0.831723000	0.000341000
1	-0.580276000	2.224462000	0.000592000
1	-3.955684000	-0.426293000	0.000050000
1	-2.421580000	-2.377054000	-0.000345000
1	0.034606000	-2.020725000	-0.000370000
1	2.631213000	1.694979000	0.000438000
1	-3.030129000	1.875744000	0.000726000

### Epoxide

Number of imaginary frequencies : 0

Electronic energy= -309.709928188 (hartree/particle)

Zero-point correction= 0.154003

Thermal correction to Energy= 0.159921

Thermal correction to Enthalpy= 0.160865

Thermal correction to Gibbs Free Energy= 0.124467

Sum of electronic and zero-point Energies= -309.555926

Sum of electronic and thermal Energies= -309.550007

Sum of electronic and thermal Enthalpies= -309.549063

Sum of electronic and thermal Free Energies= -309.585461

### Coordinates

6	1.544868000	0.552874000	-0.185413000
6	1.256118000	-0.808089000	0.449298000
6	0.116364000	-1.509368000	-0.293450000
6	-1.098765000	-0.620703000	-0.412424000
6	-0.978250000	0.844107000	-0.289678000
6	0.358840000	1.511417000	-0.029920000
8	-1.490594000	0.048758000	0.776023000
1	2.442031000	1.002446000	0.252426000
1	1.753878000	0.404127000	-1.253501000
1	2.150475000	-1.438878000	0.428130000
1	0.975082000	-0.673669000	1.500191000
1	-0.166913000	-2.437669000	0.216340000
1	0.443467000	-1.784459000	-1.304823000
1	-1.932422000	-1.020528000	-0.991858000
1	-1.740702000	1.458163000	-0.769748000
1	0.473892000	2.365254000	-0.705952000
1	0.330910000	1.913722000	0.990138000

### TRIP-TS<sub>b</sub>

Number of imaginary frequencies : 1

Electronic energy= -3634.41871713 (hartree/particle)

Zero-point correction= 1.234703  
 Thermal correction to Energy= 1.303295  
 Thermal correction to Enthalpy= 1.304239  
 Thermal correction to Gibbs Free Energy= 1.129114  
 Sum of electronic and zero-point Energies= -3633.184014  
 Sum of electronic and thermal Energies= -3633.115422  
 Sum of electronic and thermal Enthalpies= -3633.114478  
 Sum of electronic and thermal Free Energies= -3633.289603

Coordinates

6	2.270989000	2.540500000	0.265817000
6	0.939707000	2.095740000	0.471515000
6	-0.107944000	2.935370000	0.786045000
6	0.150348000	4.344827000	0.848756000
6	1.489578000	4.805375000	0.708625000
6	2.527715000	3.877255000	0.436235000
6	-0.879698000	5.309384000	1.019078000
6	-0.585512000	6.647442000	1.091509000
6	0.751533000	7.098713000	0.996834000
6	1.762949000	6.195088000	0.803897000
6	-1.460425000	2.352264000	0.997173000
6	-1.988299000	1.513533000	0.037558000
6	-3.282210000	0.932238000	0.122724000
6	-4.038636000	1.240067000	1.226172000
6	-3.534254000	2.041262000	2.282644000
6	-2.223514000	2.586880000	2.187942000
6	-4.308663000	2.288251000	3.446614000
6	-3.799245000	3.017849000	4.488586000
6	-2.480515000	3.524004000	4.414119000
6	-1.713141000	3.314683000	3.296571000
8	0.713316000	0.734909000	0.395283000
8	-1.244222000	1.248786000	-1.102210000
1	3.546396000	4.243510000	0.337576000
1	-1.909996000	4.975786000	1.081821000
1	-1.387346000	7.368521000	1.216094000
1	0.969448000	8.160097000	1.061940000
1	2.793173000	6.527515000	0.705375000
1	-5.049075000	0.846901000	1.303590000
1	-5.312834000	1.874996000	3.496890000
1	-4.397774000	3.199029000	5.375968000
1	-2.069680000	4.078374000	5.252345000
1	-0.699270000	3.697803000	3.255691000
6	4.934629000	-0.135679000	0.473171000
6	3.892709000	0.713769000	0.847235000
6	3.337972000	1.568934000	-0.121940000

