**Electronic Supplementary Information**

# Theoretical insights into the E1cB/E2 mechanistic dichotomy of elimination reactions

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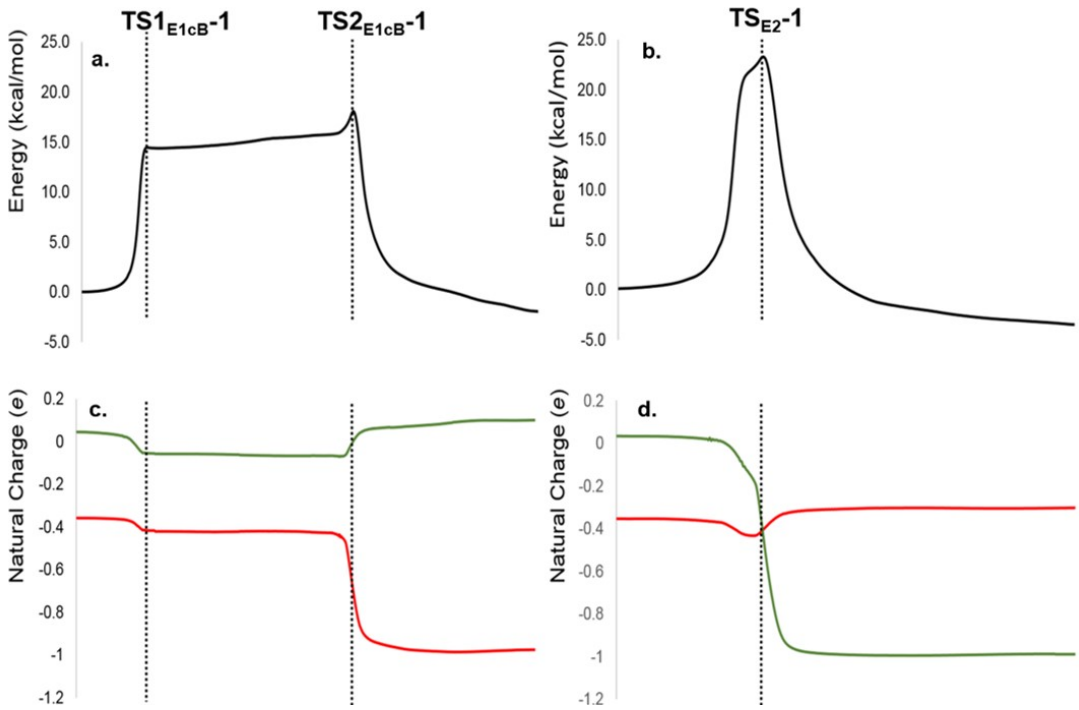


**Figure S1.** Potential energy surface along the intrinsic reaction coordinate for the expulsion of (a) phenolate and (b) thiophenolate leaving groups. Natural charge variation along the intrinsic reaction coordinate for the explusion of (c) phenolate and (d) thiophenolate moieties associated to the E1cB and E2 reaction mechanisms, respectively. Green and red lines correspond to the thiophenolate and phenolate fragments.

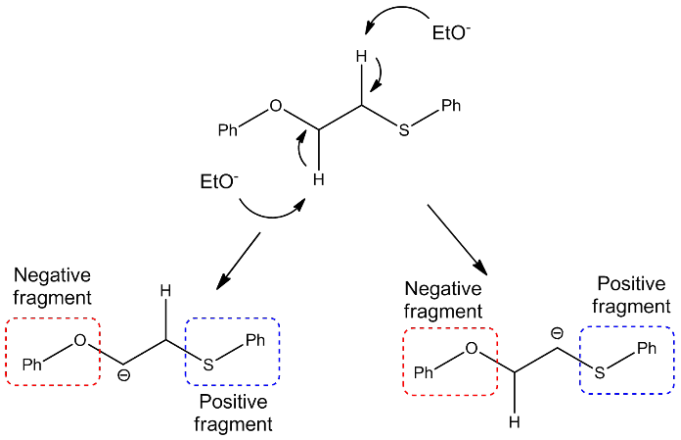


**Figure S2.** Carbanion formation process at C1 center (phenolate leaving group; E1cB) and C2 center (thiophenolate leaving group; E2).

B3LYP/6-31+G(d) method also was performed on the unsubstituted (1) β-phenylmercaptoethyl phenolate to examine the relative Gibbs free energy profiles of Figure 3 (main paper). The results are summarized in Figure S3. Calculations with B3LYP functional showed that the carbanion intermediate (**$I_{E1cB}$**) is about 1 kcal/mol above the **$TS1_{E1cB}$**. The same scenario takes place when M06-2X/6-31+G(d) method is used in ethanol. This suggests that the internal thermal energy ($E= E_t + E_r + E_v + E_e$) could be overestimated, which is independent of the functional used. Note in Figure S2 that subtracting the vibrational contribution ($E_v$) of the internal thermal energy to the Gibbs free energy the calculations predict a lower free energy of the anionic intermediate **$I_{E1cB}$** indicating that vibrational energy should be associated with some internal rotations that lead to wrong results on the thermal corrections of the enthalpy ($H_{corr}= E + k_BT$) and therefore to the Gibbs free energy ($G_{corr}= H_{corr} – TS$). Table S1 shows the corrected and non-corrected Enthalpic and Gibbs free activation and reaction energies for the E2 and E1cB mechanisms.

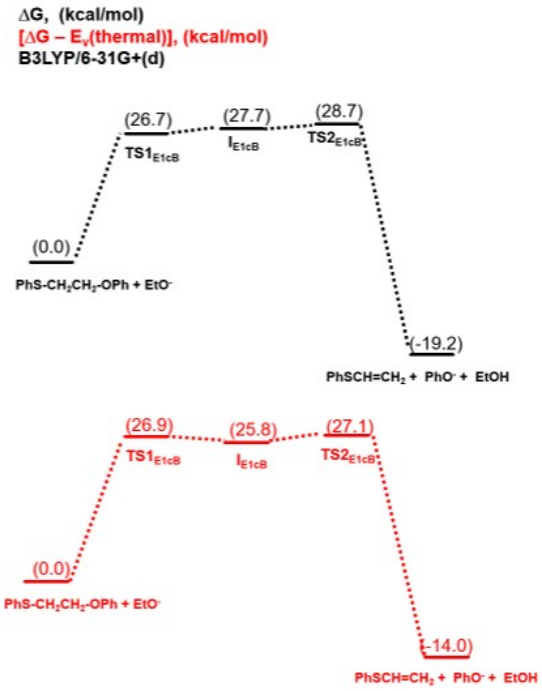


**Figure S3.** Relative Gibbs free energy (black) and corrected Gibbs free energy (red) profiles for the E1cB mechanism on the unsubstituted phenolate group. Energies are with respect to the ethoxide and β-phenylmercaptoethyl phenolate molecules.

**Table S1.** Corrected and non-corrected Enthalpic and Gibbs free activation and reaction energies of unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate systems for E2 and E1cB mechanisms. All values are given in kcal/mol.

| System | $\Delta G^{\ddagger}$ | $\Delta H^{\ddagger}$ | $\Delta G^{\circ}$ | $\Delta H^{\circ}$ | $\Delta G^{\ddagger} - E_v$ | $\Delta H^{\ddagger} - E_v$ | $\Delta G^{\circ} - E_v$ | $\Delta H^{\circ} - E_v$ | Frequencies ($cm^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|
| **$TS_{E2}$-1** | 28.07 | 18.06 | -14.68 | -3.05 | 27.1 | 17.0 | -10.1 | 1.5 | -338.65 |
| **1st step: "associated to the proton abstraction (TS1)"** | | | | | | | | | |
| **$TS1_{E1cB}$-1** | 20.3 | 7.7 | 21.6 | 9.4 | 20.4 | 7.9 | 20.1 | 7.8 | -234.05 |
| **$TS1_{E1cB}$-2** | 16.9 | 6.4 | 17.8 | 7.9 | 16.3 | 5.7 | 15.6 | 5.7 | -196.63 |
| **$TS1_{E1cB}$-3** | 18.7 | 4.6 | 20.1 | 6.6 | 18.8 | 4.7 | 18.2 | 4.7 | -399.80 |
| **$TS1_{E1cB}$-4** | 19.3 | 6.5 | 20.4 | 8.4 | 19.3 | 6.5 | 17.7 | 6.4 | -558.06 |
| **$TS1_{E1cB}$-5** | 19.2 | 6.7 | 19.3 | 8.4 | 19.4 | 6.8 | 18.3 | 6.3 | -549.95 |
| **$TS1_{E1cB}$-6** | 18.1 | 6.3 | 19.9 | 8.3 | 18.6 | 6.7 | 18.1 | 6.5 | -590.20 |
| **$TS1_{E1cB}$-7** | 18.7 | 6.3 | 21.0 | 8.4 | 19.0 | 6.7 | 19.0 | 6.5 | -642.67 |
| **$TS1_{E1cB}$-8** | 16.9 | 7.0 | 18.9 | 8.5 | 16.7 | 6.7 | 16.2 | 5.8 | -835.54 |
| **2nd step: "associated to the bond cleavage to the phenolate living group (TS2)"** | | | | | | | | | |
| **$TS2_{E1cB}$-1** | 23.58 | 12.85 | -15.02 | -2.96 | 22.3 | 11.6 | -11.5 | 1.6 | -353.62 |
| **$TS2_{E1cB}$-2** | 21.67 | 12.18 | -17.13 | -2.94 | 19.4 | 9.9 | -12.6 | 1.6 | -347.86 |
| **$TS_{E1cB}$-3** | 21.62 | 9.53 | -17.25 | -6.72 | 20.2 | 8.1 | -12.2 | -1.7 | -354.01 |
| **$TS2_{E1cB}$-4** | 22.38 | 11.56 | -21.53 | -9.42 | 20.6 | 9.8 | -16.5 | -4.4 | -357.58 |
| **$TS2_{E1cB}$-5** | 22.70 | 11.34 | -20.67 | -8.21 | 21.1 | 9.8 | -15.4 | -2.9 | -361.67 |
| **$TS2_{E1cB}$-6** | 19.87 | 10.72 | -21.89 | -9.04 | 18.5 | 9.4 | -16.6 | -3.7 | -353.42 |
| **$TS2_{E1cB}$-7** | 21.98 | 11.04 | -20.02 | -7.67 | 20.3 | 9.4 | -14.8 | -2.4 | -341.20 |
| **$TS2_{E1cB}$-8** | 19.73 | 9.75 | -25.72 | -12.38 | 17.6 | 7.6 | -21.1 | -7.8 | -348.54 |

**Table S2.** Activation energies, Distortion/Interaction analysis and $C_\beta^{\delta-}\cdots H^{\delta+}$ distance for the transition state structures associated with the proton transfer with the formation of the carbanion intermediate ($TS1_{E1cB}$) in the E1cB mechanism. All values are given in kcal/mol.

| System | $\Delta G^{\ddagger}$ | $\Delta E^{\ddagger}$ | $\Delta E^{\ddagger}_{dist}$ ($EtO^-$) | $\Delta E^{\ddagger}_{dist}$ (β-pme-phenolate -$X_n$) | $\Delta E^{\ddagger}_{int}$ | TS $C_\beta^{\delta-}\cdots H^{\delta+}$ distance (Å) |
|---|---|---|---|---|---|---|
| **$TS1_{E1cB}$-1** | 20.4 | 10.3 | 0.7 | 41.9 | -32.3 | 1.55 |
| **$TS1_{E1cB}$-2** | 16.3 | 8.1 | 0.7 | 40.3 | -32.9 | 1.56 |
| **$TS1_{E1cB}$-3** | 18.8 | 7.1 | 0.7 | 37.0 | -30.6 | 1.54 |
| **$TS1_{E1cB}$-4** | 19.3 | 8.8 | 0.6 | 37.4 | -29.1 | 1.52 |
| **$TS1_{E1cB}$-5** | 19.4 | 9.2 | 0.6 | 37.8 | -29.2 | 1.52 |
| **$TS1_{E1cB}$-6** | 18.6 | 9.1 | 0.6 | 37.2 | -28.8 | 1.51 |
| **$TS1_{E1cB}$-7** | 19.0 | 9.0 | 0.8 | 52.9 | -44.7 | 1.51 |
| **$TS1_{E1cB}$-8** | 16.7 | 9.1 | 0.5 | 33.9 | -25.3 | 1.49 |

**Table S3.** Activation energies, Distortion/Interaction analysis and $C_\alpha \cdots O$ distance for the transition state structures associated with the rate determining step ($TS2_{E1cB}$); phenolate-$X_n$ leaving group step in the E1cB mechanism. All values are given in kcal/mol

| System | $\Delta G^{\ddagger}$ | $\Delta E^{\ddagger}$ | $\Delta E^{\ddagger}_{dist}$ (EtOH) | $\Delta E^{\ddagger}_{dist}$ (PhS-olefin) | $\Delta E^{\ddagger}_{dist}$ (phenolate-$X_n$) | $\Delta E^{\ddagger}_{int}$ | TS $C_\alpha \cdots O$ distance (Å) |
|---|---|---|---|---|---|---|---|
| **$TS2_{E1cB}$-1** | 22.3 | 14.0 | 0.4 | 18.9 | 1.2 | -6.5 | 1.74 |
| **$TS2_{E1cB}$-2** | 19.4 | 12.3 | 0.3 | 18.6 | 1.3 | -7.8 | 1.74 |
| **$TS2_{E1cB}$-3** | 20.2 | 10.5 | 0.7 | 20.0 | 1.3 | -11.5 | 1.72 |
| **$TS2_{E1cB}$-4** | 20.6 | 12.1 | 0.5 | 19.8 | 1.8 | -9.9 | 1.71 |
| **$TS2_{E1cB}$-5** | 21.1 | 12.2 | 0.6 | 19.3 | 1.5 | -9.3 | 1.73 |
| **$TS2_{E1cB}$-6** | 18.5 | 11.8 | 0.5 | 20.0 | 1.5 | -10.1 | 1.72 |
| **$TS2_{E1cB}$-7** | 20.3 | 11.8 | 0.2 | 18.5 | 1.2 | -8.2 | 1.73 |
| **$TS2_{E1cB}$-8** | 17.6 | 10.0 | 0.5 | 21.8 | 2.3 | -14.5 | 1.69 |

**Table S4.** Experimental parameter values of reaction rates ($k_{obs,}$) and Gibbs free energies ($\Delta G^{\ddagger}_{obs}$), subtituent constants (σ-) and computed parameters values of nucleofugality ($v$) and Gibbs free energies ($\Delta G^{\ddagger}_{calc}$). $\log(v/v_0)$ and $\log(k/k_0)$ corresponds to the relative initial nucleofugality and experimental relative initial rates.

| System | [a]σ - | $v$ | $\log(v/v_0)$ | [b]$k_{obs}$ ($s^{-1}$) | $\log(k/k_0)$ | [c]$\Delta G^{\ddagger}_{obs}$ (kcal/mol) | [c]$\Delta G^{\ddagger}_{calc}$ (kcal/mol) |
|---|---|---|---|---|---|---|---|
| **1** | 0.0 | 0.004 | 0.0 | $6.22x10^{-5}$ | 0.0 | 23.2 | 22.3 |
| **2** | -0.17 | 0.003 | -0.09 | $2.83x10^{-5}$ | -0.34 | 23.7 | 19.4 |
| **3** | 0.19 | 0.009 | 0.38 | $2.34x10^{-4}$ | 0.58 | 22.4 | 20.2 |
| **4** | 1.13 | 0.444 | 2.07 | $3.31x10^{-3}$ | 1.73 | 20.8 | 20.6 |
| **5** | 0.84 | 0.398 | 2.02 | $1.23x10^{-3}$ | 1.30 | 21.4 | 21.1 |
| **6** | 1.0 | 0.483 | 2.10 | $2.90x10^{-3}$ | 1.67 | 20.9 | 18.5 |
| **7** | - | 0.739 | 2.29 | $2.26x10^{-3}$ | 1.56 | 21.1 | 20.3 |
| **8** | 1.27 | 0.698 | 2.26 | $1.06x10^{-2}$ | 2.23 | 20.2 | 17.6 |

[a] Values of σ - are from C. Hansch, A. Leo, and R. W. Taft, *Chem. Rev.*, 1991, **91**, 165.

[b] Values of $k_{obs}$ are from H.-Q. Xie, N. Truong, E. Buncel and J. G. Purdon, *Can. J. Chem.*, 1994, **72**, 448–453.

[c] The $k = \frac{k_B T}{h} e^{-\Delta G^{\ddagger}/RT}$ equation provides the theoretical result of the reaction rate constant ($k$) by Evans-Polanyi. The amount $\frac{k_B T}{h}$ is a fundamental term in the transition state theory and their value correspond to $6.213x10^{12}$ $s^{-1}$ at 298.15 K. $\Delta G^{\ddagger}_{obs}$ can be calculated using this equation from the experimental kinetic data ($k_{obs}$) as shown Table S4. Thus, it is possible to validate the ability of our calculated activation free energies ($\Delta G^{\ddagger}_{calc}$) to describe the experimental reaction rates, which shown a similar agreement with the experimental results.

## Linear scaling procedure

The selected reaction coordinate ξ can be replaced, by linear scaling, by a single coordinate that is a reduced or normalized reaction coordinate, according to the scheme shown below: $([\xi_{reactant} - \xi]/ [\xi_{reactant} - \xi_{product}])$. where $\xi_{reactant}$ is the coordinate ξ evaluated in the state or position of reactant and $\xi_{product}$ is the coordinate ξ evaluated in the product status or position. Its evolution from 0 to 1 will allow the change experienced by several properties to be plotted based on a single reaction coordinate scale allowing the comparison of certain properties between different chemical reactions.