6	3.787157000	1.522104000	-1.457019000
6	4.830773000	0.653373000	-1.780929000
6	3.185500000	2.403171000	-2.543626000
6	3.040273000	1.682728000	-3.888253000
6	4.523512000	1.123711000	3.249193000
6	3.407055000	0.697159000	2.288801000
1	2.179892000	2.691697000	-2.221096000
1	2.519988000	0.729742000	-3.776023000
1	2.457173000	2.306196000	-4.573186000
1	4.909871000	2.113112000	2.985366000
1	4.150325000	1.161644000	4.277775000
1	2.594818000	1.424000000	2.387667000
6	5.426010000	-0.173248000	-0.830672000
6	-4.527106000	-2.121261000	-1.737089000
6	-3.977192000	-1.334301000	-0.722370000
6	-3.795348000	0.041430000	-0.962685000
6	-4.117469000	0.590170000	-2.219713000
6	-4.651134000	-0.241263000	-3.202329000
6	-3.932378000	2.065676000	-2.540819000
6	-5.287387000	2.744218000	-2.777854000
6	-2.996959000	2.266112000	-3.737945000
6	-2.844963000	-3.311065000	0.402381000
6	-3.606760000	-1.995519000	0.598954000
1	-3.471405000	2.557344000	-1.679372000
1	-5.942437000	2.628636000	-1.908463000
1	-5.152412000	3.813972000	-2.969606000
1	-2.028505000	1.791619000	-3.558577000
1	-2.832120000	3.334263000	-3.914904000
1	-1.956986000	-3.161649000	-0.218373000
1	-2.533660000	-3.707955000	1.375833000
1	-2.942930000	-1.316139000	1.144779000
6	-4.873125000	-1.598769000	-2.978575000
6	-4.854331000	-2.248010000	1.456325000
1	-4.576853000	-2.714917000	2.408520000
1	-5.395923000	-1.322713000	1.672830000
6	2.840942000	-0.674312000	2.673388000
1	1.981457000	-0.929358000	2.045876000
1	2.500868000	-0.672455000	3.714650000
6	4.023532000	3.675110000	-2.734819000
1	3.594865000	4.300462000	-3.525139000
1	4.076002000	4.272086000	-1.820736000
15	-0.056577000	0.160752000	-0.929530000
8	-0.586112000	-1.179364000	-0.473279000
8	0.808950000	0.219001000	-2.147984000
1	1.904198000	-0.922757000	-2.332619000
6	3.236647000	-4.604423000	-2.410810000
6	3.707623000	-4.555664000	-0.955518000

6	3.609261000	-3.136327000	-0.391555000
6	2.284357000	-2.488945000	-0.662800000
6	1.528939000	-2.821166000	-1.873529000
6	1.776637000	-4.161695000	-2.521080000
8	2.428625000	-1.794234000	-2.366706000
1	3.863852000	-3.946621000	-3.024556000
1	3.343959000	-5.617067000	-2.811143000
1	3.094914000	-5.235712000	-0.349512000
1	4.743801000	-4.898927000	-0.873328000
1	4.357396000	-2.487301000	-0.858977000
1	3.800196000	-3.104533000	0.685023000
1	2.003170000	-1.595253000	-0.112669000
1	0.490560000	-2.495626000	-1.877654000
1	1.122920000	-4.885178000	-2.017385000
1	1.456740000	-4.103794000	-3.566427000
6	-1.493957000	-2.926379000	4.115273000
6	-1.943420000	-3.402701000	5.340703000
6	-1.309494000	-4.487802000	5.941925000
6	-0.224269000	-5.097873000	5.314803000
6	0.224497000	-4.630892000	4.085745000
6	-0.407965000	-3.541780000	3.477966000
6	0.020025000	-3.023187000	2.151942000
8	-0.485325000	-1.874089000	1.870071000
16	1.041138000	-3.904230000	1.144734000
1	-1.978877000	-2.081674000	3.637486000
1	-2.789238000	-2.926711000	5.826466000
1	-1.660910000	-4.858877000	6.899964000
1	0.272590000	-5.940261000	5.785265000
1	1.065945000	-5.101380000	3.588261000
1	-0.432343000	-1.575567000	0.852036000
1	5.360691000	0.417384000	3.221708000
1	3.597634000	-1.461598000	2.572703000
1	5.379825000	-0.794411000	1.219351000
1	5.180695000	0.619010000	-2.808583000
1	5.047920000	3.414110000	-3.025076000
1	4.013102000	1.504431000	-4.360028000
1	-5.798418000	2.309073000	-3.643844000
1	-3.427370000	1.840703000	-4.651468000
1	-5.543763000	-2.923792000	0.936823000
1	-4.685708000	-3.182548000	-1.559202000
1	-4.904500000	0.186371000	-4.171135000
6	-5.462264000	-2.482875000	-4.060844000
1	-5.539533000	-3.497010000	-3.647562000
6	-4.548548000	-2.542871000	-5.290093000
6	-6.871414000	-2.024868000	-4.452257000
1	-7.532880000	-1.999195000	-3.581368000
1	-6.846654000	-1.018665000	-4.885185000

1	-7.304590000	-2.700044000	-5.197764000
1	-4.452739000	-1.554267000	-5.752503000
1	-4.955738000	-3.227056000	-6.042060000
1	-3.545282000	-2.882935000	-5.017504000
6	6.596295000	-1.076755000	-1.175917000
1	6.584389000	-1.910841000	-0.459063000
6	7.919635000	-0.323540000	-0.987366000
6	6.508779000	-1.664699000	-2.586984000
1	5.520694000	-2.095076000	-2.785234000
1	6.692363000	-0.897497000	-3.346638000
1	7.265114000	-2.444085000	-2.721834000
1	7.964223000	0.533839000	-1.668198000
1	8.774084000	-0.974820000	-1.200349000
1	8.015762000	0.053923000	0.034951000
1	-3.472900000	-4.076659000	-0.065447000

### TRIP-TS<sub>b</sub>'

Number of imaginary frequencies : 1

Electronic energy= -3634.41360034 (hartree/particle)

Zero-point correction= 1.234897

Thermal correction to Energy= 1.303196

Thermal correction to Enthalpy= 1.304140

Thermal correction to Gibbs Free Energy= 1.131067

Sum of electronic and zero-point Energies= -3633.178704

Sum of electronic and thermal Energies= -3633.110404

Sum of electronic and thermal Enthalpies= -3633.109460

Sum of electronic and thermal Free Energies= -3633.282534

### Coordinates

6	-3.679133000	0.766338000	0.288634000
6	-2.465684000	1.375461000	-0.125703000
6	-2.217803000	2.729620000	-0.039515000
6	-3.216773000	3.564329000	0.561138000
6	-4.460706000	2.984289000	0.937723000
6	-4.665308000	1.590509000	0.771431000
6	-3.007525000	4.944391000	0.828413000
6	-3.995009000	5.708498000	1.396660000
6	-5.245566000	5.138818000	1.732052000
6	-5.467273000	3.805027000	1.511178000
6	-0.909417000	3.255012000	-0.517562000
6	0.254507000	2.669256000	-0.063896000
6	1.554235000	3.103872000	-0.435112000
6	1.641193000	4.179491000	-1.283687000
6	0.487817000	4.792252000	-1.836094000

6	-0.804041000	4.314081000	-1.478271000
6	0.603855000	5.854904000	-2.770402000
6	-0.508118000	6.405456000	-3.351130000
6	-1.790741000	5.904705000	-3.027365000
6	-1.935962000	4.887436000	-2.118423000
8	-1.503095000	0.554071000	-0.682054000
8	0.174179000	1.629463000	0.845827000
1	-5.622351000	1.164064000	1.061615000
1	-2.048512000	5.389762000	0.586101000
1	-3.812235000	6.759501000	1.597995000
1	-6.019268000	5.757083000	2.176453000
1	-6.414421000	3.346518000	1.783961000
1	2.621604000	4.554833000	-1.568372000
1	1.598199000	6.212824000	-3.024700000
1	-0.408196000	7.213060000	-4.069468000
1	-2.668607000	6.325031000	-3.508255000
1	-2.923938000	4.503562000	-1.887866000
6	-4.293530000	-2.710632000	-1.088578000
6	-3.992432000	-1.345150000	-1.041093000
6	-3.868686000	-0.715052000	0.208848000
6	-3.972288000	-1.475005000	1.396189000
6	-4.270181000	-2.832277000	1.293249000
6	-3.792085000	-0.862593000	2.779911000
6	-2.842160000	-1.674609000	3.668146000
6	-5.176682000	-0.604643000	-3.135470000
6	-3.856041000	-0.591883000	-2.355618000
1	-3.346994000	0.129326000	2.657070000
1	-1.858097000	-1.773351000	3.206817000
1	-2.714756000	-1.164583000	4.628718000
1	-5.989174000	-0.180512000	-2.537283000
1	-5.083609000	-0.018824000	-4.055910000
1	-3.617702000	0.452631000	-2.137297000
6	-4.456249000	-3.469613000	0.066196000
6	4.788703000	1.141549000	-0.303402000
6	3.615964000	1.710927000	-0.806859000
6	2.771830000	2.408094000	0.080459000
6	3.093631000	2.482259000	1.451180000
6	4.275226000	1.896798000	1.901479000
6	2.231195000	3.226766000	2.459888000
6	2.974768000	4.452268000	3.006468000
6	1.772827000	2.306167000	3.595977000
6	3.325100000	0.135138000	-2.784946000
6	3.339624000	1.589964000	-2.300235000
1	1.334703000	3.594606000	1.953890000
1	3.272761000	5.124307000	2.195404000
1	2.336377000	5.010072000	3.699786000
1	1.231116000	1.441488000	3.203189000