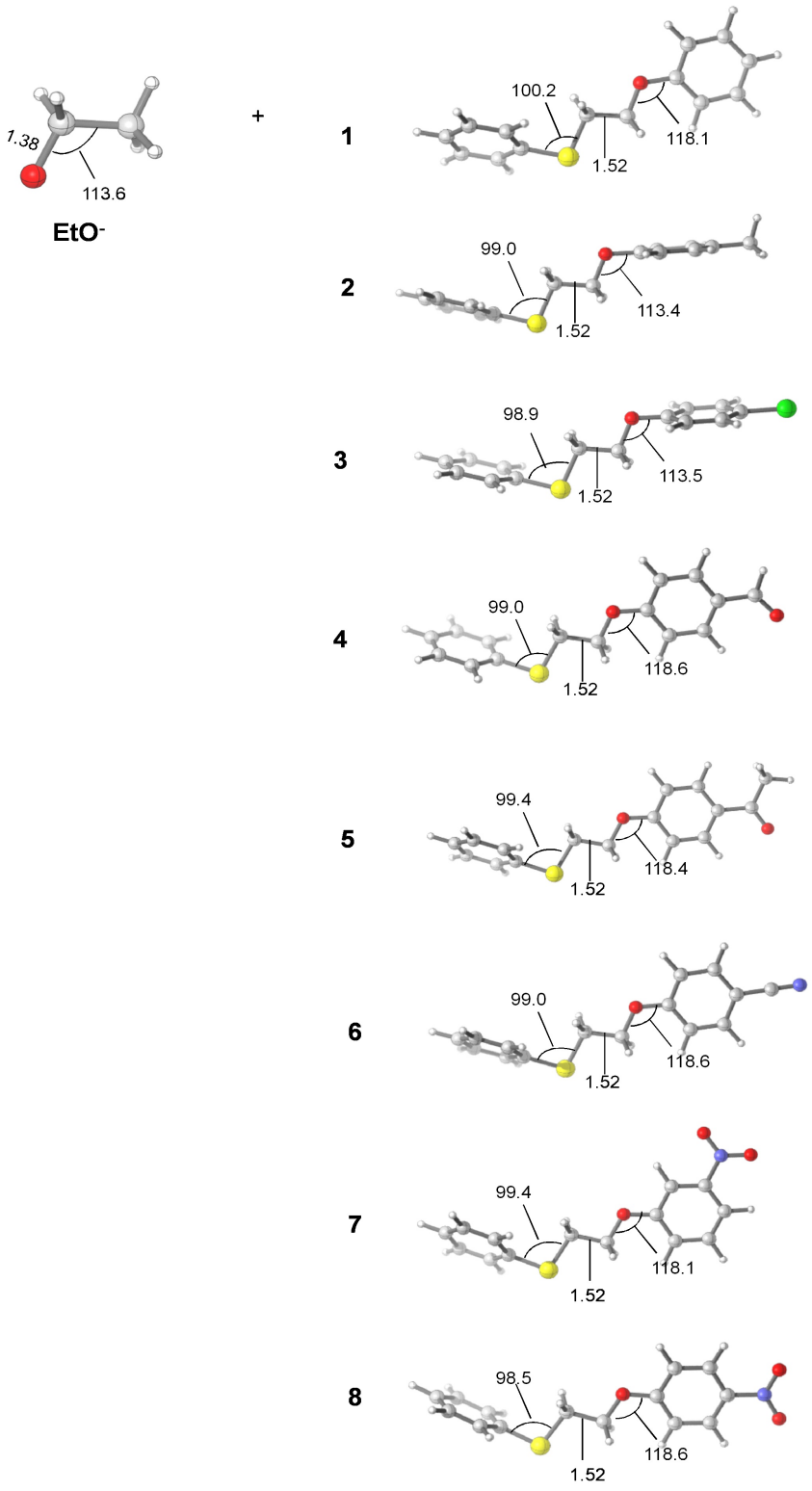


**Figure S4.** Ethoxide, unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate reactants structures.

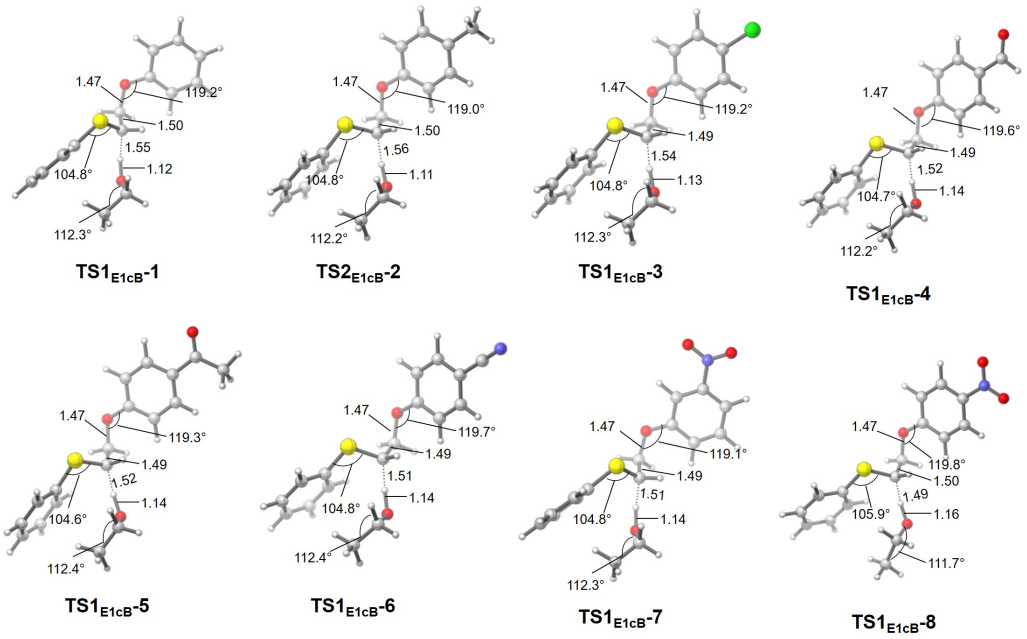


**Figure S5.** Transition state structures associated to the proton abstraction (TS1) at Cβ of unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate systems.

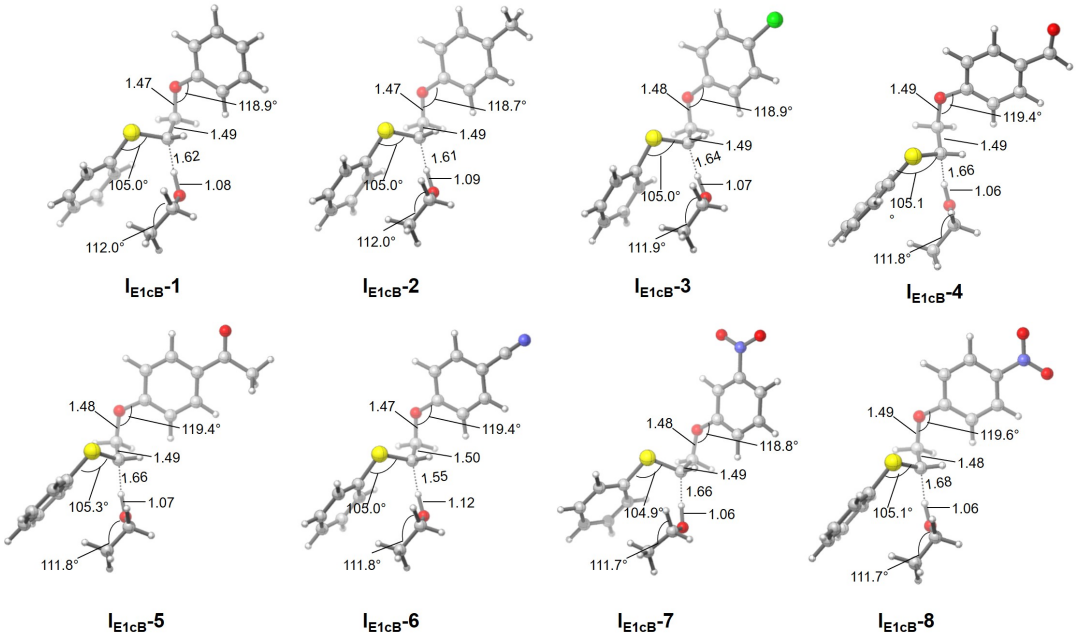


**Figure S6.** Carbanion intermediate structures (I) at Cβ of unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate systems

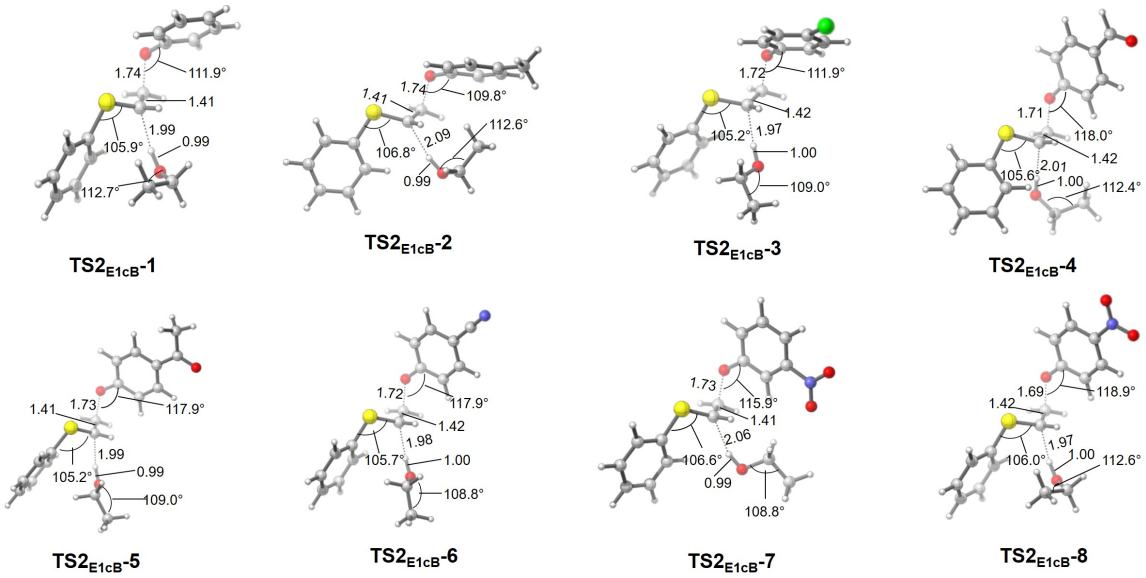


**Figure S7.** Transition state structures associated to the bond cleavage to the phenolate living group (TS2) at Cβ of unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate systems.

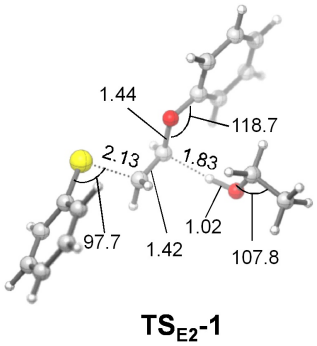


**Figure S8.** Transition state structure associated to the concerted E2 mechanism at Cα of unsubstituted (1) phenylmercaptoethyl phenolate system.

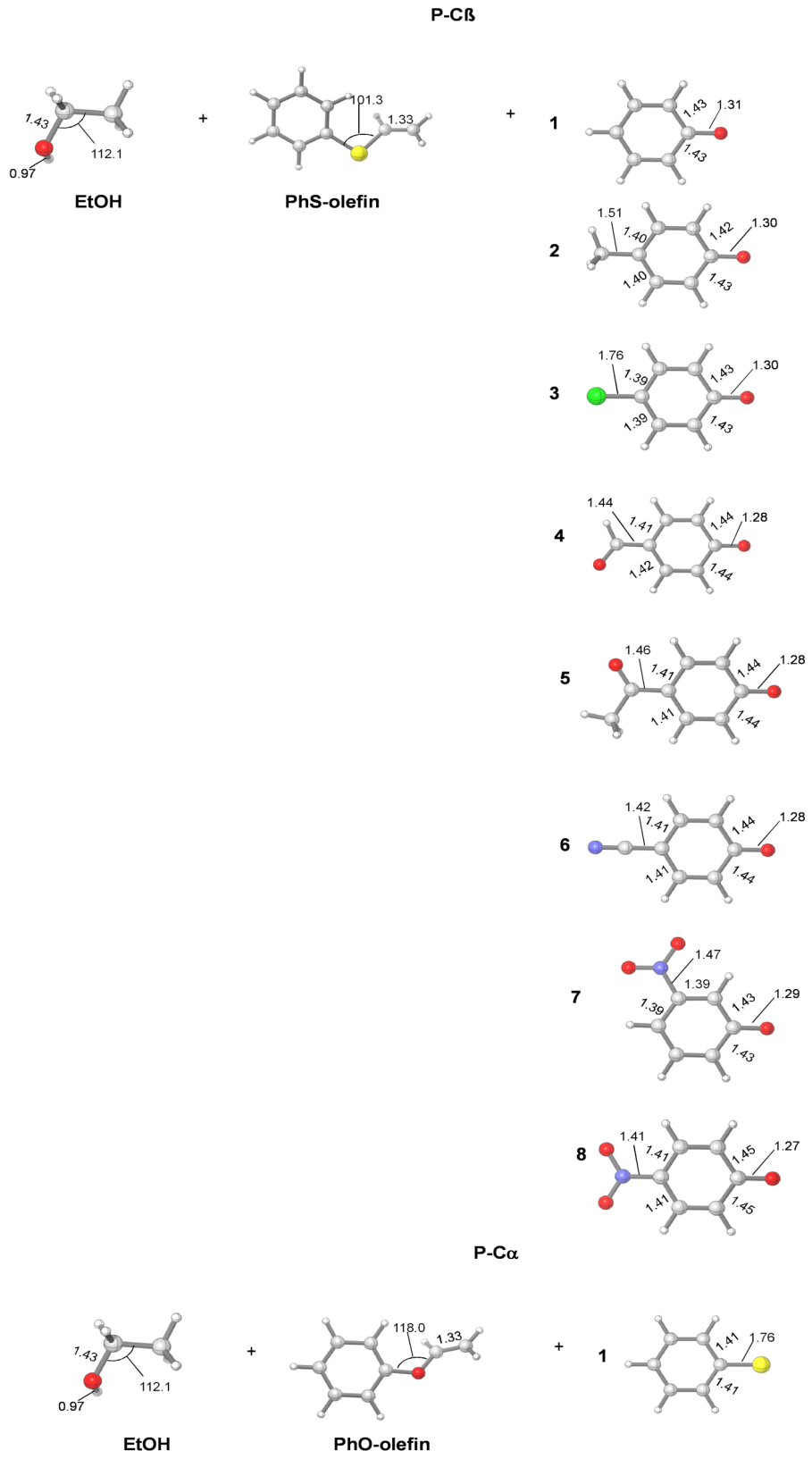


**Figure S9.** Product structures at Cβ of unsubstituted (1) and substituted (2-8) β-phenylmercaptoethyl phenolate systems. And product structures at Cα of unsubstituted (1) phenylmercaptoethyl phenolate system.