1	1.108941000	2.849299000	4.276839000
1	2.470654000	-0.400428000	-2.367219000
1	3.238190000	0.107377000	-3.876467000
1	2.346876000	2.001346000	-2.502425000
6	5.145389000	1.233242000	1.038832000
6	4.365470000	2.408939000	-3.096270000
1	4.127317000	2.387837000	-4.164853000
1	4.390218000	3.453480000	-2.769221000
6	-2.709836000	-1.153926000	-3.204157000
1	-1.759308000	-1.088221000	-2.665589000
1	-2.610059000	-0.584851000	-4.134318000
6	-5.149093000	-0.707004000	3.480189000
1	-5.023871000	-0.239587000	4.462497000
1	-5.841657000	-0.094607000	2.895630000
15	-0.244055000	0.170228000	0.276923000
8	0.782081000	-0.383015000	-0.684927000
8	-0.670882000	-0.654145000	1.454428000
1	-1.191101000	-2.124719000	1.151133000
6	0.163441000	-5.945548000	0.202768000
6	-1.153934000	-5.607519000	-0.496783000
6	-0.996090000	-4.349599000	-1.356940000
6	-0.237055000	-3.263536000	-0.652253000
6	0.209776000	-3.452875000	0.729994000
6	0.567940000	-4.850434000	1.199743000
8	-1.182541000	-3.120007000	0.944005000
1	0.088785000	-6.904955000	0.723022000
1	0.948820000	-6.052524000	-0.555959000
1	-1.477726000	-6.439804000	-1.129157000
1	-1.939069000	-5.434670000	0.248347000
1	-1.968350000	-3.927435000	-1.637262000
1	-0.469270000	-4.578526000	-2.289669000
1	-0.260571000	-2.249618000	-1.034809000
1	0.855806000	-2.666587000	1.121962000
1	1.646536000	-4.887641000	1.384006000
1	0.067936000	-4.994151000	2.164177000
6	5.356185000	-2.424760000	0.226505000
6	6.645984000	-2.873149000	0.482913000
6	7.071874000	-4.099597000	-0.023153000
6	6.204576000	-4.879114000	-0.787175000
6	4.912318000	-4.438726000	-1.042473000
6	4.479720000	-3.208019000	-0.536222000
6	3.101738000	-2.706675000	-0.770623000
8	2.818640000	-1.650217000	-0.087576000
16	2.035012000	-3.476072000	-1.822034000
1	5.009842000	-1.469311000	0.607200000
1	7.318463000	-2.266419000	1.082613000
1	8.079777000	-4.449844000	0.178602000

1	6.536155000	-5.834789000	-1.180352000
1	4.228378000	-5.041788000	-1.630269000
1	1.920949000	-1.149053000	-0.340082000
1	3.880348000	4.156121000	3.547626000
1	2.626471000	1.946047000	4.181482000
1	4.530090000	1.982026000	2.955954000
1	5.456603000	0.616171000	-0.985531000
1	-5.616617000	-1.687596000	3.628306000
1	-3.237024000	-2.674487000	3.878490000
1	-4.358868000	-3.423463000	2.203354000
1	-4.418662000	-3.178733000	-2.062382000
1	-5.461435000	-1.625016000	-3.415175000
1	-2.893040000	-2.200800000	-3.475018000
1	5.373353000	1.998079000	-2.967659000
1	4.243388000	-0.399056000	-2.512055000
6	6.479711000	0.694369000	1.521166000
1	6.863779000	0.030094000	0.734234000
6	6.369869000	-0.111014000	2.819336000
6	7.481555000	1.844571000	1.688694000
1	7.602688000	2.397592000	0.752725000
1	7.127132000	2.547304000	2.451155000
1	8.461657000	1.467992000	2.000933000
1	6.067661000	0.528851000	3.655018000
1	7.339706000	-0.549023000	3.080530000
1	5.636242000	-0.919170000	2.736828000
6	-4.880327000	-4.929274000	0.048476000
1	-4.244851000	-5.461942000	0.770094000
6	-4.726740000	-5.608942000	-1.311055000
6	-6.333469000	-5.054040000	0.530430000
1	-6.462759000	-4.623918000	1.527785000
1	-7.002063000	-4.520125000	-0.153940000
1	-6.643379000	-6.103964000	0.564405000
1	-5.428837000	-5.189887000	-2.040475000
1	-4.943036000	-6.678081000	-1.223878000
1	-3.715015000	-5.499252000	-1.714782000

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### TRIP-TS<sub>b</sub>\*

Number of imaginary frequencies : 1

Electronic energy= -3634.41758978 (hartree/particle)

Zero-point correction= 1.234695

Thermal correction to Energy= 1.303337

Thermal correction to Enthalpy= 1.304281

Thermal correction to Gibbs Free Energy= 1.127666

Sum of electronic and zero-point Energies= -3633.182895

Sum of electronic and thermal Energies= -3633.114253

Sum of electronic and thermal Enthalpies= -3633.113308  
 Sum of electronic and thermal Free Energies= -3633.289924

Coordinates

6	2.033087000	2.621436000	-0.084786000
6	0.743526000	2.131237000	0.247455000
6	-0.318734000	2.947061000	0.582049000
6	-0.132800000	4.367042000	0.512551000
6	1.164257000	4.878640000	0.229444000
6	2.226929000	3.979718000	-0.041927000
6	-1.198924000	5.291373000	0.684139000
6	-0.975549000	6.643183000	0.618364000
6	0.323481000	7.149519000	0.378770000
6	1.366651000	6.283011000	0.184389000
6	-1.624021000	2.330986000	0.943792000
6	-2.180667000	1.398983000	0.093545000
6	-3.433244000	0.768754000	0.320767000
6	-4.128087000	1.140867000	1.444527000
6	-3.591181000	2.049379000	2.392442000
6	-2.314033000	2.633383000	2.164311000
6	-4.297854000	2.361929000	3.583264000
6	-3.753794000	3.193851000	4.526224000
6	-2.466610000	3.743177000	4.320115000
6	-1.765315000	3.471073000	3.172648000
8	0.581494000	0.759595000	0.285793000
8	-1.509818000	1.080471000	-1.076622000
1	3.216688000	4.382419000	-0.242453000
1	-2.201415000	4.915063000	0.856657000
1	-1.804856000	7.332277000	0.744425000
1	0.486064000	8.221836000	0.334700000
1	2.366624000	6.655103000	-0.023852000
1	-5.111252000	0.714362000	1.626096000
1	-5.277250000	1.915414000	3.734929000
1	-4.300415000	3.423897000	5.435359000
1	-2.027781000	4.383281000	5.079305000
1	-0.775820000	3.891863000	3.029583000
6	4.964126000	0.241437000	0.164725000
6	3.834595000	0.973163000	0.528692000
6	3.149344000	1.700557000	-0.463443000
6	3.550207000	1.611564000	-1.809519000
6	4.696778000	0.873941000	-2.123059000
6	2.775594000	2.292638000	-2.929476000
6	2.646695000	1.401831000	-4.170463000
6	4.451652000	1.473390000	2.927384000
6	3.373113000	0.943207000	1.976778000
1	1.762198000	2.485768000	-2.562506000

1	2.327235000	0.392613000	-3.903572000
1	1.905025000	1.826173000	-4.853848000
1	4.747726000	2.491589000	2.656543000
1	4.080478000	1.484349000	3.957331000
1	2.499939000	1.596015000	2.073923000
6	5.434022000	0.206343000	-1.148711000
6	-4.651409000	-2.511468000	-1.117085000
6	-4.061640000	-1.599802000	-0.238606000
6	-3.972563000	-0.249753000	-0.630770000
6	-4.417040000	0.148450000	-1.906426000
6	-4.985222000	-0.803638000	-2.750781000
6	-4.322491000	1.586381000	-2.393314000
6	-5.718490000	2.184874000	-2.604643000
6	-3.478179000	1.687198000	-3.668541000
6	-2.735777000	-3.401186000	0.965068000
6	-3.541030000	-2.103020000	1.101918000
1	-3.827110000	2.184976000	-1.623542000
1	-6.309231000	2.139352000	-1.684335000
1	-5.643718000	3.232148000	-2.916268000
1	-2.484044000	1.260583000	-3.510736000
1	-3.363252000	2.735059000	-3.965510000
1	-1.948772000	-3.297788000	0.212699000
1	-2.271193000	-3.652148000	1.925312000
1	-2.865345000	-1.343570000	1.509554000
6	-5.123158000	-2.137209000	-2.371265000
6	-4.688861000	-2.316628000	2.097580000
1	-4.303037000	-2.687485000	3.053405000
1	-5.241892000	-1.392879000	2.288471000
6	2.933110000	-0.473336000	2.364470000
1	2.153986000	-0.823976000	1.681691000
1	2.526591000	-0.492191000	3.381886000
6	3.420557000	3.628777000	-3.321057000
1	2.872209000	4.089294000	-4.149795000
1	3.432417000	4.336859000	-2.488207000
15	-0.272912000	0.048971000	-0.913882000
8	-0.732874000	-1.260571000	-0.313705000
8	0.480671000	0.036495000	-2.206929000
1	1.346412000	-1.179619000	-2.624490000
6	2.835165000	-5.106901000	-1.747435000
6	3.909254000	-4.107124000	-2.177690000
6	3.832651000	-2.828545000	-1.340729000
6	2.451315000	-2.219986000	-1.348532000
6	1.301432000	-3.132189000	-1.372829000
6	1.435087000	-4.517094000	-1.935224000
8	1.963989000	-1.991990000	-2.688493000
1	2.914205000	-6.035859000	-2.320175000
1	2.982955000	-5.366913000	-0.691435000