**Optimized Cartesian coordinates and calculated thermodynamic properties (a.u.)**

**Reactants**

**$EtO^-$**
Electronic energy: -154.4703237
Vibrational energy: 0.06810573
Gibbs free energy: -154.428065
Enthalpy: -154.39844

| | | | |
|---|---|---|---|
| O | 1.40887400 | -0.01763400 | -1.02923400 |
| C | 1.60478800 | 0.77763200 | 0.08719200 |
| H | 0.64444700 | 1.15426000 | 0.50775600 |
| H | 2.07772300 | 0.21434100 | 0.92401700 |
| C | 2.48840100 | 2.00151000 | -0.17942600 |
| H | 2.03577800 | 2.63977700 | -0.94942000 |
| H | 2.63049200 | 2.60607500 | 0.72738200 |
| H | 3.47581700 | 1.68619400 | -0.54076000 |

**1**
Electronic Energy: -1015.0531667
Vibrational energy: 0.25851238
Gibbs free energy: -1014.85078
Enthalpy: -1014.790878

| | | | |
|---|---|---|---|
| C | -8.21567600 | 1.29998000 | 1.47421000 |
| C | -6.89398500 | 1.73263200 | 1.35743100 |
| C | -6.40191900 | 2.14847900 | 0.11704400 |
| C | -7.23787500 | 2.12868600 | -1.00519700 |
| C | -8.55008500 | 1.67491000 | -0.88600300 |
| C | -9.04384200 | 1.26314700 | 0.35336000 |
| H | -8.59061700 | 0.97902600 | 2.44230700 |
| H | -6.24409600 | 1.74062300 | 2.22837300 |
| H | -6.86962000 | 2.47160300 | -1.96866100 |
| H | -9.19133500 | 1.65593600 | -1.76305200 |
| H | -10.06960300 | 0.91658100 | 0.44342800 |
| S | -4.72417600 | 2.75189100 | 0.01062700 |
| C | -4.08167200 | 1.69084700 | -1.33314900 |
| H | -4.59411200 | 1.92299300 | -2.27048100 |
| H | -4.25494700 | 0.64239700 | -1.07460100 |
| C | -2.59552000 | 1.95764900 | -1.48853100 |
| H | -2.04834100 | 1.69205600 | -0.57519900 |
| H | -2.41043100 | 3.01390200 | -1.72326300 |
| O | -2.15914200 | 1.13962400 | -2.56861200 |
| C | -0.84504800 | 1.20555100 | -2.93595400 |
| C | 0.09900900 | 2.03099500 | -2.32160900 |

| | | | |
|---|---|---|---|
| C | -0.47141700 | 0.37715100 | -4.00118000 |
| C | 1.41779500 | 2.02000300 | -2.78679000 |
| H | -0.17125600 | 2.67705600 | -1.49345800 |
| C | 0.84340000 | 0.37854000 | -4.45060100 |
| H | -1.22424600 | -0.25723800 | -4.46152300 |
| C | 1.79888100 | 1.20154300 | -3.84598700 |
| H | 2.14898600 | 2.66539500 | -2.30690300 |
| H | 1.12383500 | -0.26594300 | -5.27952700 |
| H | 2.82604700 | 1.20177200 | -4.19868200 |

**2**

Electronic energy: -1054.3462961
Vibrational energy: 0.28664103
Gibbs free energy: -1054.117213
Enthalpy: -1054.055878

| | | | |
|---|---|---|---|
| C | -8.43880900 | 0.20968600 | -0.08470800 |
| C | -7.06602800 | 0.31054800 | 0.14299200 |
| C | -6.44191300 | 1.56058800 | 0.10104100 |
| C | -7.19642600 | 2.70840000 | -0.16223600 |
| C | -8.56718400 | 2.60186900 | -0.39518000 |
| C | -9.18961900 | 1.35351600 | -0.35604700 |
| H | -8.91987700 | -0.76408300 | -0.04910200 |
| H | -6.47923400 | -0.57982400 | 0.35348700 |
| H | -6.71184300 | 3.68134900 | -0.18475300 |
| H | -9.14838000 | 3.49615000 | -0.60339700 |
| H | -10.25853200 | 1.27318300 | -0.53431500 |
| S | -4.68293400 | 1.69076000 | 0.40337900 |
| C | -4.09665500 | 1.72311100 | -1.33057800 |
| H | -4.46163200 | 2.63033700 | -1.82135800 |
| H | -4.48570300 | 0.84576600 | -1.85582900 |
| C | -2.57983900 | 1.70188700 | -1.33642400 |
| H | -2.19870200 | 0.77105300 | -0.89705000 |
| H | -2.16621200 | 2.55221700 | -0.77722800 |
| O | -2.16774800 | 1.78827400 | -2.70369600 |
| C | -0.79788400 | 1.68225900 | -2.87180200 |
| C | -0.01026000 | 2.83076100 | -2.88461200 |
| C | -0.22060300 | 0.42801700 | -3.05641000 |
| C | 1.36446400 | 2.71705400 | -3.08993600 |
| H | -0.47703000 | 3.80171000 | -2.73848100 |
| C | 1.15476800 | 0.32980500 | -3.26078300 |
| H | -0.84994000 | -0.45845300 | -3.04307800 |
| C | 1.96841000 | 1.46919300 | -3.28380800 |
| H | 1.97699000 | 3.61623600 | -3.10104700 |
| H | 1.60352700 | -0.65060600 | -3.40658000 |
| C | 3.44912600 | 1.35688400 | -3.54409600 |

| | | | |
|---|---|---|---|
| H | 3.84416500 | 0.40325900 | -3.18066000 |
| H | 3.66192200 | 1.41341400 | -4.61872000 |
| H | 3.99997000 | 2.16667700 | -3.05593300 |

**3**

Electronic energy: -1474.6197201
Vibrational energy: 0.24964399
Gibbs free energy: -1474.432244
Enthalpy: -1474.366299

| | | | |
|---|---|---|---|
| C | -8.40608600 | 0.28805600 | -0.29024400 |
| C | -7.03369300 | 0.39446000 | -0.06924100 |
| C | -6.44745900 | 1.65480100 | 0.08766000 |
| C | -7.24114200 | 2.80412500 | 0.03345200 |
| C | -8.61547800 | 2.69218100 | -0.18092400 |
| C | -9.19853600 | 1.43590600 | -0.34473300 |
| H | -8.85695000 | -0.69290000 | -0.41364700 |
| H | -6.41753400 | -0.49970900 | -0.01836500 |
| H | -6.78438800 | 3.78235400 | 0.15802400 |
| H | -9.22798600 | 3.58884800 | -0.21966800 |
| H | -10.26873100 | 1.35032400 | -0.51243200 |
| S | -4.68806900 | 1.79631800 | 0.38251300 |
| C | -4.09730200 | 1.63206800 | -1.34215300 |
| H | -4.47819100 | 2.46831700 | -1.93606700 |
| H | -4.46945400 | 0.69188400 | -1.75925300 |
| C | -2.58079600 | 1.63570100 | -1.34389900 |
| H | -2.18132800 | 0.79768000 | -0.75766500 |
| H | -2.18560500 | 2.57496200 | -0.93652100 |
| O | -2.16700400 | 1.49311400 | -2.70805800 |
| C | -0.79687900 | 1.48679900 | -2.86930300 |
| C | -0.09089800 | 2.68871800 | -2.89037200 |
| C | -0.13945800 | 0.27170700 | -3.04609400 |
| C | 1.28721900 | 2.67735200 | -3.09225000 |
| H | -0.61999500 | 3.62836400 | -2.75627400 |
| C | 1.23886200 | 0.25271400 | -3.25238100 |
| H | -0.70897600 | -0.65330900 | -3.02772400 |
| C | 1.93429400 | 1.45755400 | -3.27069400 |
| H | 1.84770800 | 3.60696900 | -3.11563200 |
| H | 1.76009900 | -0.68881700 | -3.39667000 |
| Cl | 3.66751800 | 1.44128400 | -3.53203900 |

**4**

Electronic energy: -1128.3466279
Vibrational energy: 0.26966918
Gibbs free energy: -1128.138107
Enthalpy: -1128.073182

| | | | |
|---|---|---|---|
| C | -8.07008800 | 0.29847800 | 0.37066500 |
| C | -6.78567300 | 0.83787100 | 0.41043800 |
| C | -6.54187700 | 2.10227200 | -0.13668000 |
| C | -7.59000700 | 2.82822500 | -0.70809700 |
| C | -8.87705900 | 2.28845200 | -0.73458100 |
| C | -9.11794200 | 1.02373900 | -0.19971600 |
| H | -8.25278100 | -0.68533700 | 0.79455200 |
| H | -5.97256400 | 0.27950100 | 0.86798600 |
| H | -7.40023400 | 3.80983700 | -1.13416400 |
| H | -9.68895100 | 2.85694300 | -1.18012000 |
| H | -10.11987200 | 0.60400800 | -0.22508800 |
| S | -4.89741800 | 2.80621900 | -0.07962700 |
| C | -4.10521700 | 1.78382500 | -1.37398900 |
| H | -4.55386700 | 2.01644300 | -2.34400800 |
| H | -4.26686900 | 0.72665800 | -1.14467700 |
| C | -2.61868300 | 2.08472900 | -1.39720200 |
| H | -2.14708800 | 1.79924000 | -0.44937800 |
| H | -2.42768000 | 3.14730000 | -1.59200100 |
| O | -2.07645600 | 1.30189500 | -2.46077000 |
| C | -0.74307600 | 1.35487800 | -2.68881200 |
| C | 0.14847600 | 2.12656800 | -1.92816800 |
| C | -0.27826700 | 0.57306700 | -3.75667800 |
| C | 1.50171500 | 2.10090500 | -2.24035700 |
| H | -0.20081300 | 2.73790800 | -1.10382000 |
| C | 1.07293200 | 0.56027300 | -4.05660700 |
| H | -0.99175100 | -0.01186400 | -4.32967700 |
| C | 1.97715000 | 1.32138000 | -3.30067800 |
| H | 2.19953400 | 2.69337600 | -1.65422200 |
| H | 1.43886600 | -0.04493800 | -4.88361200 |
| C | 3.40389400 | 1.27833200 | -3.64003600 |
| H | 3.66974700 | 0.63471900 | -4.49822300 |
| O | 4.27942100 | 1.89142700 | -3.04622100 |

**5**

Electronic energy: -1167.6514959
Vibrational energy: 0.29961772
Gibbs free energy: -1167.416458
Enthalpy: -1107.013456

| | | | |
|---|---|---|---|
| C | -8.53508700 | 0.80744600 | 0.75038400 |
| C | -7.23862500 | 1.29579900 | 0.92186100 |
| C | -6.61627100 | 1.99928900 | -0.11262900 |
| C | -7.29461800 | 2.21278000 | -1.31763300 |
| C | -8.58199500 | 1.70786700 | -1.48974800 |
| C | -9.20571100 | 1.00728400 | -0.45520600 |

| | | | |
|---|---|---|---|
| H | -9.01595100 | 0.26486400 | 1.55975700 |
| H | -6.71086800 | 1.12818700 | 1.85694000 |
| H | -6.81787300 | 2.77443300 | -2.11727900 |
| H | -9.10204100 | 1.87225800 | -2.42967800 |
| H | -10.21231200 | 0.62063800 | -0.58879000 |
| S | -4.97296300 | 2.66043700 | 0.13273100 |
| C | -4.05670500 | 1.63980800 | -1.07808200 |
| H | -4.50432700 | 1.76235700 | -2.06826800 |
| H | -4.11290300 | 0.58858900 | -0.78142000 |
| C | -2.61122100 | 2.09996800 | -1.10344300 |
| H | -2.14355200 | 1.98998100 | -0.11739100 |
| H | -2.53706100 | 3.14608100 | -1.42472400 |
| O | -1.94510700 | 1.25959200 | -2.04472700 |
| C | -0.61665700 | 1.44293100 | -2.24533500 |
| C | 0.14517500 | 2.42327000 | -1.59772800 |
| C | -0.01386400 | 0.57490300 | -3.16630200 |
| C | 1.50347000 | 2.52003400 | -1.87981100 |
| H | -0.30299200 | 3.10611300 | -0.88472300 |
| C | 1.34000800 | 0.68637600 | -3.43691500 |
| H | -0.62443000 | -0.17818000 | -3.65631600 |
| C | 2.12073300 | 1.66200500 | -2.79573800 |
| H | 2.09687400 | 3.28012800 | -1.37955900 |
| H | 1.78721800 | 0.00340400 | -4.15308200 |
| C | 3.57699000 | 1.80678200 | -3.06607300 |
| C | 4.22138400 | 0.90248700 | -4.08330400 |
| H | 4.11509600 | -0.14632700 | -3.78480800 |
| H | 3.73893500 | 1.01811600 | -5.05995100 |
| H | 5.28100300 | 1.14965800 | -4.16807100 |
| O | 4.24091800 | 2.65018600 | -2.47115200 |

**6**

Electronic energy: -1107.2763272
Vibrational energy: 0.25909404
Gibbs free energy: -1107.076708
Enthalpy: -1107.013456

| | | | |
|---|---|---|---|
| C | -8.91630600 | 0.69173600 | -0.95109900 |
| C | -7.62546200 | 0.16070500 | -0.93205200 |
| C | -6.59311000 | 0.86150400 | -0.30318900 |
| C | -6.85645600 | 2.09275100 | 0.30708800 |
| C | -8.14344900 | 2.62584100 | 0.27078000 |
| C | -9.17617700 | 1.92508200 | -0.35555700 |
| H | -9.71579000 | 0.14248900 | -1.44086000 |
| H | -7.42018300 | -0.79372200 | -1.40946000 |
| H | -6.05727400 | 2.63121800 | 0.81053400 |
| H | -8.34065000 | 3.58499700 | 0.74205500 |

| | | | |
|---|---|---|---|
| H | -10.18039300 | 2.33942500 | -0.37737200 |
| S | -4.94783200 | 0.16037100 | -0.25439900 |
| C | -4.08862700 | 1.36946500 | -1.32579200 |
| H | -4.19417300 | 2.37094600 | -0.89953200 |
| H | -4.53956200 | 1.34918400 | -2.32212300 |
| C | -2.62095900 | 0.99496900 | -1.40776300 |
| H | -2.48990900 | -0.00599400 | -1.83654200 |
| H | -2.14841600 | 1.03202400 | -0.41863800 |
| O | -2.01675600 | 1.96412900 | -2.26447900 |
| C | -0.69125100 | 1.86477100 | -2.52031900 |
| C | -0.16810500 | 2.83714600 | -3.38653600 |
| C | 0.13800100 | 0.87558700 | -1.97966800 |
| C | 1.17529000 | 2.82310400 | -3.71225900 |
| H | -0.83483800 | 3.59166300 | -3.79308500 |
| C | 1.48959000 | 0.86485100 | -2.30920500 |
| H | -0.25075100 | 0.11872900 | -1.30815000 |
| C | 2.01226200 | 1.83242800 | -3.17257100 |
| H | 1.58349200 | 3.57140000 | -4.38482800 |
| H | 2.14046800 | 0.10143400 | -1.89334800 |
| C | 3.40616200 | 1.81338000 | -3.51094800 |
| N | 4.53198800 | 1.80063900 | -3.78703200 |

**7**

Electronic energy: -1219.4892743
Vibrational energy: 0.26368839
Gibbs free energy: -1219.288488
Enthalpy: -1219.221808

| | | | |
|---|---|---|---|
| C | -8.87652300 | 0.62336800 | -0.53779500 |
| C | -7.58441900 | 0.10799200 | -0.65542400 |
| C | -6.50496600 | 0.79964500 | -0.09995800 |
| C | -6.72187500 | 2.00763500 | 0.57216100 |
| C | -8.01149400 | 2.52609400 | 0.67061800 |
| C | -9.09160800 | 1.83358900 | 0.11955500 |
| H | -9.71228600 | 0.08019400 | -0.97073900 |
| H | -7.41574200 | -0.82818000 | -1.18109300 |
| H | -5.88584100 | 2.53801100 | 1.02183900 |
| H | -8.17354500 | 3.46732700 | 1.18904900 |
| H | -10.09686600 | 2.23687000 | 0.20516200 |
| S | -4.86138700 | 0.10554100 | -0.21494500 |
| C | -4.05382200 | 1.41199500 | -1.20792200 |
| H | -4.09443700 | 2.36068700 | -0.66591600 |
| H | -4.57796800 | 1.51477300 | -2.16235200 |
| C | -2.60888900 | 1.01526500 | -1.44500700 |
| H | -2.54507100 | 0.07357700 | -2.00405300 |
| H | -2.06782300 | 0.91120000 | -0.49624400 |

| | | | |
|---|---|---|---|
| O | -2.03102900 | 2.07017400 | -2.21277700 |
| C | -0.72239900 | 1.96603200 | -2.55945700 |
| C | -0.20650900 | 3.03505600 | -3.29667600 |
| C | 0.09710500 | 0.88281700 | -2.22594600 |
| C | 1.12484700 | 2.98206400 | -3.67654800 |
| H | -0.83950300 | 3.87639700 | -3.55548800 |
| C | 1.43266700 | 0.87226700 | -2.63349800 |
| H | -0.28974800 | 0.04604900 | -1.65518900 |
| C | 1.97218400 | 1.92204400 | -3.36562600 |
| H | 2.05804800 | 0.02461600 | -2.37114800 |
| H | 3.00703000 | 1.92101900 | -3.68563600 |
| N | 1.66549200 | 4.10922600 | -4.44570500 |
| O | 0.90973300 | 5.01583300 | -4.75896900 |
| O | 2.85107600 | 4.09112400 | -4.73794800 |

**8**

Electronic energy: -1219.4928316
Vibrational energy: 0.26242945
Gibbs free energy: -1219.291069
Enthalpy: -1219.226626

| | | | |
|---|---|---|---|
| C | -8.19496400 | 0.42081000 | 0.53420400 |
| C | -6.90111800 | 0.93075200 | 0.64027500 |
| C | -6.53294100 | 2.05834200 | -0.10040800 |
| C | -7.46471300 | 2.67784700 | -0.93838500 |
| C | -8.75782500 | 2.16435400 | -1.04047700 |
| C | -9.12360900 | 1.03603700 | -0.30588600 |
| H | -8.47604500 | -0.45611700 | 1.11089600 |
| H | -6.17732000 | 0.45512200 | 1.29718100 |
| H | -7.17878200 | 3.55741300 | -1.50930500 |
| H | -9.47866000 | 2.64785700 | -1.69430300 |
| H | -10.13148300 | 0.63813700 | -0.38669300 |
| S | -4.87332700 | 2.71475900 | 0.03543900 |
| C | -4.08810200 | 1.74180900 | -1.30125800 |
| H | -4.54423300 | 2.01024500 | -2.25853300 |
| H | -4.24723500 | 0.67691000 | -1.10879300 |
| C | -2.60311400 | 2.04829100 | -1.32607800 |
| H | -2.12100500 | 1.73815400 | -0.39160900 |
| H | -2.41737400 | 3.11591300 | -1.49565800 |
| O | -2.06510800 | 1.29533200 | -2.41557700 |
| C | -0.73954900 | 1.36121100 | -2.65413400 |
| C | 0.15676800 | 2.11362600 | -1.88287500 |
| C | -0.28180100 | 0.61146900 | -3.75117600 |
| C | 1.50733700 | 2.10748000 | -2.20773900 |
| H | -0.17983600 | 2.69925800 | -1.03556300 |
| C | 1.06053200 | 0.60582400 | -4.07536100 |

| | | | |
|---|---|---|---|
| H | -0.99824200 | 0.04055700 | -4.33368100 |
| C | 1.94294400 | 1.35668500 | -3.29439200 |
| H | 2.21254600 | 2.68199500 | -1.61749600 |
| H | 1.42292900 | 0.03074000 | -4.92013400 |
| N | 3.35581900 | 1.35087300 | -3.62490800 |
| O | 4.12032300 | 2.02182900 | -2.94286900 |
| O | 3.73060500 | 0.67330600 | -4.57359400 |