1	4.904738000	-4.549952000	-2.074486000
1	3.775469000	-3.853548000	-3.236539000
1	4.529424000	-2.072965000	-1.709226000
1	4.091886000	-3.034244000	-0.293518000
1	2.356111000	-1.328331000	-0.719833000
1	0.319922000	-2.698565000	-1.219051000
1	0.661334000	-5.146502000	-1.486960000
1	1.195300000	-4.437746000	-3.002913000
6	-0.024959000	-2.411737000	4.625396000
6	0.098531000	-2.642756000	5.990051000
6	0.927313000	-3.661783000	6.453757000
6	1.633754000	-4.451737000	5.548628000
6	1.513594000	-4.225879000	4.183680000
6	0.682228000	-3.204564000	3.711695000
6	0.532305000	-2.928191000	2.257349000
8	-0.184141000	-1.887311000	2.012847000
16	1.246157000	-3.917319000	1.096980000
1	-0.666660000	-1.620467000	4.254990000
1	-0.453716000	-2.026243000	6.692157000
1	1.024006000	-3.840368000	7.520515000
1	2.282314000	-5.244366000	5.907772000
1	2.062994000	-4.834630000	3.473818000
1	-0.360784000	-1.657771000	1.002053000
1	5.347654000	0.843575000	2.902597000
1	3.773380000	-1.176859000	2.323124000
1	5.506223000	-0.314729000	0.929368000
1	5.011505000	0.821497000	-3.161154000
1	4.455750000	3.470165000	-3.645660000
1	3.594284000	1.333403000	-4.717274000
1	-6.265496000	1.641542000	-3.383109000
1	-3.955284000	1.156395000	-4.500185000
1	-5.398268000	-3.055767000	1.707854000
1	-4.739971000	-3.554057000	-0.818911000
1	-5.334591000	-0.489952000	-3.733055000
6	-5.758500000	-3.153158000	-3.300812000
1	-5.749094000	-4.120681000	-2.781999000
6	-4.954899000	-3.305108000	-4.596801000
6	-7.217534000	-2.795760000	-3.605668000
1	-7.801567000	-2.704122000	-2.685208000
1	-7.280001000	-1.841010000	-4.139697000
1	-7.680469000	-3.562689000	-4.235813000
1	-4.949130000	-2.367181000	-5.162897000
1	-5.392923000	-4.079347000	-5.235665000
1	-3.915916000	-3.574301000	-4.385876000
6	6.725632000	-0.535078000	-1.453087000
1	6.716815000	-1.457178000	-0.853783000
6	7.925239000	0.306756000	-0.994653000

6	6.890867000	-0.927860000	-2.921286000
1	6.025855000	-1.483010000	-3.300567000
1	7.024612000	-0.042260000	-3.552239000
1	7.779672000	-1.554252000	-3.043995000
1	7.960109000	1.245882000	-1.557589000
1	8.865416000	-0.229254000	-1.162532000
1	7.852706000	0.555054000	0.068332000
1	-3.374539000	-4.245739000	0.685325000

### TRIP-TS<sub>b</sub>\*

Number of imaginary frequencies : 1

Electronic energy= -3634.41594349 (hartree/particle)

Zero-point correction= 1.234275

Thermal correction to Energy= 1.302497

Thermal correction to Enthalpy= 1.303441

Thermal correction to Gibbs Free Energy= 1.132448

Sum of electronic and zero-point Energies= -3633.181668

Sum of electronic and thermal Energies= -3633.113447

Sum of electronic and thermal Enthalpies= -3633.112503

Sum of electronic and thermal Free Energies= -3633.283496

### Coordinates

6	-3.719724000	0.988269000	0.321225000
6	-2.465447000	1.536006000	-0.056568000
6	-2.084511000	2.834862000	0.207983000
6	-2.983926000	3.666330000	0.952521000
6	-4.272763000	3.162100000	1.282482000
6	-4.612943000	1.828442000	0.939279000
6	-2.630985000	4.966016000	1.406476000
6	-3.525859000	5.733018000	2.108181000
6	-4.821998000	5.246351000	2.397882000
6	-5.181600000	3.986304000	1.997442000
6	-0.744990000	3.298340000	-0.244654000
6	0.371026000	2.547303000	0.070332000
6	1.688738000	2.897521000	-0.323814000
6	1.846632000	4.077117000	-1.010506000
6	0.743725000	4.874709000	-1.403148000
6	-0.574067000	4.468955000	-1.054073000
6	0.932128000	6.049214000	-2.178400000
6	-0.139878000	6.778493000	-2.619924000
6	-1.453513000	6.352417000	-2.312239000
6	-1.666407000	5.230008000	-1.553176000
8	-1.595563000	0.714446000	-0.752131000

8	0.216587000	1.408285000	0.844226000
1	-5.593663000	1.450071000	1.217600000
1	-1.636202000	5.345748000	1.199453000
1	-3.233750000	6.720778000	2.450911000
1	-5.521125000	5.866491000	2.950156000
1	-6.165211000	3.587694000	2.232804000
1	2.848020000	4.391684000	-1.293386000
1	1.947834000	6.346966000	-2.425914000
1	0.013094000	7.672619000	-3.216270000
1	-2.302488000	6.916220000	-2.686574000
1	-2.679208000	4.909198000	-1.335296000
6	-4.448971000	-2.346101000	-1.329360000
6	-4.134478000	-0.995581000	-1.184939000
6	-4.016650000	-0.461290000	0.114358000
6	-4.183566000	-1.297873000	1.236917000
6	-4.525292000	-2.637755000	1.035892000
6	-3.991445000	-0.816578000	2.669910000
6	-3.029300000	-1.714057000	3.458672000
6	-5.306684000	-0.067212000	-3.201568000
6	-3.978126000	-0.148587000	-2.438882000
1	-3.542230000	0.179875000	2.640828000
1	-2.059971000	-1.776941000	2.959120000
1	-2.870657000	-1.293060000	4.457207000
1	-6.103133000	0.324233000	-2.561130000
1	-5.208983000	0.589752000	-4.072107000
1	-3.711006000	0.869248000	-2.141020000
6	-4.654414000	-3.185907000	-0.235442000
6	4.808271000	0.846380000	-0.898935000
6	3.573776000	1.459359000	-1.134667000
6	2.880789000	2.035950000	-0.050552000
6	3.383903000	1.896998000	1.257562000
6	4.615917000	1.270967000	1.439326000
6	2.649810000	2.426098000	2.479394000
6	3.485549000	3.468056000	3.232117000
6	2.242001000	1.272614000	3.403263000
6	2.987966000	0.077319000	-3.174812000
6	3.039219000	1.481975000	-2.561916000
1	1.733544000	2.923368000	2.149440000
1	3.757423000	4.301899000	2.577459000
1	2.921669000	3.866496000	4.082101000
1	1.622365000	0.546247000	2.869125000
1	1.670217000	1.650062000	4.257681000
1	2.347370000	-0.584262000	-2.588452000
1	2.576478000	0.131567000	-4.188467000
1	2.011726000	1.856829000	-2.537164000
6	5.364629000	0.771431000	0.373954000
6	3.874400000	2.413348000	-3.450211000