**Transition States**

**$TS1_{E1cB}$-1**
Electronic energy: -1169.5071457
Vibrational energy: 0.32631851
Gibbs free energy: -1169.246565
Enthalpy: -1169.17705

| | | | |
|---|---|---|---|
| C | 0.23714500 | -0.05159700 | 0.03551700 |
| H | 0.17394800 | -0.17110300 | 1.58397100 |
| C | 1.63656900 | -0.00690200 | -0.48920000 |
| H | 2.24531300 | 0.70784000 | 0.08126500 |
| H | 2.12400400 | -0.98367900 | -0.42129800 |
| O | 0.01260200 | -0.13708900 | 2.68752100 |
| C | -1.37994400 | -0.05712100 | 2.89287200 |
| H | -1.63221700 | 0.88174900 | 3.41256700 |
| H | -1.89746700 | -0.02449900 | 1.91713900 |
| C | -1.91227400 | -1.23179600 | 3.70370700 |
| H | -1.41643500 | -1.27891200 | 4.68079200 |
| H | -2.99191400 | -1.13317000 | 3.87263500 |
| H | -1.72981100 | -2.17940600 | 3.18335000 |
| O | 1.80534200 | 0.31473100 | -1.91029600 |
| C | 1.55174800 | 1.57657600 | -2.33801400 |
| C | 1.33752200 | 2.67661500 | -1.49661600 |
| C | 1.53626800 | 1.76113100 | -3.72946100 |
| C | 1.12071300 | 3.93909800 | -2.05539600 |
| H | 1.33650600 | 2.56506600 | -0.41815600 |
| C | 1.32038600 | 3.02361300 | -4.26982800 |
| H | 1.70011400 | 0.89784000 | -4.36931200 |
| C | 1.10974600 | 4.12588600 | -3.43578700 |
| H | 0.95559100 | 4.78381900 | -1.39137600 |
| H | 1.31475000 | 3.14717900 | -5.34979700 |
| S | -0.81211000 | -1.25978600 | -0.80460900 |
| C | -0.97016600 | -2.61000900 | 0.35243900 |
| C | -2.19010400 | -3.29371800 | 0.43361000 |
| C | 0.10691700 | -3.05248100 | 1.13134700 |
| C | -2.33004400 | -4.39723000 | 1.27691400 |

| | | | |
|---|---|---|---|
| H | -3.03717600 | -2.95407400 | -0.15859100 |
| C | -0.03830100 | -4.14864700 | 1.97973900 |
| H | 1.05848900 | -2.52985200 | 1.07792400 |
| C | -1.25600200 | -4.82878400 | 2.05603700 |
| H | -3.28614100 | -4.91185500 | 1.33218100 |
| H | 0.80623700 | -4.47529200 | 2.58154100 |
| H | -1.36626700 | -5.68401600 | 2.71710400 |
| H | -0.26730900 | 0.91405800 | -0.09199200 |
| H | 0.93818900 | 5.11187700 | -3.85765000 |

**$TS1_{E1cB}$-2**
Electronic energy: -1208.8037003
Vibrational energy: 0.35576348
Gibbs free energy: -1208.518284
Enthalpy: -1208.44416

| | | | |
|---|---|---|---|
| C | 0.25893500 | -0.05272700 | 0.04276100 |
| H | 0.17339700 | -0.16643800 | 1.59643900 |
| C | 1.66116600 | -0.00914100 | -0.47560900 |
| H | 2.26694600 | 0.70589100 | 0.09799200 |
| H | 2.14800100 | -0.98605300 | -0.40338600 |
| O | -0.01080000 | -0.12871600 | 2.69375200 |
| C | -1.40866600 | -0.06129100 | 2.86809400 |
| H | -1.68208900 | 0.88070800 | 3.37107300 |
| H | -1.90484900 | -0.04610100 | 1.88122900 |
| C | -1.94485200 | -1.23257500 | 3.68076100 |
| H | -1.47836100 | -1.25697200 | 4.67300000 |
| H | -3.03061900 | -1.15072900 | 3.81597400 |
| H | -1.73046000 | -2.18412400 | 3.18017200 |
| O | 1.83676600 | 0.31112500 | -1.89513800 |
| C | 1.57256600 | 1.57372800 | -2.32255900 |
| C | 1.36422800 | 2.67528500 | -1.48672500 |
| C | 1.54075800 | 1.76102700 | -3.71328400 |
| C | 1.13715400 | 3.93656500 | -2.04822500 |
| H | 1.37476700 | 2.57146100 | -0.40729700 |
| C | 1.31504900 | 3.02191400 | -4.24984200 |
| H | 1.70084700 | 0.90056700 | -4.35822800 |
| C | 1.10617900 | 4.13942000 | -3.42769600 |
| H | 0.97748600 | 4.78143600 | -1.38114100 |
| H | 1.29781900 | 3.14327100 | -5.33167000 |
| S | -0.78567300 | -1.26040200 | -0.80461400 |
| C | -0.95379200 | -2.60958800 | 0.35214400 |
| C | -2.17467900 | -3.29267400 | 0.42443700 |
| C | 0.11662600 | -3.05150400 | 1.14040400 |
| C | -2.32183700 | -4.39533500 | 1.26759700 |
| H | -3.01685600 | -2.95323900 | -0.17483100 |

| | | | |
|---|---|---|---|
| C | -0.03575800 | -4.14694200 | 1.98856400 |
| H | 1.06874200 | -2.52912200 | 1.09409400 |
| C | -1.25422100 | -4.82667300 | 2.05565200 |
| H | -3.27861400 | -4.90941200 | 1.31578800 |
| H | 0.80378900 | -4.47329400 | 2.59748800 |
| H | -1.37011400 | -5.68126300 | 2.71659000 |
| H | -0.24384600 | 0.91319300 | -0.09016100 |
| C | 0.84645700 | 5.49987500 | -4.02425700 |
| H | 1.63099600 | 5.77937400 | -4.73641000 |
| H | -0.10595400 | 5.52175000 | -4.56691700 |
| H | 0.80653300 | 6.26914000 | -3.24703600 |

**$TS1_{E1cB}$-3**
Electronic energy: -1629.0787988
Vibrational energy: 0.31763816
Gibbs free energy: -1628.830464
Enthalpy: -1628.757384

| | | | |
|---|---|---|---|
| C | 0.23597100 | -0.05028100 | 0.03503600 |
| H | 0.17625400 | -0.17142800 | 1.56480900 |
| C | 1.63816300 | -0.00487100 | -0.48113400 |
| H | 2.24348300 | 0.71209000 | 0.08996400 |
| H | 2.12693600 | -0.98052600 | -0.41127500 |
| O | 0.01936000 | -0.13787500 | 2.67919100 |
| C | -1.37121400 | -0.05267600 | 2.88995900 |
| H | -1.61904200 | 0.88619500 | 3.41230500 |
| H | -1.89300800 | -0.01598800 | 1.91615900 |
| C | -1.90690800 | -1.22659400 | 3.70022700 |
| H | -1.40863000 | -1.27769300 | 4.67590400 |
| H | -2.98571200 | -1.12372000 | 3.87222300 |
| H | -1.72984000 | -2.17406700 | 3.17770200 |
| O | 1.81175900 | 0.31605200 | -1.90324600 |
| C | 1.55358900 | 1.57316900 | -2.33166000 |
| C | 1.33090600 | 2.67313300 | -1.49283300 |
| C | 1.54051900 | 1.75887200 | -3.72269100 |
| C | 1.10751800 | 3.93617000 | -2.04376800 |
| H | 1.32790300 | 2.56797200 | -0.41410600 |
| C | 1.32018200 | 3.01543900 | -4.27117400 |
| H | 1.71005000 | 0.90029400 | -4.36649200 |
| C | 1.10385100 | 4.09915800 | -3.42233800 |
| H | 0.93489800 | 4.78551200 | -1.38941000 |
| H | 1.31499400 | 3.14904300 | -5.34887400 |
| S | -0.80754200 | -1.26038800 | -0.81030400 |
| C | -0.96869300 | -2.60936300 | 0.34778700 |
| C | -2.19043300 | -3.28946700 | 0.43003700 |
| C | 0.10785600 | -3.05402300 | 1.12612500 |

| | | | |
|---|---|---|---|
| C | -2.33270700 | -4.39212100 | 1.27413000 |
| H | -3.03693200 | -2.94790000 | -0.16181300 |
| C | -0.03987800 | -4.14897900 | 1.97559400 |
| H | 1.06093400 | -2.53429000 | 1.07165200 |
| C | -1.25936500 | -4.82578400 | 2.05294700 |
| H | -3.29004600 | -4.90430700 | 1.33021700 |
| H | 0.80404700 | -4.47732200 | 2.57730200 |
| H | -1.37151400 | -5.68019200 | 2.71475700 |
| H | -0.26880900 | 0.91483400 | -0.09489800 |
| Cl | 0.81906700 | 5.68979000 | -4.10698700 |

**$TS1_{E1cB}$-4**
Electronic energy: -1282.80285
Vibrational energy: 0.337751
Gibbs free energy: -1282.535362
Enthalpy: -1282.461329

| | | | |
|---|---|---|---|
| C | 0.05447000 | -0.08289500 | -0.07231200 |
| H | -0.05732300 | -0.09039000 | 1.44100000 |
| C | 1.46428300 | 0.05240600 | -0.54841700 |
| H | 1.99586200 | 0.84488500 | -0.00597200 |
| H | 2.02665800 | -0.87574800 | -0.42009800 |
| O | -0.27243800 | 0.00946000 | 2.55226000 |
| C | -1.66927700 | -0.09346100 | 2.70280500 |
| H | -2.08170800 | 0.85100300 | 3.09578600 |
| H | -2.13983000 | -0.25189800 | 1.71509900 |
| C | -2.06609900 | -1.23192700 | 3.63417800 |
| H | -1.62558300 | -1.08547300 | 4.62789000 |
| H | -3.15612600 | -1.28420200 | 3.74844700 |
| H | -1.71358300 | -2.19404700 | 3.24383100 |
| O | 1.64896700 | 0.32013900 | -1.98403100 |
| C | 1.37840600 | 1.54152600 | -2.46950500 |
| C | 1.01893800 | 2.65172700 | -1.68679700 |
| C | 1.49453300 | 1.68078000 | -3.86988400 |
| C | 0.79439200 | 3.87523600 | -2.30860500 |
| H | 0.91548900 | 2.57272800 | -0.61108900 |
| C | 1.26877500 | 2.90146200 | -4.47214200 |
| H | 1.76918500 | 0.80674200 | -4.45373500 |
| C | 0.91509100 | 4.01916100 | -3.69445600 |
| H | 0.51908200 | 4.73742600 | -1.70415700 |
| H | 1.36336800 | 3.00504100 | -5.55005400 |
| S | -0.84069900 | -1.45489500 | -0.83883300 |
| C | -0.88217400 | -2.72392300 | 0.41605200 |
| C | -2.02708800 | -3.52217300 | 0.53387200 |
| C | 0.22007800 | -2.99541200 | 1.23683400 |
| C | -2.06684200 | -4.57367900 | 1.45114100 |

| | | | |
|---|---|---|---|
| H | -2.89457500 | -3.31497300 | -0.08922200 |
| C | 0.17421400 | -4.04010800 | 2.15824500 |
| H | 1.11468900 | -2.38307800 | 1.15776800 |
| C | -0.96730000 | -4.83735200 | 2.26854400 |
| H | -2.96578800 | -5.17962700 | 1.53278900 |
| H | 1.03756500 | -4.23415700 | 2.78999500 |
| H | -0.99964300 | -5.65234400 | 2.98649700 |
| H | -0.53259300 | 0.81473100 | -0.30166600 |
| C | 0.67245400 | 5.32850700 | -4.29823000 |
| O | 0.75362300 | 5.57259800 | -5.49561600 |
| H | 0.39969500 | 6.13497400 | -3.59322200 |

**$TS1_{E1cB}$-5**
Electronic energy: -1322.1072047
Vibrational energy: 0.36749079
Gibbs free energy: -1321.81386
Enthalpy: -1321.735937

| | | | |
|---|---|---|---|
| C | 0.08560400 | -0.09156600 | -0.06197000 |
| H | -0.04902500 | -0.08897700 | 1.45150300 |
| C | 1.49549100 | 0.04163500 | -0.54094000 |
| H | 2.03187200 | 0.82773400 | 0.00613900 |
| H | 2.05454800 | -0.88967300 | -0.41957000 |
| O | -0.28951700 | 0.02187100 | 2.55568600 |
| C | -1.69058000 | -0.06846500 | 2.67263100 |
| H | -2.10260800 | 0.87858100 | 3.05967800 |
| H | -2.13888200 | -0.21830600 | 1.67340500 |
| C | -2.12310100 | -1.20591800 | 3.58922100 |
| H | -1.70229000 | -1.07055100 | 4.59296700 |
| H | -3.21609000 | -1.24215300 | 3.67884900 |
| H | -1.77710500 | -2.17174700 | 3.20202200 |
| O | 1.67372200 | 0.31838800 | -1.97416300 |
| C | 1.38258500 | 1.54233700 | -2.44941200 |
| C | 1.04778200 | 2.65029300 | -1.65482500 |
| C | 1.44816900 | 1.69105400 | -3.84853800 |
| C | 0.79742100 | 3.87842700 | -2.26004400 |
| H | 0.98062100 | 2.56938200 | -0.57623500 |
| C | 1.19536900 | 2.91697800 | -4.43388700 |
| H | 1.70347700 | 0.82352800 | -4.45080400 |
| C | 0.86554500 | 4.03600200 | -3.64907900 |
| H | 0.54349000 | 4.72139700 | -1.62368700 |
| H | 1.25015700 | 3.02193800 | -5.51375900 |
| S | -0.80797200 | -1.46395000 | -0.82910800 |
| C | -0.84129600 | -2.73544900 | 0.42233900 |
| C | -1.96106300 | -3.57358900 | 0.50222600 |
| C | 0.24205700 | -2.96904900 | 1.27895400 |

| | | | |
|---|---|---|---|
| C | -1.99597100 | -4.62401900 | 1.42049700 |
| H | -2.81360700 | -3.39727300 | -0.15037600 |
| C | 0.20067700 | -4.01376000 | 2.20065300 |
| H | 1.11670300 | -2.32589400 | 1.22830400 |
| C | -0.91654900 | -4.84842800 | 2.27595200 |
| H | -2.87566500 | -5.26073100 | 1.47290800 |
| H | 1.04872200 | -4.17776400 | 2.86103600 |
| H | -0.94552300 | -5.66261500 | 2.99495100 |
| H | -0.50007900 | 0.80552400 | -0.29782400 |
| C | 0.60137600 | 5.33955400 | -4.30637600 |
| C | 0.25424700 | 6.53183500 | -3.45242100 |
| H | -0.65225000 | 6.33694600 | -2.86929300 |
| H | 1.06236400 | 6.74585600 | -2.74476500 |
| H | 0.09358900 | 7.40002600 | -4.09381800 |
| O | 0.66594900 | 5.45072100 | -5.52853200 |

**$TS1_{E1cB}$-6**
Electronic energy: -1261.7322134
Vibrational energy: 0.32650337
Gibbs free energy: -1261.475865
Enthalpy: -1261.401934

| | | | |
|---|---|---|---|
| C | 0.21632300 | -0.03583700 | 0.04157900 |
| H | 0.16926000 | -0.16735100 | 1.55000100 |
| C | 1.61935400 | 0.01897100 | -0.46805000 |
| H | 2.21900400 | 0.74279000 | 0.09902700 |
| H | 2.11585800 | -0.95237800 | -0.40043800 |
| O | 0.02425200 | -0.14157000 | 2.67820100 |
| C | -1.36325500 | -0.05837900 | 2.90359200 |
| H | -1.60781100 | 0.87734700 | 3.43363200 |
| H | -1.89586300 | -0.01654600 | 1.93529200 |
| C | -1.89134200 | -1.23698100 | 3.71248800 |
| H | -1.38429200 | -1.29284100 | 4.68341100 |
| H | -2.96875200 | -1.13629400 | 3.89448000 |
| H | -1.71796300 | -2.18157500 | 3.18344500 |
| O | 1.78918400 | 0.34043500 | -1.89481000 |
| C | 1.54380800 | 1.58727800 | -2.32872500 |
| C | 1.29958700 | 2.69005600 | -1.49259700 |
| C | 1.56293600 | 1.76471500 | -3.72505400 |
| C | 1.08715200 | 3.94412700 | -2.05204000 |
| H | 1.27550300 | 2.58364000 | -0.41472100 |
| C | 1.35171300 | 3.01346000 | -4.27874000 |
| H | 1.74964600 | 0.90082000 | -4.35615600 |
| C | 1.11045900 | 4.11538400 | -3.44101400 |
| H | 0.89995500 | 4.79680900 | -1.40597500 |
| H | 1.36944000 | 3.14549300 | -5.35648200 |

| | | | |
|---|---|---|---|
| S | -0.81789900 | -1.24966500 | -0.81052900 |
| C | -0.97394500 | -2.60325600 | 0.34302600 |
| C | -2.19726900 | -3.27938800 | 0.43152800 |
| C | 0.10783100 | -3.05556300 | 1.10963900 |
| C | -2.33599000 | -4.38661500 | 1.27028600 |
| H | -3.04748600 | -2.93153500 | -0.15117600 |
| C | -0.03654500 | -4.15467700 | 1.95423700 |
| H | 1.06247200 | -2.53927000 | 1.04976600 |
| C | -1.25756300 | -4.82802900 | 2.03747600 |
| H | -3.29435900 | -4.89626300 | 1.33124700 |
| H | 0.81118900 | -4.48924000 | 2.54703100 |
| H | -1.36688100 | -5.68607500 | 2.69502500 |
| H | -0.29319700 | 0.92701300 | -0.08531200 |
| C | 0.88727900 | 5.41228000 | -4.00797500 |
| N | 0.70629700 | 6.46174500 | -4.46746500 |