1	3.471372000	2.435837000	-4.468170000
1	3.888817000	3.437958000	-3.066566000
6	-2.856470000	-0.672666000	-3.342265000
1	-1.895165000	-0.655601000	-2.820297000
1	-2.766189000	-0.046300000	-4.236022000
6	-5.338323000	-0.720543000	3.398079000
1	-5.199291000	-0.341339000	4.415938000
1	-6.036313000	-0.057341000	2.877870000
15	-0.358411000	0.087557000	0.094603000
8	0.613020000	-0.407209000	-0.956634000
8	-0.824177000	-0.869050000	1.150513000
1	-1.510242000	-2.292874000	0.711483000
6	-0.004945000	-6.011419000	-0.660053000
6	-1.381610000	-5.673847000	-1.238263000
6	-1.382153000	-4.280145000	-1.868876000
6	-0.866672000	-3.224978000	-0.922799000
6	0.214207000	-3.591023000	-0.001671000
6	0.397481000	-5.018121000	0.432506000
8	-1.574223000	-3.231325000	0.340826000
1	0.001958000	-7.023980000	-0.245402000
1	0.746903000	-5.984864000	-1.459547000
1	-1.669771000	-6.415722000	-1.989793000
1	-2.135502000	-5.711469000	-0.442441000
1	-2.386817000	-3.982918000	-2.188536000
1	-0.734381000	-4.261463000	-2.754536000
1	-0.790331000	-2.230546000	-1.359872000
1	0.645425000	-2.779289000	0.576749000
1	1.435476000	-5.159254000	0.744401000
1	-0.227161000	-5.156567000	1.323793000
6	4.627363000	-2.259886000	1.606370000
6	5.748059000	-2.649182000	2.329684000
6	6.537558000	-3.705323000	1.879477000
6	6.192551000	-4.390199000	0.714631000
6	5.057353000	-4.024556000	0.001305000
6	4.276289000	-2.948425000	0.437760000
6	3.066691000	-2.511075000	-0.300727000
8	2.615505000	-1.372843000	0.082179000
16	2.309632000	-3.469285000	-1.473079000
1	4.017899000	-1.423151000	1.930445000
1	6.010656000	-2.120999000	3.241391000
1	7.420758000	-3.998861000	2.438918000
1	6.807650000	-5.213277000	0.365323000
1	4.770905000	-4.556027000	-0.900464000
1	1.754768000	-0.993266000	-0.441781000
1	3.984014000	-0.372978000	-3.247650000
1	4.912052000	2.064555000	-3.505847000
1	5.351903000	0.429771000	-1.743631000

1	5.025020000	1.188050000	2.446519000
1	4.411257000	3.030691000	3.621990000
1	3.126553000	0.756099000	3.795513000
1	-4.657237000	-3.273138000	1.906972000
1	-4.549867000	-2.761451000	-2.332654000
1	-5.617980000	-1.054950000	-3.559407000
1	-3.061377000	-1.696774000	-3.676731000
1	-3.430579000	-2.724902000	3.590023000
1	-5.809021000	-1.708267000	3.466756000
6	-5.012066000	-4.642710000	-0.468998000
1	-4.374970000	-5.001064000	-1.291735000
6	-6.472232000	-4.767581000	-0.925231000
6	-4.756331000	-5.536151000	0.744322000
1	-3.751577000	-5.381159000	1.151324000
1	-5.478142000	-5.329926000	1.542664000
1	-4.864156000	-6.589997000	0.469202000
1	-7.143169000	-4.407389000	-0.137601000
1	-6.725362000	-5.811026000	-1.141286000
1	-6.661367000	-4.173133000	-1.824127000
6	6.769425000	0.253485000	0.624756000
1	6.776149000	-0.191952000	1.628504000
6	7.752934000	1.432836000	0.630148000
6	7.229482000	-0.817213000	-0.364050000
1	6.500809000	-1.628726000	-0.449828000
1	7.388540000	-0.391841000	-1.361383000
1	8.182392000	-1.245339000	-0.036357000
1	7.759600000	1.921471000	-0.350695000
1	8.770460000	1.091605000	0.850084000
1	7.468198000	2.181410000	1.375876000

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**Table S3.** BSSE energy values of key intermediates and transition states.

Geometries	BSSE energy (a.u)
<b>1</b>	0.00366
<b>1'</b>	0.00336
<b>TS<sub>tauto</sub></b>	0.00512
<b>1''</b>	0.00369
<b>2<sub>a</sub></b>	0.00861
<b>TS<sub>a</sub></b>	0.01150
<b>TS<sub>a</sub>'</b>	0.01132
<b>TS<sub>a</sub>*</b>	0.01130
<b>TS<sub>a</sub>'*</b>	0.01146
<b>3<sub>a</sub></b>	0.00650
<b>2<sub>b</sub></b>	0.00835
<b>TS<sub>b</sub></b>	0.00983
<b>TS<sub>b</sub>'</b>	0.01030
<b>TS<sub>b</sub>*</b>	0.01005
<b>TS<sub>b</sub>'*</b>	0.01047
<b>3<sub>b</sub></b>	0.00574
<b>TRIP-TS<sub>b</sub></b>	0.00967
<b>TRIP-TS<sub>b</sub>'</b>	0.00977
<b>TRIP-TS<sub>b</sub>*</b>	0.00971
<b>TRIP-TS<sub>b</sub>'*</b>	0.01030