**$TS1_{E1cB}$-7**
Electronic energy: -1373.9452102
Vibrational energy: 0.33125708
Gibbs free energy: -1373.686756
Enthalpy: -1373.610176

| | | | |
|---|---|---|---|
| C | -0.00042300 | 0.19106600 | -0.08444400 |
| H | -0.14658200 | 0.38786400 | 1.40715100 |
| C | 1.42634800 | 0.16653800 | -0.52793700 |
| H | 1.98780400 | 1.00723300 | -0.09934300 |
| H | 1.92942000 | -0.75645900 | -0.22883700 |
| O | -0.38488400 | 0.65003000 | 2.49180300 |
| C | -1.78823800 | 0.72387800 | 2.58474300 |
| H | -2.09987400 | 1.74511700 | 2.86139400 |
| H | -2.23848700 | 0.51700200 | 1.59635900 |
| C | -2.35200400 | -0.25863600 | 3.60359000 |
| H | -1.94353300 | -0.05492200 | 4.60084800 |
| H | -3.44523000 | -0.18299300 | 3.65946600 |
| H | -2.09163600 | -1.28917300 | 3.33352300 |
| O | 1.66566400 | 0.17719200 | -1.98001000 |
| C | 1.35593800 | 1.28252500 | -2.68705600 |
| C | 1.06699500 | 2.53752600 | -2.12874000 |
| C | 1.35802200 | 1.13707200 | -4.07991300 |
| C | 0.79220300 | 3.62653000 | -2.95701700 |
| H | 1.05755700 | 2.67802000 | -1.05409800 |
| C | 1.07988600 | 2.24635200 | -4.86388600 |
| H | 1.57346200 | 0.17058900 | -4.52156000 |
| C | 0.79170000 | 3.50392700 | -4.34170400 |
| H | 0.57401600 | 4.58991800 | -2.50637600 |
| S | -0.97514600 | -1.20012600 | -0.70521500 |

| | | | |
|---|---|---|---|
| C | -1.15771200 | -2.29073900 | 0.69568800 |
| C | -2.36475300 | -2.98242900 | 0.85881100 |
| C | -0.11058900 | -2.53267900 | 1.59423700 |
| C | -2.52168200 | -3.89745400 | 1.90107500 |
| H | -3.18877600 | -2.79611000 | 0.17329000 |
| C | -0.27431100 | -3.43837600 | 2.64083400 |
| H | 0.83202000 | -2.00397700 | 1.47770300 |
| C | -1.47876900 | -4.12780500 | 2.79884900 |
| H | -3.46710200 | -4.42171500 | 2.01645700 |
| H | 0.54643100 | -3.60985700 | 3.33299200 |
| H | -1.60232400 | -4.83580600 | 3.61375800 |
| H | -0.51534800 | 1.09168900 | -0.44068100 |
| N | 1.08823600 | 2.07813100 | -6.32084100 |
| H | 0.57967000 | 4.34578700 | -4.98930400 |
| O | 0.78267100 | 3.03576600 | -7.01577100 |
| O | 1.39964300 | 0.98995700 | -6.78041200 |

**$TS1_{E1cB}$-8**
Electronic energy: -1373.9486741
Vibrational energy: 0.33091446
Gibbs free energy: -1373.692178
Enthalpy: -1373.613983

| | | | |
|---|---|---|---|
| C | -0.28066100 | 0.20965700 | -0.01973200 |
| H | -0.27395100 | 0.50087000 | 1.43720800 |
| C | 1.13591800 | 0.09886600 | -0.48844700 |
| H | 1.76098900 | 0.89318300 | -0.06050800 |
| H | 1.57836300 | -0.86119600 | -0.21089600 |
| O | -0.28967500 | 0.86369600 | 2.53616800 |
| C | -1.61156900 | 0.71868400 | 2.99660200 |
| H | -2.13070300 | 1.69303400 | 3.00957500 |
| H | -2.18363900 | 0.07241700 | 2.30515800 |
| C | -1.65648600 | 0.11740200 | 4.39402300 |
| H | -1.11338500 | 0.75455400 | 5.10221800 |
| H | -2.68948100 | 0.01429200 | 4.74859100 |
| H | -1.18880100 | -0.87446500 | 4.39928600 |
| O | 1.34805600 | 0.11865900 | -1.94460700 |
| C | 1.20211500 | 1.26247500 | -2.62102300 |
| C | 0.98341200 | 2.51981200 | -2.02684000 |
| C | 1.30079500 | 1.16176100 | -4.02424400 |
| C | 0.87676400 | 3.64874700 | -2.82533300 |
| H | 0.89920500 | 2.62829200 | -0.95259900 |
| C | 1.19423400 | 2.28435500 | -4.81958600 |
| H | 1.46538100 | 0.18324900 | -4.46480200 |
| C | 0.98246700 | 3.52427200 | -4.20879700 |
| H | 0.71194800 | 4.62065800 | -2.37352600 |

| | | | |
|---|---|---|---|
| H | 1.27261800 | 2.20785500 | -5.89828800 |
| S | -1.34090100 | -1.12359700 | -0.62288700 |
| C | -1.42829100 | -2.31148300 | 0.69904000 |
| C | -2.47388800 | -3.24713200 | 0.66720300 |
| C | -0.48042600 | -2.39135400 | 1.72563000 |
| C | -2.57098700 | -4.23413100 | 1.64587100 |
| H | -3.21971900 | -3.19610000 | -0.12377800 |
| C | -0.58774400 | -3.37706900 | 2.70791200 |
| H | 0.33713900 | -1.67786100 | 1.76130300 |
| C | -1.62977600 | -4.30389300 | 2.67567500 |
| H | -3.39086800 | -4.94706500 | 1.60727400 |
| H | 0.15514300 | -3.41898200 | 3.50105800 |
| H | -1.70771400 | -5.07076700 | 3.44134500 |
| H | -0.75390100 | 1.12971900 | -0.38318900 |
| N | 0.87271600 | 4.70640100 | -5.03306800 |
| O | 0.96755300 | 4.58527300 | -6.24986600 |
| O | 0.69051700 | 5.79050400 | -4.48929700 |

**$I_{E1cB}$-1**
Electronic Energy: -1169.5072695
Vibrational energy: 0.32907225
Gibbs free energy: -1169.244423
Enthalpy: -1169.174421

| | | | |
|---|---|---|---|
| C | 0.35441000 | 0.28487000 | -0.21107800 |
| H | 0.36646700 | 0.30680600 | 1.40666500 |
| C | 1.70603700 | 0.25686900 | -0.84317700 |
| H | 2.38256700 | 0.97863100 | -0.36521800 |
| H | 2.16807500 | -0.73156200 | -0.76407300 |
| O | 0.23828700 | 0.44669800 | 2.47334800 |
| C | -1.14967700 | 0.57112800 | 2.70797000 |
| H | -1.37052600 | 1.56658200 | 3.12509100 |
| H | -1.69346100 | 0.49967500 | 1.75054000 |
| C | -1.66408700 | -0.49693100 | 3.66213700 |
| H | -1.13580900 | -0.44062600 | 4.62153500 |
| H | -2.73611200 | -0.36395800 | 3.85364100 |
| H | -1.50967200 | -1.49883200 | 3.24449500 |
| O | 1.77518300 | 0.50432600 | -2.29212100 |
| C | 1.53073300 | 1.75462700 | -2.75585700 |
| C | 1.39479100 | 2.89255300 | -1.94889100 |
| C | 1.43814700 | 1.88680800 | -4.15036400 |
| C | 1.17810100 | 4.13817800 | -2.54415500 |
| H | 1.45348800 | 2.82342100 | -0.86829500 |
| C | 1.22295300 | 3.13305800 | -4.72730300 |
| H | 1.54115500 | 0.99561400 | -4.76445500 |
| C | 1.09048400 | 4.27219200 | -3.92774100 |

| | | | |
|---|---|---|---|
| H | 1.07566600 | 5.01230500 | -1.90566400 |
| H | 1.15705300 | 3.21489100 | -5.80945200 |
| S | -0.77581800 | -0.96040600 | -0.86049900 |
| C | -0.87027000 | -2.20823600 | 0.41406300 |
| C | -2.07586700 | -2.89868400 | 0.59310700 |
| C | 0.23878200 | -2.57073800 | 1.18890800 |
| C | -2.17046100 | -3.93020200 | 1.52841400 |
| H | -2.94752500 | -2.62149200 | 0.00347600 |
| C | 0.13953000 | -3.59624500 | 2.12757000 |
| H | 1.17875700 | -2.04002600 | 1.05921400 |
| C | -1.06402600 | -4.28296700 | 2.30243800 |
| H | -3.11645100 | -4.45022300 | 1.65878100 |
| H | 1.00953000 | -3.86226800 | 2.72320900 |
| H | -1.13897600 | -5.08221000 | 3.03490400 |
| H | -0.14273000 | 1.25058400 | -0.36253300 |
| H | 0.92127200 | 5.24579300 | -4.37863200 |

**$I_{E1cB}$-2**
Electronic energy: -1208.803771 Hartree
Vibrational energy: 0.35825428
Gibbs free energy: -1208.516973
Enthalpy: -1208.44174

| | | | |
|---|---|---|---|
| C | 0.35292600 | 0.28014600 | -0.21210000 |
| H | 0.36677800 | 0.29933600 | 1.39489300 |
| C | 1.70654600 | 0.24974500 | -0.84221200 |
| H | 2.38211800 | 0.97053100 | -0.36078600 |
| H | 2.16670000 | -0.73942000 | -0.75984500 |
| O | 0.24257800 | 0.43672200 | 2.46738200 |
| C | -1.14355400 | 0.56676500 | 2.70667900 |
| H | -1.35997200 | 1.56337100 | 3.12380800 |
| H | -1.69118300 | 0.49665300 | 1.75110200 |
| C | -1.65960500 | -0.49842900 | 3.66334600 |
| H | -1.12814600 | -0.44352700 | 4.62109500 |
| H | -2.73052200 | -0.36103300 | 3.85797200 |
| H | -1.51040400 | -1.50128200 | 3.24613800 |
| O | 1.77986800 | 0.49713000 | -2.28855300 |
| C | 1.53593600 | 1.75175400 | -2.74895200 |
| C | 1.39903200 | 2.88809000 | -1.94510200 |
| C | 1.44193400 | 1.89229700 | -4.14232300 |
| C | 1.17997500 | 4.13520700 | -2.54026800 |
| H | 1.45481100 | 2.82190500 | -0.86398600 |
| C | 1.22583600 | 3.13993200 | -4.71264900 |
| H | 1.54214800 | 1.00537400 | -4.76335800 |
| C | 1.09016100 | 4.29140700 | -3.92312400 |
| H | 1.07410900 | 5.00650900 | -1.89639500 |

| | | | |
|---|---|---|---|
| H | 1.15829900 | 3.22298800 | -5.79629700 |
| S | -0.77865000 | -0.96351000 | -0.86437100 |
| C | -0.87752700 | -2.21050500 | 0.41039800 |
| C | -2.08656100 | -2.89409600 | 0.59267100 |
| C | 0.23145600 | -2.57928900 | 1.18249000 |
| C | -2.18461600 | -3.92506400 | 1.52827300 |
| H | -2.95813300 | -2.61203600 | 0.00524700 |
| C | 0.12873200 | -3.60406100 | 2.12155700 |
| H | 1.17414100 | -2.05407500 | 1.05037300 |
| C | -1.07824700 | -4.28402700 | 2.29948200 |
| H | -3.13322200 | -4.43967100 | 1.66108900 |
| H | 0.99867200 | -3.87481700 | 2.71513300 |
| H | -1.15588100 | -5.08271700 | 3.03225900 |
| H | -0.14228900 | 1.24617700 | -0.36806400 |
| C | 0.86716300 | 5.64135600 | -4.55711700 |
| H | 1.76346600 | 5.98414300 | -5.08817600 |
| H | 0.05130900 | 5.60877000 | -5.28782700 |
| H | 0.61817100 | 6.39473100 | -3.80344600 |

**$I_{E1cB}$-3**
Electronic energy: -1629.078839
Vibrational energy: 0.32083493
Gibbs free energy: -1628.828208
Enthalpy: -1628.754228

| | | | |
|---|---|---|---|
| C | 0.37681700 | 0.28833400 | -0.20624300 |
| H | 0.38281600 | 0.30058500 | 1.43248700 |
| C | 1.72753800 | 0.25921000 | -0.83505000 |
| H | 2.40451700 | 0.98182200 | -0.35932300 |
| H | 2.19005900 | -0.72899200 | -0.75904800 |
| O | 0.24512800 | 0.43357000 | 2.48965900 |
| C | -1.14472600 | 0.56952000 | 2.71090600 |
| H | -1.36060700 | 1.56776000 | 3.12338700 |
| H | -1.67988600 | 0.49924000 | 1.74898600 |
| C | -1.67338100 | -0.49236700 | 3.66353200 |
| H | -1.15173500 | -0.43736500 | 4.62656500 |
| H | -2.74571100 | -0.35128900 | 3.84690300 |
| H | -1.52295100 | -1.49622700 | 3.24906900 |
| O | 1.80025700 | 0.50668000 | -2.28844500 |
| C | 1.54090300 | 1.74958800 | -2.75271200 |
| C | 1.40150300 | 2.88932400 | -1.94907200 |
| C | 1.43399700 | 1.87961100 | -4.14624000 |
| C | 1.16631000 | 4.13358900 | -2.53634100 |
| H | 1.47246700 | 2.82940300 | -0.86901900 |
| C | 1.20116000 | 3.11732500 | -4.73109200 |
| H | 1.53896500 | 0.99190300 | -4.76411400 |

| | | | |
|---|---|---|---|
| C | 1.06769100 | 4.23990400 | -3.91680700 |
| H | 1.06021500 | 5.01360300 | -1.90838500 |
| H | 1.12252100 | 3.20573700 | -5.81074100 |
| S | -0.75861900 | -0.94615900 | -0.86248900 |
| C | -0.86402500 | -2.19832100 | 0.40731900 |
| C | -2.07279100 | -2.88517900 | 0.57855000 |
| C | 0.24016000 | -2.56702300 | 1.18598100 |
| C | -2.17525000 | -3.91907800 | 1.51045400 |
| H | -2.94076700 | -2.60343800 | -0.01436500 |
| C | 0.13309700 | -3.59490700 | 2.12118400 |
| H | 1.18243800 | -2.03904900 | 1.06194000 |
| C | -1.07365900 | -4.27790100 | 2.28857400 |
| H | -3.12363800 | -4.43616100 | 1.63497800 |
| H | 0.99949100 | -3.86570100 | 2.71992000 |
| H | -1.15477700 | -5.07882400 | 3.01851100 |
| H | -0.11570700 | 1.25860800 | -0.34129000 |
| Cl | 0.76630800 | 5.80708000 | -4.64723800 |

**$I_{E1cB}$-4**
Electronic energy: -1282.8030838
Vibrational energy: 0.34112147
Gibbs free energy: -1282.533725
Enthalpy: -1282.458185

| | | | |
|---|---|---|---|
| C | 0.37281700 | 0.28731900 | -0.21233800 |
| H | 0.36650200 | 0.31301500 | 1.44991200 |
| C | 1.72329600 | 0.27191800 | -0.83372300 |
| H | 2.39597300 | 0.99946000 | -0.36146400 |
| H | 2.19383400 | -0.71280300 | -0.76932800 |
| O | 0.21118800 | 0.45557500 | 2.49338300 |
| C | -1.18518400 | 0.57146200 | 2.69089300 |
| H | -1.42087600 | 1.56743100 | 3.09701800 |
| H | -1.70252000 | 0.49094600 | 1.72055300 |
| C | -1.71263700 | -0.49610300 | 3.63748500 |
| H | -1.20870600 | -0.42995600 | 4.60915000 |
| H | -2.78997100 | -0.37110200 | 3.80217600 |
| H | -1.53973000 | -1.49871000 | 3.22875000 |
| O | 1.79409700 | 0.52978500 | -2.29467400 |
| C | 1.55260800 | 1.76442100 | -2.75606000 |
| C | 1.39039900 | 2.90214000 | -1.94636900 |
| C | 1.48365000 | 1.89329900 | -4.16092500 |
| C | 1.17201900 | 4.13735500 | -2.54588500 |
| H | 1.43362300 | 2.83297400 | -0.86581800 |
| C | 1.26530900 | 3.12593300 | -4.74143000 |
| H | 1.60877900 | 0.99986300 | -4.76658100 |
| C | 1.10562800 | 4.26855300 | -3.93683100 |

| | | | |
|---|---|---|---|
| H | 1.04870100 | 5.01913500 | -1.91950500 |
| H | 1.21485900 | 3.21939200 | -5.82339400 |
| S | -0.74751300 | -0.95902600 | -0.86632500 |
| C | -0.85254300 | -2.20593600 | 0.40950000 |
| C | -2.05530000 | -2.90590600 | 0.56901700 |
| C | 0.24588400 | -2.55710000 | 1.20390900 |
| C | -2.15730700 | -3.93610000 | 1.50498100 |
| H | -2.91905800 | -2.63717200 | -0.03599800 |
| C | 0.13926800 | -3.58170200 | 2.14282400 |
| H | 1.18331200 | -2.01840300 | 1.08870300 |
| C | -1.06136500 | -4.27796500 | 2.29860900 |
| H | -3.10102600 | -4.46372500 | 1.62041800 |
| H | 1.00134000 | -3.83971800 | 2.75334700 |
| H | -1.14218600 | -5.07627000 | 3.03143500 |
| H | -0.12832400 | 1.25379900 | -0.34007500 |
| C | 0.87174100 | 5.58964600 | -4.51686800 |
| H | 0.76092200 | 6.41536900 | -3.79023400 |
| O | 0.79419700 | 5.82439800 | -5.71656900 |

**$I_{E1cB}$-5**
Electronic energy: -1322.1072591
Vibrational energy: 0.37038158
Gibbs free energy: -1321.813734
Enthalpy: -1321.7331

| | | | |
|---|---|---|---|
| C | 0.31615700 | 0.30770400 | -0.22365200 |
| H | 0.24238700 | 0.39123800 | 1.42976000 |
| C | 1.68961200 | 0.38310500 | -0.79099600 |
| H | 2.27105900 | 1.19070800 | -0.32704900 |
| H | 2.24080400 | -0.55109800 | -0.65349900 |
| O | 0.03751900 | 0.55325100 | 2.46450100 |
| C | -1.36887300 | 0.52442200 | 2.61812500 |
| H | -1.72185500 | 1.50104100 | 2.98426400 |
| H | -1.84387500 | 0.36147600 | 1.63654900 |
| C | -1.80997900 | -0.56487800 | 3.58453200 |
| H | -1.36132700 | -0.40671800 | 4.57265200 |
| H | -2.90075700 | -0.56394800 | 3.70118200 |
| H | -1.50059700 | -1.55288100 | 3.22418800 |
| O | 1.80748000 | 0.57193800 | -2.25721100 |
| C | 1.46341200 | 1.75123700 | -2.79908600 |
| C | 1.14593100 | 2.90656100 | -2.06588500 |
| C | 1.44993300 | 1.80588000 | -4.20701900 |
| C | 0.82654800 | 4.08239400 | -2.73814200 |
| H | 1.14503800 | 2.90034900 | -0.98226500 |
| C | 1.13281700 | 2.98189500 | -4.85963900 |
| H | 1.69562100 | 0.90556000 | -4.76350700 |

| | | | |
|---|---|---|---|
| C | 0.81248200 | 4.14416300 | -4.13638500 |
| H | 0.58327800 | 4.96146800 | -2.14793900 |
| H | 1.12735400 | 3.01206100 | -5.94577400 |
| S | -0.67255600 | -1.04794000 | -0.87624200 |
| C | -0.74451500 | -2.25652400 | 0.43885200 |
| C | -1.91505800 | -3.00904700 | 0.59619200 |
| C | 0.35191100 | -2.52790100 | 1.26690700 |
| C | -1.98719000 | -4.01551700 | 1.56021900 |
| H | -2.77779400 | -2.79941700 | -0.03319300 |
| C | 0.27474800 | -3.52901300 | 2.23385800 |
| H | 1.26555000 | -1.94857400 | 1.15547200 |
| C | -0.89313700 | -4.27982800 | 2.38505500 |
| H | -2.90665400 | -4.58500200 | 1.67285700 |
| H | 1.13447300 | -3.72637800 | 2.86997500 |
| H | -0.95040200 | -5.06019600 | 3.13928400 |
| H | -0.25774700 | 1.22258200 | -0.41070200 |
| C | 0.47044700 | 5.38936800 | -4.86600000 |
| C | 0.11763000 | 6.62535800 | -4.07891400 |
| H | -0.75510700 | 6.43928600 | -3.44358900 |
| H | 0.94736000 | 6.91566700 | -3.42531700 |
| H | -0.10292200 | 7.44118900 | -4.76963200 |
| O | 0.47159700 | 5.41792700 | -6.09476500 |

**$I_{E1cB}$-6**
Electronic energy: -1261.7325391
Vibrational energy: 0.33015112
Gibbs free energy: -1261.475865
Enthalpy: -1261.398612

| | | | |
|---|---|---|---|
| C | 0.36502000 | 0.30610500 | -0.20107100 |
| H | 0.38512000 | 0.30137900 | 1.46298700 |
| C | 1.70778400 | 0.27707400 | -0.83882900 |
| H | 2.39218500 | 0.99872400 | -0.37429500 |
| H | 2.17039300 | -0.71167700 | -0.77847600 |
| O | 0.25414400 | 0.42123400 | 2.51231300 |
| C | -1.13538300 | 0.55140600 | 2.74595500 |
| H | -1.34903100 | 1.54621300 | 3.16702800 |
| H | -1.67794200 | 0.48620800 | 1.78824300 |
| C | -1.65073400 | -0.51858800 | 3.69615200 |
| H | -1.11833800 | -0.46979500 | 4.65355700 |
| H | -2.72109300 | -0.38028900 | 3.89230000 |
| H | -1.50379500 | -1.51901400 | 3.27245100 |
| O | 1.76606800 | 0.53044000 | -2.30095200 |
| C | 1.52292900 | 1.76459900 | -2.76495100 |
| C | 1.38278800 | 2.90737900 | -1.95775500 |
| C | 1.43021600 | 1.89054600 | -4.16456200 |

| | | | |
|---|---|---|---|
| C | 1.16404700 | 4.14592300 | -2.54778700 |
| H | 1.44504200 | 2.84314300 | -0.87787300 |
| C | 1.21210000 | 3.12400900 | -4.74880100 |
| H | 1.53620700 | 0.99807900 | -4.77462700 |
| C | 1.07680700 | 4.26445300 | -3.93969500 |
| H | 1.05942300 | 5.02868200 | -1.92334000 |
| H | 1.14425100 | 3.21437400 | -5.82906900 |
| S | -0.78253500 | -0.91553700 | -0.85481500 |
| C | -0.87655500 | -2.18171100 | 0.40237100 |
| C | -2.08382300 | -2.86973400 | 0.57874300 |
| C | 0.23569500 | -2.55926100 | 1.16489000 |
| C | -2.17696300 | -3.91328300 | 1.50082700 |
| H | -2.95771600 | -2.58173100 | -0.00240400 |
| C | 0.13795700 | -3.59682100 | 2.09041200 |
| H | 1.17694200 | -2.03056300 | 1.03645100 |
| C | -1.06740400 | -4.28082200 | 2.26341800 |
| H | -3.12426200 | -4.43122200 | 1.62988600 |
| H | 1.01035100 | -3.87405400 | 2.67737900 |
| H | -1.14130800 | -5.08922000 | 2.98586800 |
| H | -0.12354800 | 1.28116100 | -0.31087900 |
| C | 0.85039600 | 5.54624400 | -4.53800200 |
| N | 0.66845200 | 6.58410600 | -5.02296500 |

**$I_{E1cB}$-7**
Electronic energy: -1373.9455189
Vibrational energy: 0.33493352
Gibbs free energy: -1373.683091
Enthalpy: -1373.606809

| | | | |
|---|---|---|---|
| C | 0.39849600 | 0.28225100 | -0.21522900 |
| H | 0.39965800 | 0.29287300 | 1.44851500 |
| C | 1.74499600 | 0.23772000 | -0.84441700 |
| H | 2.43398900 | 0.95216700 | -0.37496600 |
| H | 2.19673200 | -0.75572900 | -0.77823300 |
| O | 0.25232600 | 0.42581200 | 2.49414700 |
| C | -1.13929300 | 0.57612600 | 2.70092600 |
| H | -1.34832300 | 1.57905300 | 3.10474800 |
| H | -1.66565400 | 0.50376300 | 1.73489000 |
| C | -1.68359700 | -0.47489000 | 3.65625100 |
| H | -1.16953300 | -0.41705300 | 4.62312000 |
| H | -2.75614800 | -0.32419300 | 3.82986300 |
| H | -1.53744200 | -1.48257100 | 3.24961800 |
| O | 1.81695800 | 0.48760100 | -2.30520100 |
| C | 1.55319700 | 1.72443900 | -2.76593100 |
| C | 1.42727500 | 2.87022900 | -1.96369800 |
| C | 1.42522900 | 1.84781900 | -4.15577400 |

| | | | |
|---|---|---|---|
| C | 1.19006200 | 4.11453500 | -2.54914800 |
| H | 1.51678800 | 2.80499600 | -0.88539100 |
| C | 1.19293200 | 3.10407000 | -4.69382100 |
| H | 1.51449600 | 0.97014200 | -4.78631700 |
| C | 1.06974700 | 4.25872300 | -3.92637100 |
| H | 1.09817600 | 4.98848800 | -1.91120500 |
| S | -0.75472900 | -0.93483900 | -0.86658900 |
| C | -0.86774400 | -2.18775600 | 0.40242000 |
| C | -2.08023400 | -2.86829700 | 0.57227800 |
| C | 0.23399600 | -2.56236900 | 1.18149600 |
| C | -2.18889200 | -3.90152000 | 1.50423900 |
| H | -2.94619200 | -2.58229300 | -0.02157200 |
| C | 0.12069100 | -3.58962300 | 2.11670300 |
| H | 1.17909900 | -2.03935900 | 1.05803400 |
| C | -1.08986500 | -4.26602500 | 2.28336600 |
| H | -3.14007700 | -4.41360800 | 1.62803000 |
| H | 0.98523500 | -3.86504200 | 2.71600700 |
| H | -1.17583700 | -5.06628200 | 3.01345300 |
| H | -0.08179100 | 1.26077500 | -0.33211100 |
| H | 0.88554500 | 5.22174800 | -4.38679000 |
| N | 1.06745800 | 3.21553200 | -6.15054000 |
| O | 1.10675700 | 2.19430400 | -6.81997100 |
| O | 0.92757300 | 4.32864100 | -6.63557500 |

**$I_{E1cB}$-8**
Electronic energy:-1373.9501245 Hartree
Vibrational energy: 0.33486499
Gibbs free energy: -1373.688982
Enthalpy: -1373.611482

| | | | |
|---|---|---|---|
| C | 0.38961500 | 0.29850700 | -0.20033800 |
| H | 0.37962600 | 0.30593600 | 1.48036900 |
| C | 1.74134500 | 0.29019900 | -0.81119200 |
| H | 2.40842000 | 1.02240100 | -0.33912000 |
| H | 2.21795900 | -0.69153500 | -0.75161000 |
| O | 0.21693300 | 0.43646800 | 2.51718000 |
| C | -1.18097800 | 0.56120700 | 2.70310700 |
| H | -1.41323200 | 1.55910000 | 3.10601600 |
| H | -1.69082000 | 0.48191700 | 1.72903700 |
| C | -1.71967700 | -0.50243300 | 3.64709300 |
| H | -1.22183800 | -0.43786800 | 4.62193700 |
| H | -2.79735700 | -0.37198800 | 3.80459100 |
| H | -1.54897700 | -1.50615300 | 3.24002100 |
| O | 1.82020000 | 0.55054800 | -2.27919000 |
| C | 1.55954300 | 1.77258900 | -2.74522700 |
| C | 1.38123800 | 2.91417300 | -1.93819400 |

| | | | |
|---|---|---|---|
| C | 1.48369700 | 1.89700300 | -4.14896100 |
| C | 1.13820200 | 4.14492300 | -2.52819800 |
| H | 1.43355300 | 2.85161900 | -0.85804600 |
| C | 1.24078400 | 3.12117900 | -4.73702800 |
| H | 1.62182500 | 1.00780300 | -4.75672900 |
| C | 1.06758700 | 4.24045700 | -3.91670800 |
| H | 1.00301200 | 5.02733100 | -1.91203800 |
| H | 1.18282000 | 3.21488100 | -5.81576200 |
| S | -0.72860300 | -0.94000800 | -0.86775800 |
| C | -0.84408100 | -2.19502900 | 0.39971100 |
| C | -2.04993400 | -2.89150100 | 0.55043200 |
| C | 0.25033900 | -2.55536100 | 1.19525000 |
| C | -2.15874900 | -3.92744800 | 1.47936600 |
| H | -2.91062400 | -2.61587800 | -0.05583500 |
| C | 0.13695500 | -3.58555900 | 2.12719400 |
| H | 1.19016400 | -2.01955000 | 1.08631500 |
| C | -1.06674300 | -4.27842300 | 2.27437100 |
| H | -3.10471800 | -4.45243000 | 1.58822700 |
| H | 0.99609100 | -3.85061900 | 2.73880600 |
| H | -1.15288400 | -5.08105300 | 3.00181800 |
| H | -0.11069300 | 1.26752500 | -0.30785800 |
| N | 0.80563000 | 5.52455800 | -4.52285400 |
| O | 0.74764200 | 5.59670600 | -5.74640700 |
| O | 0.64906100 | 6.50052400 | -3.79592900 |

**$TS2_{E1cB}$-1**
Electronic energy: -1169.50122
Vibrational energy: 0.32860692
Gibbs free energy: -1169.241273
Enthalpy: -1169.168836

| | | | |
|---|---|---|---|
| C | -0.06099200 | 0.00018500 | -0.03314700 |
| H | -0.07475900 | 0.07248600 | 1.95925900 |
| C | 1.32585300 | 0.02999400 | -0.29315400 |
| H | 1.87482900 | 0.80936700 | 0.24157200 |
| H | 1.85101100 | -0.92492000 | -0.30903900 |
| O | -0.14307300 | 0.27838800 | 2.93015500 |
| C | -1.37521600 | 0.95594800 | 3.14856600 |
| H | -1.39039200 | 1.22897600 | 4.20880800 |
| H | -1.40055900 | 1.89012500 | 2.56870200 |
| C | -2.58398400 | 0.09891500 | 2.80646500 |
| H | -2.56316100 | -0.84320400 | 3.36684800 |
| H | -3.50888400 | 0.63179500 | 3.05711900 |
| H | -2.60495600 | -0.13565500 | 1.73577800 |
| O | 1.83485800 | 0.46752900 | -1.89651100 |
| C | 1.27786400 | 1.61643900 | -2.30078800 |

| | | | |
|---|---|---|---|
| C | 1.88671900 | 2.85432400 | -2.01659200 |
| C | 0.05162300 | 1.61972200 | -2.99113400 |
| C | 1.30113200 | 4.04829400 | -2.43355200 |
| H | 2.83075700 | 2.85924400 | -1.47571900 |
| C | -0.52901300 | 2.81854400 | -3.40625000 |
| H | -0.42591700 | 0.66682800 | -3.20756000 |
| C | 0.09033000 | 4.03962300 | -3.13221700 |
| H | 1.79404400 | 4.99258700 | -2.21370400 |
| H | -1.47333600 | 2.79759400 | -3.94552100 |
| H | -0.36289800 | 4.97168300 | -3.45836400 |
| S | -1.06010800 | -1.25155900 | -0.78596100 |
| C | -1.44311900 | -2.42325900 | 0.51590000 |
| C | -2.66085400 | -3.11157400 | 0.45351300 |
| C | -0.55449100 | -2.70522400 | 1.55802200 |
| C | -2.98913900 | -4.05623100 | 1.42633500 |
| H | -3.36174100 | -2.89576200 | -0.35032800 |
| C | -0.88942500 | -3.64279700 | 2.53450500 |
| H | 0.39783800 | -2.18321500 | 1.60664700 |
| C | -2.10808800 | -4.32213400 | 2.47577300 |
| H | -3.94244100 | -4.57568500 | 1.36905000 |
| H | -0.19099800 | -3.84618500 | 3.34266500 |
| H | -2.36736100 | -5.05115200 | 3.23856200 |
| H | -0.58007600 | 0.95489400 | 0.07057600 |

**$TS2_{E1cB}$-2**
Electronic energy: -1208.7970849
Vibrational energy: 0.35840248
Gibbs free energy: -1208.510743
Enthalpy: -1169.168836

| | | | |
|---|---|---|---|
| C | 0.10443800 | -0.06349300 | -0.00411200 |
| H | 0.54103700 | -0.16994900 | 2.03722100 |
| C | 1.48614300 | 0.03041500 | -0.27935000 |
| H | 2.09288700 | 0.51933500 | 0.48868700 |
| H | 1.96080000 | -0.86407500 | -0.68268500 |
| O | 0.71529300 | 0.04790300 | 2.98253000 |
| C | 0.11708600 | 1.31169700 | 3.26122400 |
| H | -0.93853800 | 1.30098000 | 2.95526600 |
| H | 0.14322700 | 1.42506600 | 4.34964800 |
| C | 0.84971400 | 2.46501900 | 2.59385300 |
| H | 0.78700900 | 2.39511200 | 1.50154300 |
| H | 0.40966700 | 3.42268700 | 2.89702100 |
| H | 1.90782400 | 2.46496000 | 2.88027300 |
| O | 1.96255900 | 1.07167400 | -1.58361100 |
| C | 1.78087400 | 2.35500000 | -1.23090900 |
| C | 2.78814100 | 3.06207200 | -0.54446800 |

| | | | |
|---|---|---|---|
| C | 0.56638800 | 3.01674500 | -1.47665200 |
| C | 2.58097600 | 4.37179900 | -0.12314100 |
| H | 3.73361300 | 2.56131000 | -0.34545500 |
| C | 0.37030000 | 4.33154200 | -1.04616500 |
| H | -0.22008300 | 2.48946900 | -2.01194900 |
| C | 1.36623200 | 5.03245900 | -0.36002600 |
| H | 3.37717500 | 4.89538200 | 0.40484400 |
| H | -0.58154400 | 4.82018000 | -1.24821200 |
| S | -0.90014900 | -0.98659700 | -1.12474900 |
| C | -1.57613400 | -2.36136200 | -0.20008700 |
| C | -2.40839100 | -3.25196000 | -0.89533600 |
| C | -1.33152100 | -2.58232500 | 1.15753800 |
| C | -2.97849900 | -4.34229400 | -0.24302600 |
| H | -2.60993000 | -3.08955800 | -1.95279900 |
| C | -1.90641700 | -3.67663200 | 1.80690500 |
| H | -0.69066400 | -1.89603900 | 1.70336600 |
| C | -2.73110900 | -4.56283000 | 1.11454100 |
| H | -3.61872300 | -5.02316700 | -0.79851600 |
| H | -1.70487100 | -3.83334700 | 2.86392900 |
| H | -3.17655900 | -5.41308100 | 1.62337600 |
| H | -0.40159600 | 0.80541000 | 0.42016900 |
| C | 1.15320800 | 6.44827700 | 0.11530500 |
| H | 1.20881300 | 6.51398700 | 1.20852300 |
| H | 1.91411900 | 7.12609800 | -0.28855100 |
| H | 0.17225300 | 6.82341900 | -0.19234300 |

**$TS2_{E1cB}$-3**
Electronic energy: -1629.0733502
Vibrational energy: 0.32002219
Gibbs free energy: -1628.825854
Enthalpy: -1628.74955

| | | | |
|---|---|---|---|
| C | 0.04467700 | -0.18733000 | -0.08923500 |
| H | -0.15835800 | -0.14066500 | 1.87025900 |
| C | 1.42726500 | -0.09331500 | -0.37725900 |
| H | 1.93939000 | 0.73117200 | 0.12592700 |
| H | 2.00096300 | -1.01987900 | -0.35646900 |
| O | -0.43686300 | 0.05574800 | 2.80670600 |
| C | -1.84706900 | -0.11147100 | 2.88830600 |
| H | -2.32784800 | 0.31811100 | 1.99717100 |
| H | -2.10123800 | -1.18178400 | 2.91867500 |
| C | -2.35293700 | 0.57731000 | 4.14060700 |
| H | -2.13862000 | 1.65111100 | 4.10688500 |
| H | -3.43531300 | 0.44318600 | 4.24122300 |
| H | -1.87164100 | 0.15606300 | 5.03038700 |
| O | 1.87503100 | 0.30284000 | -1.98875800 |

| | | | |
|---|---|---|---|
| C | 1.26954300 | 1.41744000 | -2.41526800 |
| C | 1.83596900 | 2.68373700 | -2.17753400 |
| C | 0.03142900 | 1.35572200 | -3.07944500 |
| C | 1.20266300 | 3.84685900 | -2.60708900 |
| H | 2.78892300 | 2.74464200 | -1.65741900 |
| C | -0.61010600 | 2.51440000 | -3.51391000 |
| H | -0.41678600 | 0.38285900 | -3.26406900 |
| C | -0.01721100 | 3.74951500 | -3.27250500 |
| H | 1.65394000 | 4.81860500 | -2.42686900 |
| H | -1.56333900 | 2.45452200 | -4.03161200 |
| S | -0.89344400 | -1.52054000 | -0.78438300 |
| C | -1.21180000 | -2.63586300 | 0.58382900 |
| C | -2.44364500 | -3.29730600 | 0.64468500 |
| C | -0.25068000 | -2.89264700 | 1.56729400 |
| C | -2.71697500 | -4.18672800 | 1.68532600 |
| H | -3.19857900 | -3.10164700 | -0.11391400 |
| C | -0.53036600 | -3.77136700 | 2.61219100 |
| H | 0.71265600 | -2.39059300 | 1.51949500 |
| C | -1.76568700 | -4.42072200 | 2.67879000 |
| H | -3.68243700 | -4.68475600 | 1.72575400 |
| H | 0.22208800 | -3.95328600 | 3.37562600 |
| H | -1.98233800 | -5.10382800 | 3.49550400 |
| H | -0.52140000 | 0.74452200 | -0.03356100 |
| Cl | -0.82282900 | 5.21444000 | -3.81430600 |

**$TS2_{E1cB}$-4**
Electronic energy: -1282.7976128
Vibrational energy: 0.34063064
Gibbs free energy: -1282.530512
Enthalpy: -1282.453205

| | | | |
|---|---|---|---|
| C | -0.01541800 | 0.01800400 | -0.04431000 |
| H | 0.01058300 | -0.02718600 | 1.96369000 |
| C | 1.39734100 | 0.04922000 | 0.05787600 |
| H | 1.81870300 | 0.99326300 | 0.40842400 |
| H | 1.87009800 | -0.81014900 | 0.53440600 |
| O | 0.12816100 | -0.05955100 | 2.95297800 |
| C | -0.44131400 | 1.12099100 | 3.50327900 |
| H | -1.52028900 | 1.15799700 | 3.29100800 |
| H | -0.32649900 | 1.04188100 | 4.58930100 |
| C | 0.23492900 | 2.38415200 | 2.99287000 |
| H | 0.09088100 | 2.49588000 | 1.91180200 |
| H | -0.18604700 | 3.26911400 | 3.48401200 |
| H | 1.31098000 | 2.35416200 | 3.19772000 |
| O | 2.28556900 | -0.13456400 | -1.39024100 |
| C | 1.95487800 | 0.62243500 | -2.41948900 |

| | | | |
|---|---|---|---|
| C | 1.44087800 | 1.93866600 | -2.27854500 |
| C | 2.13192000 | 0.10654100 | -3.72580200 |
| C | 1.13338500 | 2.69346600 | -3.39621800 |
| H | 1.30762600 | 2.36145900 | -1.28825600 |
| C | 1.82655100 | 0.87394600 | -4.83538100 |
| H | 2.51661300 | -0.90426300 | -3.83229300 |
| C | 1.31832600 | 2.17607600 | -4.68997200 |
| H | 0.74803200 | 3.70356200 | -3.27789500 |
| H | 1.97244600 | 0.46675500 | -5.83465600 |
| S | -0.71328100 | -1.51747700 | -0.59588200 |
| C | -2.03420100 | -1.88187300 | 0.54904600 |
| C | -2.53685300 | -3.19047700 | 0.58137200 |
| C | -2.62388200 | -0.90744700 | 1.36071300 |
| C | -3.59913500 | -3.51780700 | 1.42187300 |
| H | -2.08794100 | -3.95741900 | -0.04693600 |
| C | -3.68334900 | -1.24156000 | 2.20496500 |
| H | -2.25104800 | 0.11307100 | 1.32935300 |
| C | -4.17673600 | -2.54624000 | 2.24254300 |
| H | -3.97074400 | -4.53926800 | 1.44121200 |
| H | -4.12869800 | -0.47297800 | 2.83238900 |
| H | -5.00214300 | -2.80320100 | 2.90057100 |
| H | -0.50856000 | 0.90294300 | -0.44746000 |
| C | 0.99800800 | 2.95209700 | -5.88007700 |
| H | 1.18673600 | 2.44240700 | -6.84342100 |
| O | 0.54677400 | 4.09377100 | -5.88165800 |

**$TS2_{E1cB}$-5**
Electronic energy: -1322.1024524
Vibrational energy: 0.37020788
Gibbs free energy: -1321.808352
Enthalpy: -1321.728467

| | | | |
|---|---|---|---|
| C | 0.05762300 | 0.00605000 | 0.00076900 |
| H | 0.04098100 | -0.01964000 | 1.99201800 |
| C | 1.41389000 | 0.02879000 | -0.39583300 |
| H | 2.02463200 | 0.80522800 | 0.06716900 |
| H | 1.93059000 | -0.92920600 | -0.44086500 |
| O | -0.14785200 | 0.14618900 | 2.95444900 |
| C | -1.54394700 | -0.03292200 | 3.16502700 |
| H | -2.10738000 | 0.39777600 | 2.32451500 |
| H | -1.78576000 | -1.10522900 | 3.21164400 |
| C | -1.93922500 | 0.64375200 | 4.46277300 |
| H | -1.73673700 | 1.71946400 | 4.41838400 |
| H | -3.00729300 | 0.49968000 | 4.65817100 |
| H | -1.37769100 | 0.22019100 | 5.30299900 |
| O | 1.74291900 | 0.37629600 | -2.05477200 |

| | | | |
|---|---|---|---|
| C | 1.15431500 | 1.42787500 | -2.59462800 |
| C | 0.84176000 | 2.60279800 | -1.86656700 |
| C | 0.82889800 | 1.39677000 | -3.97120300 |
| C | 0.25329900 | 3.68515900 | -2.50014600 |
| H | 1.08284000 | 2.66343600 | -0.81030400 |
| C | 0.24599000 | 2.48789500 | -4.59329700 |
| H | 1.05535100 | 0.49461100 | -4.53360000 |
| C | -0.05687600 | 3.65537800 | -3.87000200 |
| H | 0.02959400 | 4.58269500 | -1.92902600 |
| H | 0.01949400 | 2.42565100 | -5.65431800 |
| S | -1.00787500 | -1.25916200 | -0.63428600 |
| C | -1.21547800 | -2.42124100 | 0.71603800 |
| C | -2.45863500 | -3.03898700 | 0.89239500 |
| C | -0.16003200 | -2.75489600 | 1.57138500 |
| C | -2.64802500 | -3.96266800 | 1.92174000 |
| H | -3.28681400 | -2.78234000 | 0.23507100 |
| C | -0.35483100 | -3.66791200 | 2.60604300 |
| H | 0.81098000 | -2.28500900 | 1.43423300 |
| C | -1.59989400 | -4.27503700 | 2.78822000 |
| H | -3.62222800 | -4.42668700 | 2.05409500 |
| H | 0.47171700 | -3.91035000 | 3.26955800 |
| H | -1.74963700 | -4.98597400 | 3.59611500 |
| H | -0.45359400 | 0.95860900 | 0.14069100 |
| C | -0.67788400 | 4.83505800 | -4.50672000 |
| C | -0.99996900 | 4.78724800 | -5.98011100 |
| H | -0.09437900 | 4.60664700 | -6.56896400 |
| H | -1.70039800 | 3.97273800 | -6.19446200 |
| H | -1.44575900 | 5.73641000 | -6.28274500 |
| O | -0.93375400 | 5.84857100 | -3.85544400 |

**$TS2_{E1cB}$-6**
Electronic energy: -1261.7278848
Vibrational energy: 0.32930332
Gibbs free energy: -1261.47311
Enthalpy: -1261.394805

| | | | |
|---|---|---|---|
| C | -0.03485100 | -0.04917600 | -0.02280700 |
| H | -0.05065500 | -0.07281300 | 1.96002600 |
| C | 1.33818400 | -0.06828400 | -0.36542600 |
| H | 1.95543600 | 0.67753100 | 0.13820300 |
| H | 1.82269000 | -1.04344100 | -0.40196500 |
| O | -0.21825600 | 0.04550800 | 2.93437000 |
| C | -1.62652500 | 0.12422800 | 3.11964800 |
| H | -2.02096500 | 1.02971200 | 2.63528800 |
| H | -2.11880700 | -0.74265100 | 2.65482900 |
| C | -1.92342200 | 0.15320100 | 4.60519400 |

| | | | |
|---|---|---|---|
| H | -1.44612400 | 1.01716000 | 5.08078400 |
| H | -3.00299600 | 0.21772500 | 4.77797000 |
| H | -1.55097400 | -0.75760900 | 5.08736900 |
| O | 1.74617700 | 0.29303300 | -1.99579100 |
| C | 1.21292100 | 1.36978700 | -2.54232200 |
| C | 0.89584800 | 2.53695300 | -1.80624400 |
| C | 0.95487900 | 1.36794600 | -3.93449100 |
| C | 0.36256600 | 3.64841000 | -2.44012500 |
| H | 1.08796600 | 2.57367600 | -0.73943300 |
| C | 0.42933800 | 2.47922300 | -4.56776900 |
| H | 1.18618000 | 0.46978200 | -4.50055900 |
| C | 0.12432000 | 3.63204400 | -3.82295900 |
| H | 0.13077900 | 4.54119100 | -1.86550800 |
| H | 0.24408200 | 2.46316200 | -5.63828500 |
| S | -1.11727200 | -1.25617100 | -0.73784600 |
| C | -1.46788200 | -2.42839000 | 0.57245700 |
| C | -2.73742600 | -3.01591100 | 0.62547500 |
| C | -0.50426100 | -2.80038300 | 1.51548000 |
| C | -3.04467700 | -3.94464800 | 1.62068600 |
| H | -3.49439700 | -2.73053300 | -0.10205100 |
| C | -0.81859300 | -3.71657000 | 2.51799000 |
| H | 0.48825300 | -2.35883700 | 1.47165400 |
| C | -2.09012200 | -4.29200900 | 2.57763400 |
| H | -4.03826200 | -4.38435600 | 1.65575000 |
| H | -0.06338700 | -3.98766800 | 3.25174800 |
| H | -2.33268700 | -5.00548500 | 3.36038600 |
| H | -0.51583100 | 0.92047300 | 0.10753000 |
| C | -0.42424600 | 4.78305500 | -4.47144800 |
| N | -0.86799800 | 5.71658700 | -4.99985200 |

**$TS2_{E1cB}$-7**
Electronic energy: -1373.940858
Vibrational energy: 0.33442197
Gibbs free energy: -1373.681531
Enthalpy: -1373.602659

| | | | |
|---|---|---|---|
| C | -0.19932500 | 0.23798800 | 0.12622700 |
| H | -0.67677300 | 0.49883900 | 2.11508100 |
| C | 1.17688600 | 0.02188300 | 0.35637300 |
| H | 1.62323400 | 0.59110800 | 1.17412600 |
| H | 1.51527500 | -1.01378600 | 0.34902500 |
| O | -0.80859500 | 0.93096000 | 2.99292800 |
| C | -0.39075200 | 2.28756000 | 2.86783200 |
| H | 0.68978300 | 2.33230700 | 2.66593500 |
| H | -0.91164800 | 2.76489400 | 2.02596800 |
| C | -0.70629600 | 3.01665500 | 4.15749800 |

| | | | |
|---|---|---|---|
| H | -0.18854800 | 2.54870200 | 5.00192800 |
| H | -0.38269000 | 4.06102100 | 4.09108000 |
| H | -1.78320700 | 3.00028900 | 4.35706100 |
| O | 2.26180400 | 0.50655000 | -0.89853900 |
| C | 2.10891700 | 1.74342400 | -1.34928400 |
| C | 1.64106200 | 2.79837100 | -0.54116400 |
| C | 2.43009300 | 2.03934400 | -2.69252400 |
| C | 1.52705000 | 4.06939700 | -1.09251000 |
| H | 1.38871100 | 2.63998600 | 0.49916800 |
| C | 2.31397600 | 3.32831700 | -3.20233800 |
| H | 2.78145100 | 1.22816900 | -3.32504000 |
| C | 1.85148200 | 4.37784100 | -2.40853700 |
| H | 2.57850200 | 3.52069200 | -4.23810300 |
| S | -1.03393800 | -0.76446700 | -1.05865900 |
| C | -2.06625100 | -1.89867900 | -0.13134300 |
| C | -3.06047200 | -2.59092700 | -0.83773700 |
| C | -1.90213800 | -2.15234600 | 1.23301100 |
| C | -3.87661200 | -3.51429400 | -0.18742100 |
| H | -3.19999900 | -2.40033200 | -1.90033100 |
| C | -2.72697100 | -3.07256700 | 1.88179200 |
| H | -1.12400200 | -1.63157900 | 1.78448100 |
| C | -3.71775200 | -3.75857200 | 1.17863300 |
| H | -4.64523400 | -4.03875700 | -0.74973200 |
| H | -2.58718800 | -3.25696200 | 2.94424700 |
| H | -4.35772800 | -4.47447800 | 1.68681500 |
| H | -0.59093100 | 1.25342500 | 0.18438100 |
| H | 1.74425000 | 5.38375600 | -2.79519900 |
| N | 1.03680600 | 5.14425200 | -0.22356000 |
| O | 0.74297800 | 4.87502800 | 0.93284100 |
| O | 0.93842800 | 6.27085700 | -0.68963000 |

**$TS2_{E1cB}$-8**
Electronic energy: -1373.9472653
Vibrational energy: 0.33395983
Gibbs free energy: -1373.687695
Enthalpy: -1373.609528

| | | | |
|---|---|---|---|
| C | -0.02540700 | 0.04598300 | 0.14777500 |
| H | 0.19604300 | -0.18878400 | 2.09496800 |
| C | 1.30073000 | -0.01634800 | -0.35980300 |
| H | 2.02286400 | 0.62480600 | 0.14989600 |
| H | 1.70340700 | -1.01323200 | -0.53863700 |
| O | 0.24245600 | -0.13274100 | 3.09026200 |
| C | -0.82651500 | 0.69815400 | 3.52636400 |
| H | -0.72411600 | 0.78676500 | 4.61295100 |
| H | -0.71720800 | 1.70804600 | 3.10393100 |

| | | | |
|---|---|---|---|
| C | -2.19134400 | 0.12856300 | 3.17061600 |
| H | -2.30581800 | -0.88373900 | 3.57640200 |
| H | -2.98643000 | 0.75967700 | 3.58493100 |
| H | -2.32489200 | 0.08099700 | 2.08367300 |
| O | 1.53819900 | 0.48555300 | -1.95647000 |
| C | 1.09346500 | 1.66566900 | -2.32414800 |
| C | 0.91094200 | 2.74921500 | -1.42628800 |
| C | 0.79390700 | 1.87065800 | -3.69649700 |
| C | 0.46260200 | 3.97384900 | -1.88560400 |
| H | 1.14293300 | 2.63058400 | -0.37430200 |
| C | 0.35053900 | 3.09216800 | -4.15705400 |
| H | 0.92601900 | 1.03873300 | -4.38196100 |
| C | 0.18214800 | 4.14188400 | -3.24470100 |
| H | 0.33336900 | 4.80226200 | -1.19752100 |
| H | 0.12729100 | 3.23933900 | -5.20815200 |
| S | -1.26007600 | -0.98743300 | -0.59124200 |
| C | -1.59182200 | -2.28880900 | 0.59629500 |
| C | -2.88249300 | -2.82912400 | 0.64919200 |
| C | -0.60104800 | -2.81004800 | 1.43371600 |
| C | -3.17918600 | -3.86466000 | 1.53601800 |
| H | -3.66237800 | -2.42675900 | 0.00575900 |
| C | -0.90283400 | -3.83768500 | 2.32671900 |
| H | 0.40652300 | -2.40381300 | 1.39051000 |
| C | -2.19263700 | -4.36967700 | 2.38438200 |
| H | -4.18850600 | -4.26700700 | 1.57209100 |
| H | -0.12315600 | -4.22788400 | 2.97642900 |
| H | -2.42531400 | -5.17025000 | 3.08115300 |
| H | -0.41690800 | 1.02850900 | 0.41443400 |
| N | -0.28383300 | 5.41592900 | -3.71477800 |
| O | -0.43348000 | 6.33107400 | -2.90701400 |
| O | -0.52052900 | 5.55701500 | -4.91329600 |

**$TS_{E2}$-1**
Electronic energy: -1169.4925464
Vibrational energy: 0.32823721
Gibbs free energy: -1169.234109
Enthalpy: -1169.160532

| | | | |
|---|---|---|---|
| C | 0.27559800 | -1.08572000 | 0.11531400 |
| C | 0.29506800 | -1.11909300 | 1.50949200 |
| C | 1.06110700 | -0.19632300 | 2.24345900 |
| C | 1.80942100 | 0.75731700 | 1.53217700 |
| C | 1.78017500 | 0.79623400 | 0.13841500 |
| C | 1.01508400 | -0.12600700 | -0.57821500 |
| H | -0.32494200 | -1.80976400 | -0.42992700 |
| H | -0.29588800 | -1.86155700 | 2.04097700 |

| | | | |
|---|---|---|---|
| H | 2.41456600 | 1.47441700 | 2.08141500 |
| H | 2.36186800 | 1.54820000 | -0.38918700 |
| H | 0.99569900 | -0.09727900 | -1.66426100 |
| S | 1.11461700 | -0.27111100 | 4.01199400 |
| C | 2.33797000 | -2.00995500 | 4.18730800 |
| H | 3.23252800 | -1.63851100 | 3.68829500 |
| H | 1.74397500 | -2.66427200 | 3.54637000 |
| C | 2.58307600 | -2.48136900 | 5.50433600 |
| H | 3.11771700 | -1.79707100 | 6.17272600 |
| H | 3.48634700 | -4.02808500 | 5.13745200 |
| O | 1.36740700 | -2.94137600 | 6.12369000 |
| C | 1.45270500 | -3.65955800 | 7.26508700 |
| C | 0.24753300 | -4.18107300 | 7.76356900 |
| C | 2.64724800 | -3.89278100 | 7.95997200 |
| C | 0.24061000 | -4.93211000 | 8.93239200 |
| H | -0.67035300 | -3.98893200 | 7.21362300 |
| C | 2.62171400 | -4.65182100 | 9.13356000 |
| H | 3.58553900 | -3.49880100 | 7.58672700 |
| C | 1.43003100 | -5.17645800 | 9.62857100 |
| H | -0.69999300 | -5.33201400 | 9.30285900 |
| H | 3.55458000 | -4.83049700 | 9.66290300 |
| H | 1.42298600 | -5.76386300 | 10.54214900 |
| O | 3.83896500 | -4.96172500 | 4.91799600 |
| C | 2.72741100 | -5.84366200 | 4.86852900 |
| H | 2.38755000 | -6.08901600 | 5.88710500 |
| H | 1.88536000 | -5.36099400 | 4.34973400 |
| C | 3.12478400 | -7.11387500 | 4.14118000 |
| H | 2.28796300 | -7.82063800 | 4.11376600 |
| H | 3.42380000 | -6.89153400 | 3.11099000 |
| H | 3.96611100 | -7.59996900 | 4.64787800 |

**Products**

**EtOH**
Electronic energy: -154.972774
Vibrational energy: 0.0823079
Gibbs free energy: -154.917062
Enthalpy: -154.886689

| | | | |
|---|---|---|---|
| H | 0.56922400 | -0.34640000 | -0.75211000 |
| O | 1.39837900 | 0.11886800 | -0.94756400 |
| C | 1.88699900 | 0.69672100 | 0.26422100 |
| H | 2.08402400 | -0.09338700 | 1.00022900 |
| H | 2.84325800 | 1.15855700 | 0.00264500 |
| C | 0.93029700 | 1.72770100 | 0.83231900 |

| | | | |
|---|---|---|---|
| H | -0.03156900 | 1.26613100 | 1.08472000 |
| H | 1.34413300 | 2.16967600 | 1.74559900 |
| H | 0.75208200 | 2.52981200 | 0.10827900 |

**PhS-olefin**
Electronic energy: -707.669251
Vibrational energy: 0.1409301
Gibbs free energy: -707.568189
Enthalpy: -707.524545

| | | | |
|---|---|---|---|
| C | -0.75018300 | -1.97351600 | -0.49003800 |
| C | -1.54918300 | -1.14456200 | -1.16239600 |
| H | -1.53966300 | -0.08059300 | -0.94026900 |
| H | -2.23462000 | -1.49415500 | -1.93111500 |
| S | -0.82395000 | -3.73036900 | -0.68077800 |
| C | 0.89603300 | -4.17227700 | -0.51552500 |
| C | 1.20497500 | -5.41962300 | 0.03751300 |
| C | 1.92254300 | -3.33115600 | -0.95618900 |
| C | 2.53522300 | -5.82069300 | 0.14726900 |
| H | 0.40960200 | -6.07311700 | 0.38792400 |
| C | 3.25153200 | -3.73257300 | -0.82251300 |
| H | 1.69039700 | -2.37010700 | -1.40828400 |
| C | 3.56317000 | -4.97678600 | -0.27485000 |
| H | 2.76608600 | -6.79168300 | 0.57732100 |
| H | 4.04443700 | -3.07043000 | -1.16022500 |
| H | 4.59972800 | -5.28736900 | -0.17869200 |
| H | -0.06080200 | -1.61468100 | 0.27298700 |

**PhO-olefin**
Electronic energy: -384.7054228
Vibrational energy: 0.1434145
Gibbs free energy: -384.599664
Enthalpy: -384.558232

| | | | |
|---|---|---|---|
| C | -1.04441000 | -1.59332500 | -0.81645700 |
| C | -1.11348600 | -0.53648000 | -1.61851200 |
| H | -1.37671500 | 0.43063600 | -1.20457300 |
| H | -0.92509400 | -0.61904600 | -2.68546100 |
| C | -0.17739400 | -3.76527600 | -0.50347900 |
| C | -0.45624100 | -5.11048700 | -0.74585700 |
| C | 0.72920500 | -3.38521700 | 0.48491200 |
| C | 0.17619400 | -6.08573200 | 0.01988700 |
| H | -1.16328900 | -5.37327500 | -1.52793400 |
| C | 1.34891400 | -4.37518900 | 1.25015500 |
| H | 0.96267500 | -2.33668200 | 0.64675500 |
| C | 1.07748700 | -5.72346200 | 1.02398000 |

| | | | |
|---|---|---|---|
| H | -0.04082900 | -7.13393900 | -0.16700900 |
| H | 2.05572400 | -4.08218700 | 2.02186000 |
| H | 1.56651300 | -6.48786300 | 1.62082300 |
| H | -1.22236900 | -1.55538600 | 0.25690200 |
| O | -0.80671900 | -2.85022000 | -1.31918300 |

**1-Cβ**
Electronic energy: -306.8807864
Vibrational energy: 0.09365594
Gibbs free energy: -306.8216033
Enthalpy: -306.7852112

| | | | |
|---|---|---|---|
| O | -3.43465400 | -1.43385700 | -1.47577200 |
| C | -4.22109000 | -1.01654500 | -0.51816100 |
| C | -3.88735500 | 0.10194600 | 0.31086800 |
| C | -5.47337600 | -1.64805600 | -0.22891300 |
| C | -4.73094100 | 0.54159300 | 1.33255300 |
| H | -2.94285100 | 0.61347800 | 0.12606000 |
| C | -6.30753000 | -1.19858300 | 0.79569100 |
| H | -5.76762300 | -2.50408900 | -0.83580900 |
| C | -5.95239900 | -0.09882300 | 1.59259300 |
| H | -4.43127000 | 1.39821900 | 1.93614600 |
| H | -7.25083500 | -1.71382100 | 0.97668200 |
| H | -6.60636900 | 0.24770300 | 2.38949000 |

**2-Cβ**
Electronic energy: -346.1758328
Vibrational energy: 0.1242945
Gibbs free energy: -346.08732
Enthalpy: -346.047762

| | | | |
|---|---|---|---|
| O | -3.29694800 | -1.54799700 | -1.60960100 |
| C | -4.09535000 | -1.07795400 | -0.69303100 |
| C | -3.78358900 | 0.08003000 | 0.07325100 |
| C | -5.34799200 | -1.68838400 | -0.38626500 |
| C | -4.64835000 | 0.57617600 | 1.04807700 |
| H | -2.83748300 | 0.58405700 | -0.12025400 |
| C | -6.19774800 | -1.17901200 | 0.59056300 |
| H | -5.63309800 | -2.57933900 | -0.94427500 |
| C | -5.87489800 | -0.03392100 | 1.33454500 |
| H | -4.35877000 | 1.46815000 | 1.60419200 |
| H | -7.14482000 | -1.68534200 | 0.78248200 |
| C | -6.80880200 | 0.50846600 | 2.38973600 |
| H | -7.78802500 | 0.77286500 | 1.97134600 |
| H | -6.98871900 | -0.21908200 | 3.19096300 |
| H | -6.39405200 | 1.41105600 | 2.85145100 |

**3-Cβ**
Electronic energy: -766.4545222
Vibrational energy: 0.08653413
Gibbs free energy: -766.402541
Enthalpy: -766.364212

| | | | |
|---|---|---|---|
| O | -3.46971700 | -1.50048900 | -1.47717500 |
| C | -4.30344500 | -1.04723900 | -0.59431300 |
| C | -3.98730300 | 0.05326300 | 0.25808200 |
| C | -5.60080100 | -1.61431000 | -0.40891300 |
| C | -4.88079100 | 0.54041300 | 1.20630800 |
| H | -3.00968000 | 0.52010400 | 0.15375900 |
| C | -6.49588100 | -1.12920100 | 0.53785800 |
| H | -5.88697200 | -2.45634000 | -1.03616600 |
| C | -6.13408600 | -0.05207500 | 1.34488500 |
| H | -4.60206600 | 1.38207000 | 1.83613900 |
| H | -7.47533200 | -1.58877200 | 0.64911100 |
| Cl | -7.26850900 | 0.56265100 | 2.54575300 |

**4-Cβ**
Electronic energy: -420.1857109
Vibrational energy: 0.1065386
Gibbs free energy: -420.115229
Enthalpy: -420.075396

| | | | |
|---|---|---|---|
| O | -3.23849900 | -1.59831300 | -1.26948900 |
| C | -4.06874600 | -1.03009100 | -0.48324800 |
| C | -3.69635100 | 0.10761900 | 0.32245300 |
| C | -5.42732100 | -1.48330200 | -0.34661800 |
| C | -4.58920400 | 0.71699500 | 1.17144700 |
| H | -2.67448300 | 0.47166800 | 0.23643000 |
| C | -6.30970000 | -0.86070600 | 0.50829400 |
| H | -5.73818900 | -2.33947900 | -0.94143200 |
| C | -5.92021700 | 0.25031900 | 1.28932000 |
| H | -4.27751700 | 1.57351100 | 1.76657000 |
| H | -7.33265500 | -1.22782300 | 0.59208000 |
| C | -6.87470800 | 0.86818900 | 2.17287800 |
| H | -7.88467800 | 0.41498400 | 2.16912200 |
| O | -6.65989100 | 1.83610000 | 2.91184600 |

**5-Cβ**
Electronic energy: -459.4882149
Vibrational energy: 0.1360394
Gibbs free energy: -459.392216
Enthalpy: -459.348398

| | | | |
|---|---|---|---|
| O | -3.43254100 | -1.64324700 | -1.19201200 |
| C | -4.26363900 | -1.07513500 | -0.40008600 |
| C | -3.91006600 | 0.08097200 | 0.37792800 |
| C | -5.60756300 | -1.55174400 | -0.23076700 |
| C | -4.80973100 | 0.68478800 | 1.22860900 |
| H | -2.89934800 | 0.47129900 | 0.27511000 |
| C | -6.49664600 | -0.93460200 | 0.62539500 |
| H | -5.91137600 | -2.42593500 | -0.80310400 |
| C | -6.12883500 | 0.20078800 | 1.38148000 |
| H | -4.50521900 | 1.55800200 | 1.80149400 |
| H | -7.50159200 | -1.34187600 | 0.71401300 |
| C | -7.05481200 | 0.86987300 | 2.29313800 |
| C | -8.46341300 | 0.33650800 | 2.43415800 |
| H | -8.97472500 | 0.31737900 | 1.46587200 |
| H | -8.45132500 | -0.68826100 | 2.82139100 |
| H | -9.02202600 | 0.97267200 | 3.12361500 |
| O | -6.71785900 | 1.86131400 | 2.95553000 |

**6-Cβ**
Electronic energy: -399.1143052
Vibrational energy: 0.09546308
Gibbs free energy: -399.054413
Enthalpy: -399.015065

| | | | |
|---|---|---|---|
| O | -3.43106800 | -1.63981500 | -1.25654200 |
| C | -4.28229700 | -1.13542700 | -0.44253300 |
| C | -3.96015400 | -0.02074300 | 0.40329200 |
| C | -5.61774200 | -1.65001300 | -0.31948500 |
| C | -4.87803200 | 0.52150700 | 1.27925000 |
| H | -2.95748100 | 0.39592600 | 0.33721000 |
| C | -6.53279200 | -1.10562000 | 0.55739100 |
| H | -5.89626900 | -2.49546400 | -0.94465400 |
| C | -6.18068700 | -0.01011400 | 1.37349400 |
| H | -4.60058700 | 1.36684400 | 1.90490300 |
| H | -7.53623800 | -1.51975100 | 0.62632900 |
| C | -7.12614500 | 0.54843800 | 2.27992800 |
| N | -7.89784800 | 1.00531400 | 3.02092300 |

**7-Cβ**
Electronic energy: -511.3252078
Vibrational energy: 0.1001977
Gibbs free energy: -511.263206
Enthalpy: -511.221233

| | | | |
|---|---|---|---|
| O | -3.43413100 | -1.53210500 | -1.37794500 |
| C | -4.25840200 | -1.07916100 | -0.49598000 |

| | | | |
|---|---|---|---|
| C | -3.92038500 | 0.00315400 | 0.36957900 |
| C | -5.56906700 | -1.62386300 | -0.31786900 |
| C | -4.83913100 | 0.45982400 | 1.30499300 |
| H | -2.94044600 | 0.46055600 | 0.28452400 |
| C | -6.45711500 | -1.13354300 | 0.63107600 |
| H | -5.86175000 | -2.45302900 | -0.95875400 |
| C | -6.11581900 | -0.07266600 | 1.47295400 |
| H | -7.44198300 | -1.58493500 | 0.72437100 |
| H | -6.80124200 | 0.31613700 | 2.21504000 |
| N | -4.43945900 | 1.57215900 | 2.17429500 |
| O | -3.31682800 | 2.04277000 | 2.05106900 |
| O | -5.24337300 | 1.99293000 | 2.99664700 |

**8-Cβ**
Electronic energy: -511.337344
Vibrational energy: 0.1000017
Gibbs free energy: -511.274864
Enthalpy: -511.233566

| | | | |
|---|---|---|---|
| O | -3.01769200 | -1.73044500 | -0.99153500 |
| C | -3.91971400 | -1.13034800 | -0.33384200 |
| C | -3.66730800 | 0.12075000 | 0.34465400 |
| C | -5.26008700 | -1.65786600 | -0.21644200 |
| C | -4.64269700 | 0.76754300 | 1.05733200 |
| H | -2.66758200 | 0.54189500 | 0.27293800 |
| C | -6.23418200 | -1.00789000 | 0.49609100 |
| H | -5.47937100 | -2.59765900 | -0.71686400 |
| C | -5.93844200 | 0.21207900 | 1.14204400 |
| H | -4.42821800 | 1.70574100 | 1.55905300 |
| H | -7.23416600 | -1.42369100 | 0.56921400 |
| N | -6.93779800 | 0.87831700 | 1.87158000 |
| O | -8.07594700 | 0.38754500 | 1.94380000 |
| O | -6.67144300 | 1.95038900 | 2.43838700 |

**1-Cα**
Electronic energy: -629.8466319
Vibrational energy: 0.09359697
Gibbs free energy: -629.785519
Enthalpy: -629.749257

| | | | |
|---|---|---|---|
| C | -4.12416300 | -0.92822000 | -0.50175500 |
| C | -3.75917700 | 0.04723500 | 0.45318800 |
| C | -5.19266100 | -1.78180700 | -0.14569400 |
| C | -4.41661600 | 0.16245700 | 1.67716800 |
| H | -2.94029400 | 0.72499300 | 0.22122300 |
| C | -5.85049200 | -1.66777700 | 1.07788700 |

| | | | |
|---|---|---|---|
| H | -5.50619800 | -2.54844300 | -0.85129500 |
| C | -5.47071600 | -0.69364600 | 2.00467600 |
| H | -4.10066900 | 0.92953100 | 2.38164400 |
| H | -6.66861200 | -2.34759100 | 1.30808800 |
| H | -5.98393200 | -0.60435000 | 2.95839000 |
| S | -3.29352100 | -1.07113300 | -2.04842800 |